MULTIPLE MODULAR VALUES FOR $\mathrm{SL}_2(\mathbb{Z})$

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1. Introduction

The purpose of this paper is to define and study a common generalisation of multiple zeta values, which are iterated integrals on the projective line minus 3 points and periods of mixed Tate motives over $\mathbb{Z}$, and the special values of L-functions of modular forms at all integers. Multiple modular values are regularised iterated integrals of modular forms on an (orbifold) quotient $\Gamma\backslash\backslash\mathfrak{H}$ of the upper-half plane $\mathfrak{H}$ by a subgroup $\Gamma \leq \mathrm{SL}_2(\mathbb{Z})$ of finite index, building on those first considered by Manin [31, 32]. They are periods of a hypothetical Tannakian category of mixed modular motives $\mathcal{MMM}$ ($\mathcal{M}^3$) consisting of iterated extensions of motives of modular forms. By Belyi's theorem [2], the simple objects in $\mathcal{M}^3$ should include the motives of algebraic curves over number fields. The goal is to understand this category through iterated integrals.

The motivations for this work are numerous. First of all, there are modular phenomena in the ring of multiple zeta values relating to the depth filtration which are not fully understood, and a geometric understanding of these phenomena seems to require placing multiple zeta values and modular forms for $\mathrm{SL}_2(\mathbb{Z})$ in a common framework. Secondly, there is no prescription, conjectural or otherwise, for constructing the objects of the category of mixed Tate motives over the ring of S-integers $\mathbb{Z}[S^{-1}]$ where S is a finite set of primes. Indeed, it is known [21] that the motivic fundamental group of the projective line minus roots of unity fails to generate the corresponding category of mixed Tate motives over cyclotomic fields. It is my hope that these categories can be constructed from the multiple modular motives generated by congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$. Finally, multiple zeta values and polylogarithms play an important role in high-energy physics as the Feynman amplitudes of a very large class of physical processes. However, there is an increasing supply of examples which are not of this type, and whose underlying motives are mixed modular and hence objects in $\mathcal{M}^3$. Therefore, in order to express the basic quantities in quantum field theory, we are forced to enlarge the class of known periods to incorporate periods of modular forms.

1.1. **Philosophy.** A programme for the study of multiple modular motives could go something along the following lines. The motivic fundamental groupoid of $\Gamma\backslash\backslash\mathfrak{H}$, with tangential base-points at the cusps, should define a pro-object in the category $\mathcal{M}^3$, and in a suitable realisation ω, will admit an action of the Tannaka group $\pi_1(\mathcal{M}^3, \omega)$. We wish to study this action using motivic periods in a category of Betti-de Rham realisations [9]. The Betti realisation of the fundamental groupoid of $\Gamma\backslash\backslash\mathfrak{H}$ should be the unipotent completion of Γ relative to the embedding $\Gamma \to \mathrm{SL}_2(\mathbb{Q})$. Its de Rham version, together with its mixed Hodge structure, was worked out by Hain [22], [24].

As a prototype, we have in mind the analogous story for the projective line minus three points which goes back to [19, 14, 17, 27]. The de Rham Tannaka group $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ of the category $\mathcal{MT}(\mathbb{Z})$ of mixed Tate motives over $\mathbb{Z}$ acts on the de Rham realisation of the motivic fundamental groupoid of $\mathbb{P}^1\backslash\{0, 1, \infty\}$ with respect to suitable tangential base points at 0 and 1. The periods of this fundamental groupoid are iterated integrals on $\mathbb{P}^1\backslash\{0,1,\infty\}$ and are expressible in terms of multiple zeta values. The non-vanishing of the $\zeta(2n+1)$, or rather, their motivic versions, proves that the generators of the Lie algebra of $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ act non-trivially on the de Rham fundamental group [16]. The ℓ-adic analogue of this result was previously proved by Hain and Matsumoto [25], and was called the 'generation' conjecture. Next, one needs a formula for the action of $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ on the de Rham fundamental groupoid of $\mathbb{P}^1\backslash\{0,1,\infty\}$, which was first computed by Ihara. The dual coaction on motivic multiple zeta values is given by a version of a formula due to Goncharov [21], [9]. Finally, the freeness of this action was proved in [6], which implies that $\mathcal{MT}(\mathbb{Z})$ is actually generated by the motivic fundamental groupoid of $\mathbb{P}^1\backslash\{0,1,\infty\}$. See [9], [15] for an overview.

A key ingredient in this picture is the upper bound on the Ext groups of mixed Tate motives which come from Borel's deep theorems on the rational algebraic K-theory of $\mathbb{Q}$. Analogous results for the motives of modular forms are presently unavailable, but we can nonetheless follow a similar programme for multiple modular motives.

The first step is to write down the periods of $\mathcal{M}^3$ which are iterated integrals of modular forms and study their structure. An analogue of the 'generation' part of the previous story is partly carried out in the present paper in the case $\Gamma = \mathrm{SL}_2(\mathbb{Z})$. We prove that for every cusp form g of weight k for $\mathrm{SL}_2(\mathbb{Z})$, and for every $n \geq 0$, the L-value $L(g,n)$ multiplied by a suitable power of $2\pi i$, is a multiple modular value for $\mathrm{SL}_2(\mathbb{Z})$, and, in particular, a period in the sense of [28]. It occurs as a certain part of an iterated integral of two Eisenstein series (or of an Eisenstein series and the cusp form g). The second step is to study the motivic periods corresponding to multiple modular values (in a category of Betti and de Rham realisations), and the action of the Tannaka group upon them. This will be the topic of a future paper in the general context of relative unipotent completions of discrete groups. The formula for the motivic action is actually derived in the present paper in the case of $\mathrm{SL}_2(\mathbb{Z})$, since it is required for the final chapters. One of our goals is ultimately to study the freeness of this action. Perhaps surprisingly, this action is combinatorially simpler than the action of the motivic Galois on the projective line minus three points.

1.2. **Contents.** Apart from the motivic philosophy described above, this paper is almost entirely analytic, and I have tried to stay as close as possible to the language of classical modular forms.

Section 2 consists of background material, and can be consulted when required. The next section §3 is a brief reminder of Manin's theory of iterated Shimura integrals. In §4, I explain how to regularise these iterated integrals with respect to a tangential base point at the cusp. One obtains explicit and highly convergent formulae which are very well suited to numerical computation. In §5, I explain how the generating series of regularised iterated integrals defines a canonical cocycle $\mathcal{C}$ for $\mathrm{SL}_2(\mathbb{Z})$ in a certain non-abelian pro-unipotent group. Its coefficients can be thought of as higher period polynomials for iterated modular forms: and in length one, it gives precisely the generating series of period polynomials for modular forms. These are recalled in §7, together with standard facts about Hecke operators and the Eichler-Shimura theorem.

The work begins in §8, where a curious phenomenon of transference of periods is described, related to the fact that the compactly supported cohomology of $\mathcal{M}^{an}_{1,1}$ is non-zero in degree 2. It gives rise to a higher analogue of the Peterssen inner product for iterated integrals and implies that periods are transferred between iterated integrals of quite different types: for example, certain coefficients in an iterated integral of two Eisenstein series also occur as iterated integrals of an Eisenstein series and a cusp form.

In §9, we compute a certain group $\mathcal{A}$ of automorphisms of the space of non-abelian $\mathrm{SL}_2(\mathbb{Z})$-cocycles with coefficients in its relative completion. The action of the motivic Galois group of $\mathcal{M}^3$ should factor through $\mathcal{A}$, which is the direct analogue of the Ihara action of the motivic Galois group on the fundamental groupoid of the projective line minus three points. It is the group which preserves the following (motivic) structures: the shuffle and cocycle relations between iterated integrals, and the local monodromy at the cusp (which is mixed Tate and computed in §6). One could further constrain the image of the motivic Galois group by adding information about the mixed Hodge structure on the de Rham relative completion of $\mathrm{SL}_2(\mathbb{Z})$ [22, 24] and the action of Hecke operators. A more detailed study of this group in a more general context will be undertaken in [5].

The main theorems are proved in §11. The imaginary part of an iterated integral of two Eisenstein series is computed using a generalisation of Haberlund's formula and the Rankin-Selberg method. The periods can be expressed as special values of L-functions of cusp forms f at all integers n where n is greater than or equal to the weight of f. The basic ideas for such a computation can presumably be traced back to Beilinson's original work on his conjecture on L-values. The computations of §11 should also give a new proof of his conjecture for modular forms. As a bonus we also obtain the extended regulators for motives of modular forms as the real part of double Eisenstein integrals. In the light of the transference principle, I have the feeling that the general method can be pushed much further.

In the final section, I describe in detail the periods of double Eisenstein integrals. I briefly explain how the presence of the L-values described above gives rise to the depth-defect for double zeta values and hence relates to the Broadhurst-Kreimer conjecture. In this sense, multiple modular values give a kind of resolution of the depth-defect.

1.3. **Applications, and further remarks.** A first application of the results of §11 is to compute cup products in the Deligne cohomology of $\mathcal{M}_{1,1}$. This will be undertaken in a forthcoming joint work with R. Hain. It implies in particular that the relations between certain derivations on a free Lie algebra with two generators studied by Pollack are motivic [35]. I believe that a special case of this computation was also obtained by Terasoma. The results of §10.1 should also compute the quadratic part of the action of $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ on this Lie algebra.

All the results in this paper can easily be transposed to the case of general congruence subgroups. I preferred to restrict to the case of $\mathrm{SL}_2(\mathbb{Z})$ for the time being because of the special connection with multiple zeta values, and in order not to condemn this work to the graveyard of unfinished manuscripts. The key remark to achieve this is to view a modular curve as a finite cover of $\mathcal{M}^{an}_{1,1}$ and push all geometric structures down to $\mathcal{M}^{an}_{1,1}$. This idea was recently used by Pasol and Popa [34] in their work on period polynomials for modular forms of higher level. Using Shapiro's lemma, all computations can be performed using $\mathrm{SL}_2(\mathbb{Z})$-cocycles (as opposed to general Γ-cocyles, which are hard to manage), and therefore the methods described here should carry through with only minor modifications.

There is a class of relations between multiple modular values which I did not touch upon here, which relate to multiple elliptic zeta values, but goes in the opposite direction from the main philosophical thrust of the present paper. This is very easily seen using the formulae from [10]: iterated integrals on the universal elliptic curve restricted to the zero section can be expressed as certain iterated integrals of Eisenstein series (see also [18]). One immediately deduces that the corresponding multiple modular values are multiple zeta values. In the language of Hain and Matsumoto, this should be equivalent to computing the image of $\mathcal{O}(\mathfrak{u}^{\mathrm{eis}})$ inside the affine ring of the relative completion of Γ.

1.4. **Acknowledgements.** I am greatly indebted to Andrey Levin for discussions in 2013 and encouragement. As part of our project to study multiple elliptic polylogarithms [10], it was our intention to prove that multiple elliptic zeta values are orthogonal to cusp forms in order to explain the depth-defect of multiple zeta values. This results of §11 imply this result and were inspired by our joint work. Many thanks also to Dick Hain for numerous discussions and his patient explanation of his joint work with Matsumoto. See his notes [24] for much background, as well as his IHES lectures in May 2014. Many thanks also to Yuri I. Manin and Pierre Cartier for their interest. This work is part of the ERC grant PAGAP 257638. Some of the numerical checks of §12 were computed during a stay at Humboldt University in summer 2013.

2. Basic notation and reminders

All tensor products are over $\mathbb{Q}$ unless stated otherwise.

2.1. Modular forms.

2.1.1. Let $\Gamma = \mathrm{SL}_2(\mathbb{Z})$, acting on the left on $\mathfrak{H} = \{\tau \in \mathbb{C} : \mathrm{Im}(\tau) > 0\}$ via

$$\tau \mapsto \frac{a\tau + b}{c\tau + d} \quad \text{where} \quad \gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \Gamma \ .$$

Recall that the group Γ is generated by matrices S, T defined by

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

If we set $U = TS$, then $S^2 = U^3 = -1$. Let Γ_∞ denote the subgroup of Γ consisting of matrices with a 0 in the lower left hand corner. It is generated by $-1, T$ and is the stabilizer of the cusp $\tau = i\infty$. Write $q = \exp(2\pi i \tau)$ for $\tau \in \mathfrak{H}$.

2.1.2. For $n \geq 0$, let V_n denote the vector space of homogeneous polynomials in X, Y of degree n with rational coefficients, and write $V_\infty = \bigoplus_{n\geq 0} V_n \subset \mathbb{Q}[X,Y]$. The graded vector space V_∞ admits the following right action of $\mathrm{SL}_2(\mathbb{Q})$

$$P(X,Y)\big|_\gamma = P(aX + bY, cX + dY) \quad \text{ where } \gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \ .$$

We shall identify $V_\infty^{\otimes n}$ with the vector space of (multi-)homogeneous polynomials in $X_1, Y_1, \ldots, X_n, Y_n$. Thus a tensor $X^{i_1}Y^{j_1} \otimes \ldots \otimes X^{i_n}Y^{j_n}$ will be denoted by $X_1^{i_1}Y_1^{j_1} \ldots X_n^{i_n}Y_n^{j_n}$. We shall view V_n, V_∞, and their various tensor products as trivial bundles over $\mathfrak{H}$, equipped with the action of Γ.

2.1.3. Let $\mathcal{M}_k(\Gamma)$ denote the vector space over $\mathbb{Q}$ spanned by modular forms $f(\tau)$ for Γ of weight k. Every such modular form admits a Fourier expansion

$$f(q) = \sum_{n\geq 0} a_n(f)\, q^n \quad \text{ where } \ a_n(f) \in \mathbb{Q} \ .$$

Let $\mathcal{M}_k(\Gamma) = \mathcal{E}_k(\Gamma) \oplus \mathcal{S}_k(\Gamma)$ denote the decomposition into Eisenstein series and cusp forms. The Eisenstein series of weight $2k \geq 4$ will be denoted by

$$E_{2k}(q) = -\frac{\mathsf{b}_{2k}}{4k} + \sum_{n\geq 0} \sigma_{2k-1}(n) q^n \ ,$$

where b_{2k} is the $2k^{\text{th}}$ Bernoulli number, and σ denotes the divisor function. For every modular form $f(\tau) \in \mathcal{M}_{2k}(\Gamma)$ of weight $2k \geq 4$ we shall write:

$$\underline{f}(\tau) = (2\pi i)^{2k-1} f(\tau)(X - \tau Y)^{2k-2} d\tau \ . \tag{2.1}$$

It is viewed as a section of $\Omega^1(\mathfrak{H}; V_{2k-2} \otimes \mathbb{C})$. The modularity of f is equivalent to

$$\underline{f}(\gamma(\tau))\big|_\gamma = \underline{f}(\tau) \quad \text{ for all } \gamma \in \Gamma \ . \tag{2.2}$$

2.1.4. Let $f \in \mathcal{M}_{2k}(\Gamma) \otimes \mathbb{C}$ with Fourier expansion $f(q) = \sum_{n \geq 0} a_n(f)\, q^n$. Recall that its L-function is the Dirichlet series, defined for $\mathrm{Re}(s) > 2k$, by

$$L(f, s) = \sum_{n \geq 1} \frac{a_n(f)}{n^s} \ . \tag{2.3}$$

By Hecke, it has a meromorphic continuation to $\mathbb{C}$, and the completed L-function

$$\Lambda(f, s) = (2\pi)^{-s} \Gamma(s) L(f, s)$$

admits a functional equation of the form $\Lambda(f, s) = (-1)^k \Lambda(f, 2k - s)$. The L-function of the normalised Eisenstein series is

$$L(E_{2k}, s) = \zeta(s)\zeta(s - 2k + 1) \ . \tag{2.4}$$

When f is a cusp form, (2.3) converges for $\mathrm{Re}(s) > k + 1$ and is entire. Recall Euler's formula for the special values of the Riemann zeta function at even integers

$$\zeta(2n) = -\frac{\mathsf{b}_{2n}}{2} \frac{(2\pi i)^{2n}}{(2n)!} \qquad \text{for } n \geq 1 \ .$$

2.1.5. Let $\mathcal{M}_{1,1}^{an}$ denote the orbifold quotient $\Gamma \backslash\!\backslash \mathfrak{H}$. Let $\overline{\mathcal{M}}_{1,1}^{an}$ denote its compactification, and denote the cusp, corresponding to the point $i\infty$ on the boundary of $\mathfrak{H}$, by p. There is a canonical tangential base point at p which is often denoted by $\partial/\partial q$ [24]. Here it will be written as $\vec{1}_\infty$.

2.2. **Tensor algebras.**

2.2.1. Let $W = \bigoplus_{m \geq 0} W_m$ be a graded vector space over $\mathbb{Q}$ whose graded pieces W_m are finite-dimensional. Its graded dual is defined to be $W^\vee = \bigoplus_{m \geq 0} W_m^\vee$. All infinite-dimensional vector spaces considered in this paper will be of this type. Let

$$T(W) = \bigoplus_{n \geq 0} W^{\otimes n}$$

denote the tensor algebra on W. It is a graded Hopf algebra for the grading given by the length of tensors, and the coproduct for which each $w \in W$ is primitive. Its graded dual (in the above sense, i.e., using the grading W_m on W) is the tensor coalgebra

$$T^c(W) \quad \text{(sometimes denoted by } \mathbb{Q}\langle W \rangle)$$

which is a commutative graded Hopf algebra whose generators will be denoted using the bar notation $[w_1|\dots|w_n]$, where $w_i \in W$. The coproduct is

$$\Delta([w_1|\dots|w_n]) = \sum_{0 \leq i \leq n} [w_1|\dots|w_i] \otimes [w_{i+1}|\dots|w_n] \ .$$

The antipode is the linear map defined on generators by

$$S : [w_1|\dots|w_n] \mapsto (-1)^n [w_n|\dots|w_1] \ .$$

The multiplication on $T^c(W)$ is given by the shuffle product, denoted by ш [11].

2.2.2. Often it is convenient to work with a basis $X = \bigcup_{m\geq 0} X_m$ of $W = \bigoplus_{m\geq 0} W_m$. Then we shall sometimes denote by $T(X)$ (or $T^c(X)$) the tensor algebra (or tensor coalgebra) on the vector space W generated by X over $\mathbb{Q}$.

The topological dual of $T^c(X)$ is isomorphic to the ring

$$\mathbb{Q}\langle\langle X\rangle\rangle = \{S = \sum_{w\in X^*} S_w w, \text{ where } S_w \in \mathbb{Q}\}$$

of non-commutative formal power series in X, where X^* denotes the free monoid generated by X. It is a complete Hopf algebra equipped with the coproduct for which the elements of X are primitive. A series S in $\mathbb{Q}\langle\langle X\rangle\rangle$ is invertible if and only if $S_1 \neq 0$, where $1 \in X^*$ denotes the empty word. A series S is group-like if and only if its coefficients satisfy the shuffle equations: the linear map defined on generators by

$$w \mapsto S_w : T^c(X) \longrightarrow \mathbb{Q}$$

is a homomorphism for the shuffle product ш.

By the previous paragraph, $\mathrm{Spec}\, T^c(X)$ is an affine group scheme over $\mathbb{Q}$. It is pro-unipotent. For any commutative unitary ring R, its group of R points is

$$\{S \in R\langle\langle X\rangle\rangle^\times : S \text{ is group-like}\} .$$

2.2.3. Let W be a vector space over $\mathbb{Q}$ as above. The algebra $\mathrm{Sym}(W)$ defines a commutative and cocommutative Hopf subalgebra

$$\begin{array}{ccc} \mathrm{Sym}(W) & \subset & T^c(W) \\ w_1 \dots w_n & \mapsto & \sum_\sigma w_{\sigma(1)} \otimes \dots w_{\sigma(n)} \end{array}$$

where the sum is over all permutations of n letters, and $\mathrm{Sym}(W)$ is equipped with the coproduct for which the elements of W are primitive. The affine group scheme $\mathrm{Spec}\,(\mathrm{Sym} W)$ can be identified with the abelianization of $\mathrm{Spec}\, T^c(W)$. Its group of R-points is the abelian group $\mathrm{Hom}(W, R)$.

2.3. **Group cohomology.**

2.3.1. Let G be a (finitely-generated) group, and let V be a right G-module over a $\mathbb{Q}$-algebra R. Recall that the group of i-cochains for G is the abelian group generated by maps from the product of i copies of G to V:

$$C^i(G; V) = \langle f : G^i \longrightarrow V\rangle_R .$$

These form a complex with respect to differentials $\delta^i : C^i(G; V) \to C^{i+1}(G; V)$, whose i^{th} homology group is denoted $H^i(G; V)$. The group of i cocycles is denoted $Z^i(G; V)$. We shall only need the following special cases:

- A 0-cochain is an element $v \in V$. Its coboundary is

$$\delta^0(v)(g) = v|_g - v .$$

  In particular $H^0(G; V) \cong Z^0(G; V) \cong V^G$, the group of G-invariants of V.

- A 1-cochain is a map $f : G \to V$. Its coboundary is

$$\delta^1 f(g, h) = f(gh) - f(g)\big|_h - f(h) .$$

We will often denote the value of a cochain f on $g \in G$ by a subscript f_g.

2.3.2. *Cup products.* There is a cup product on cochains

$$\cup : C^i(G; V_1) \otimes_R C^j(G; V_2) \longrightarrow C^{i+j}(G; V_1 \otimes_R V_2) \ ,$$

which satisfies a version of the Leibniz rule $\delta(\alpha \cup \beta) = (-1)^\beta \delta(\alpha) \cup \beta + \alpha \cup \delta(\beta)$. In particular, cup products of cocycles are cocycles. Some special cases:

$$\begin{array}{lrcl} (i,j) = (0,1): & (v \cup \phi)(g) & = & v|_g \otimes \phi(g) \\ (i,j) = (1,0): & (\phi \cup v)(g) & = & \phi(g) \otimes v \\ (i,j) = (1,1): & (\phi_1 \cup \phi_2)(g,h) & = & \phi_1(g)|_h \otimes \phi_2(h) \ . \end{array}$$

2.3.3. *Relative cohomology.* Let $H \leq G$ be a subgroup, and let $C^i(G, H; V)$ denote the cone of the restriction morphism:

$$i^* : C^i(G, V) \longrightarrow C^i(H, V) \ .$$

Denote the homology of $C^i(G, H; V)$ by $H^i(G, H; V)$. Chains in $C^i(G, H; V)$ can be represented by pairs (α, β), where $\alpha \in C^i(G; V)$ and $\beta \in C^{i-1}(H; V)$, with differential

$$\delta(\alpha, \beta) = (\delta\alpha, i^*\alpha - \delta\beta)$$

where i^* denotes restriction to H. There is a long exact cohomology sequence

$$\cdots \rightarrow H^i(G; V) \rightarrow H^i(H; V) \rightarrow H^{i+1}(G, H; V) \rightarrow H^{i+1}(G; V) \rightarrow \cdots \ . \tag{2.5}$$

2.4. **Representations of** SL_2**.**

2.4.1. *Tensor products.* Let $m, n \geq 0$. There is an isomorphism of SL_2-representations

$$V_m \otimes V_n \xrightarrow{\sim} V_{m+n} \oplus V_{m+n-2} \oplus \ldots \oplus V_{|m-n|}$$

Identifying $V_m = \bigoplus_{i+j=m} X^i Y^j \mathbb{Q}$, we can define an explicit SL_2-equivariant map $\partial^k : V_m \otimes V_n \rightarrow V_{m+n-2k}$ for all $k \geq 0$ as follows. First of all, let us denote the projection onto the top component

$$\pi_d : V_{m_1} \otimes \cdots \otimes V_{m_n} \longrightarrow V_{m_1 + \ldots + m_n} \tag{2.6}$$

It is given by the diagonal map $\mathbb{Q}[X_1, \ldots, X_n, Y_1, \ldots, Y_n] \longrightarrow \mathbb{Q}[X, Y]$ which sends every (X_i, Y_i) to (X, Y). Now define

$$\partial^k : \mathbb{Q}[X_1, X_2, Y_1, Y_2] \longrightarrow \mathbb{Q}[X, Y]$$

to be the operator $\pi_d(\partial_{12})^k$ where

$$\partial_{12} = \frac{\partial}{\partial X_1}\frac{\partial}{\partial Y_2} - \frac{\partial}{\partial Y_1}\frac{\partial}{\partial X_2} \ .$$

The operator ∂^k decreases the degree by $2k$ and is evidently SL_2-equivariant. It is $(-1)^k$ symmetric with respect to the involution $v \otimes w \mapsto w \otimes v : V_m \otimes V_n \xrightarrow{\sim} V_n \otimes V_m$.

2.4.2. *Equivariant inner product.* In particular, the operator $(k!)^2 \partial^k : V_k \otimes V_k \rightarrow V_0$ defines a Γ-invariant pairing commonly denoted by

$$\langle \ , \ \rangle : V_k \otimes V_k \longrightarrow \mathbb{Q} \ .$$

It is uniquely determined by the property that for all $P(X, Y) \in V_k$

$$\langle P, (aX + bY)^k \rangle = P(-b, a) \ . \tag{2.7}$$

In particular $\langle P|_\gamma, Q|_\gamma \rangle = \langle P, Q \rangle$ for all $\gamma \in \Gamma$ and $P, Q \in V_k$.

Now suppose that $P, Q : \Gamma \rightarrow V_k \otimes \mathbb{C}$ are two Γ-cocycles, and suppose that Q is cuspidal (i.e., $Q_T = 0$). Define the Peterssen-Haberlund pairing [29, 34] by

$$\{P, Q\} = \langle P_S, Q_S\big|_{T-T^{-1}} \rangle - 2 \,\langle P_T, Q_S\Big|_{1+T} \rangle \tag{2.8}$$

It will be derived in §8.2 and §11.3.2. It has the property that $\{P, Q\} = 0$ whenever P is the cocycle of a Hecke normalised Eisenstein series (proved in §8.4).

3. Iterated Shimura integrals

I recall some basic properties of iterated Shimura integrals on modular curves which are essentially contained in Manin [31]. I only consider the special case $\Gamma = \mathrm{SL}_2(\mathbb{Z})$. For simplicity, I prefer to work entirely on the universal covering space.

3.1. **Generalities on iterated integrals.** Let $\omega_1, \ldots, \omega_n$ be smooth 1-forms on a differentiable manifold M. For any piecewise smooth path $\gamma : [0,1] \to M$, the iterated integral of $\omega_1, \ldots, \omega_n$ along γ is defined by

$$\int_\gamma \omega_1 \ldots \omega_n = \int_{0<t_1<\ldots<t_n<1} \gamma^*(\omega_1)(t_1) \ldots \gamma^*(\omega_n)(t_n) \ .$$

The empty iterated integral $n = 0$ is defined to be the constant 1. Well-known results due to Chen [12] state that there is the composition of paths formula:

$$\int_{\gamma_1\gamma_2} \omega_1 \ldots \omega_n = \sum_{i=0}^{n} \int_{\gamma_1} \omega_1 \ldots \omega_i \int_{\gamma_2} \omega_{i+1} \ldots \omega_n \ , \tag{3.1}$$

whenever $\gamma_1(1) = \gamma_2(0)$ and $\gamma_1\gamma_2$ denotes the path γ_1 followed by γ_2. The shuffle product formula states that iterated integration along a path γ is a homomorphism for the shuffle product. Extending the definition by linearity, this reads

$$\int_\gamma \omega_1 \ldots \omega_m \int_\gamma \omega'_1 \ldots \omega'_n = \int_\gamma \omega_1 \ldots \omega_m \,ш\, \omega'_1 \ldots \omega'_n \ .$$

Finally, recall that the reversal of paths formula states that

$$\int_{\gamma^{-1}} \omega_1 \ldots \omega_n = (-1)^n \int_\gamma \omega_n \ldots \omega_1$$

where γ^{-1} denotes the reversed path $t \mapsto \gamma(1-t)$. Many basic properties of iterated integrals can be found in [12]. One often writes iterated integrals using bar notation

$$\int_\gamma \omega_1 \ldots \omega_n = \int_\gamma [\omega_1| \ldots |\omega_n] \ .$$

It is convenient to work with generating series of iterated integrals, indexed by non-commuting symbols, as follows.

3.2. **Notations.** Most of the constructions in this paper will be defined intrinsically, but it can be useful to fix a rational basis $\mathcal{B}$ of $\mathcal{M}(\Gamma)$. We assume that $\mathcal{B} = \cup_k \mathcal{B}_k$ where $\mathcal{B}_k$ is a basis of $\mathcal{M}_k(\Gamma)$, and that $\mathcal{B}_k$ is compatible with the action of Hecke operators. This means that $\mathcal{B}_k$ is a disjoint union of subsets, each of which is a basis for generalised eigenspaces with respect to the action of Hecke operators. For every k, define a $\mathbb{Q}$-vector space with a basis consisting of certain symbols indexed by $\mathcal{B}_k$

$$M_k = \langle \mathsf{a}_f : f \in \mathcal{B}_k \rangle_{\mathbb{Q}} \ .$$

In order to distinguish between vector spaces and their duals, we shall reserve upper case letters (to be consistent with [31, 32]) for the dual vector space

$$M_k^\vee = \langle \mathsf{A}_f : f \in \mathcal{B}_k \rangle_{\mathbb{Q}} \ ,$$

where $\langle \mathsf{a}_f, \mathsf{A}_g \rangle = \delta_{f,g}$, and δ is the Kronecker delta. We can assume $\mathcal{B}_{2n}$ contains the Hecke normalised Eisenstein series E_{2n}, and write

$$\mathbf{e}_{2n} \quad \text{for} \quad \mathsf{a}_{E_{2n}} \quad , \quad \text{and} \quad \mathbf{E}_{2n} \quad \text{for} \quad \mathsf{A}_{E_{2n}} \tag{3.2}$$

Consider the graded right SL_2-module

$$M^\vee = \bigoplus_{k\geq 0} M_k^\vee \otimes V_{k-2}$$

which has one copy of V_{k-2} for every element of $\mathcal{B}_k$. For any commutative unitary $\mathbb{Q}$-algebra R, let $R\langle\langle M^\vee\rangle\rangle$ denote the ring of formal power series in $M^\vee$. It is a complete Hopf algebra with respect to the coproduct which makes every element of $M^\vee$ primitive. Its elements can be represented by infinite R-linear combinations of

$$\mathsf{A}_{f_1}\ldots\mathsf{A}_{f_n}\otimes X_1^{i_1-1}Y_1^{k_1-i_1-1}\ldots X_n^{i_n-1}Y_n^{k_n-i_n-1} \tag{3.3}$$

where $f_j\in\mathcal{B}_{k_j}$ and $1\leq i_j\leq k_j-1$.

Remark 3.1. Hain's notations are equivalent but slightly different. Given a Hecke eigenform f of weight n he writes $S^{n-2}(e_f)$ for the SL_2 representation $\mathsf{A}_f\otimes V_{n-2}$, where e_f denotes the highest weight vector $\mathsf{A}_f\otimes X^{n-2}$. Note, however, that he works with left SL_2-modules as opposed to the right ones we consider here.

3.3. **Iterated Shimura integrals.** Consider the trivial bundle

$$\mathfrak{H}\times\mathbb{C}\langle\langle M^\vee\rangle\rangle\longrightarrow\mathfrak{H}$$

on $\mathfrak{H}$. The corresponding holomorphic vector bundle has a connection

$$\nabla:\Omega^0(\mathfrak{H},\mathbb{C}\langle\langle M^\vee\rangle\rangle)\longrightarrow\Omega^1(\mathfrak{H},\mathbb{C}\langle\langle M^\vee\rangle\rangle)$$

defined by $\nabla=d+\Omega(\tau)$, where $d(\mathsf{A}_f)=0$,

$$\Omega(\tau)=\sum_{f\in\mathcal{B}}\mathsf{A}_f\,\underline{f}(\tau)\ , \tag{3.4}$$

and A_f acts on $\mathbb{C}\langle\langle M^\vee\rangle\rangle$ by concatenation on the left. Clearly ∇ is flat because $d\Omega(\tau)=0$ and $\Omega(\tau)\wedge\Omega(\tau)=0$. By the invariance (2.2) of $\underline{f}(\tau)$, we have

$$\Omega(\gamma(\tau))\big|_\gamma=\Omega(\tau)\text{ for all }\gamma\in\Gamma\ .$$

Horizontal sections of this vector bundle can be written down using iterated integrals. Let $\gamma:[0,1]\to\mathfrak{H}$ denote a piecewise smooth path, with endpoints $\gamma(0)=\tau_0$, and $\gamma(1)=\tau_1$, and consider the iterated integral

$$I_\gamma=1+\int_\gamma\Omega(\tau)+\int_\gamma\Omega(\tau)\Omega(\tau)+\ldots \tag{3.5}$$

Since the connection ∇ is flat and $\mathfrak{H}$ is simply connected, I_γ only depends on the homotopy class of γ relative to its endpoints. As a consequence we can write I_γ as

$$I(\tau_0;\tau_1)\in\mathbb{C}\langle\langle M^\vee\rangle\rangle\ ,$$

It is a well-defined function on $\mathfrak{H}\times\mathfrak{H}$, and for all $\tau_1\in\mathfrak{H}$, the map $\tau\mapsto I(\tau;\tau_1)$ defines a horizontal section of the bundle $(\mathbb{C}\langle\langle M^\vee\rangle\rangle,\nabla)$.

3.4. **Properties.**

Proposition 3.2. *The integrals $I(\tau_0;\tau_1)$ have the following properties:*

i). (Differential equation).

$$dI(\tau_0;\tau_1)=I(\tau_0;\tau_1)\,\Omega(\tau_1)-\Omega(\tau_0)\,I(\tau_0;\tau_1)\ .$$

ii). (Composition of paths). For all $\tau_0,\tau_1,\tau_2\in\mathfrak{H}$,

$$I(\tau_0;\tau_2)=I(\tau_0;\tau_1)I(\tau_1;\tau_2)\ .$$

iii). (Shuffle product).

$$I(\tau_0;\tau_1)\in\mathbb{C}\langle\langle M^\vee\rangle\rangle\textit{ is invertible and group-like}\ .$$

iv). (Γ-invariance). For all $\gamma \in \Gamma$, and $\tau_0, \tau_1 \in \mathfrak{H}$, we have

$$I(\gamma(\tau_0); \gamma(\tau_1))\big|_{\gamma} = I(\tau_0; \tau_1) \ .$$

Proof. Properties *i)*-*iii)* are general properties of iterated integrals. The last property *iv)* follows because Ω is Γ-invariant, and therefore, for any $\tau_1 \in \mathfrak{H}$, $I(\gamma(\tau); \gamma(\tau_1))|_{\gamma}$ satisfies the differential equation $\nabla F = 0$, as does $I(\tau; \tau_1)$. Both solutions are equal to 1 when $\tau = \tau_1$, which fixes the constant of integration. □

3.5. **A group scheme.** Consider the following graded ring and its dual

$$M = \bigoplus_{k \geq 2} M_k \otimes V_{k-2}^{\vee} \qquad \text{and} \qquad M^{\vee} = \bigoplus_{k \geq 2} M_k^{\vee} \otimes V_{k-2}$$

Then M a graded left SL_2-module, and $M^{\vee}$ is a graded right SL_2-module. Let $T^c(M)$ denote the tensor coalgebra on M. It is a graded Hopf algebra over $\mathbb{Q}$ whose graded pieces are finite-dimensional left SL_2-representations. Let us define

$$\Pi = \mathrm{Spec}\,(T^c(M)) \ . \tag{3.6}$$

It is a non-commutative pro-unipotent affine group scheme over $\mathbb{Q}$, and for any commutative $\mathbb{Q}$-algebra R, its group of R-points is given by formal power series

$$\Pi(R) = \{S \in R\langle\langle M^{\vee}\rangle\rangle^{\times} \text{ such that } S \text{ is group-like}\} \ .$$

The group $\Pi(R)$ admits a right action of SL_2 and hence Γ which we write

$$S\big|_{\gamma} T\big|_{\gamma} = ST\big|_{\gamma} \qquad \text{for} \qquad S, T \in \Pi(R) \ .$$

Property *iii)* of proposition 3.2 states that the elements $I(\tau_0; \tau_1) \in \Pi(\mathbb{C})$ for all $\tau_0, \tau_1 \in \mathfrak{H} \times \mathfrak{H}$, and in fact the iterated integral $I : \mathfrak{H} \times \mathfrak{H} \to \Pi(\mathbb{C})$ defines an element of the constant groupoid $\Pi(\mathbb{C})$ over $\mathfrak{H}$ by property *ii)*.

3.6. **Representation as linear maps.** Any element $S \in R\langle\langle M^{\vee}\rangle\rangle$ can be viewed as a collection of maps (also denoted by S):

$$S : M_{k_1} \otimes \ldots \otimes M_{k_n} \longrightarrow V_{k_1-2} \otimes \ldots \otimes V_{k_n-2} \otimes R \tag{3.7}$$

which to any n-tuple of modular forms associates a multi-homogeneous polynomial in n pairs of variables. The right-hand side carries a right action of SL_2. This map sends $\mathsf{a}_{f_1} \ldots \mathsf{a}_{f_n}$ to the coefficient of $\mathsf{A}_{f_1} \ldots \mathsf{A}_{f_n}$ in S. A series S is group-like if and only if the following shuffle relation holds

$$\begin{aligned} S(\mathsf{a}_{f_1} \ldots \mathsf{a}_{f_p})(X_1, \ldots, X_p)\, S(\mathsf{a}_{f_{p+1}} \ldots \mathsf{a}_{f_{p+q}})(X_{p+1}, \ldots, X_{p+q}) \\ = \sum_{\sigma \in \mathfrak{S}_{p,q}} S(\mathsf{a}_{f_{\sigma(1)}} \ldots \mathsf{a}_{f_{\sigma(p+q)}})(X_{\sigma(1)}, \ldots, X_{\sigma(p+q)}) \end{aligned} \tag{3.8}$$

and if the leading term of S is 1. In this formula, $\mathfrak{S}_{p,q}$ denotes the set of shuffles of type p, q, and we dropped the variables Y_i for simplicity. Note, for example, that the polynomial $S(\mathsf{a}_f \mathsf{a}_f)$ in four variables X_1, Y_1, X_2, Y_2 is not completely determined by $S(\mathsf{a}_f)(X_1, Y_1)$ by the relation (3.8); however, its image under π_d (2.6) is.

4. Regularization

We explain how to regularise the iterated integrals of §3 at a tangential base point at infinity. This defines canonical iterated Eichler integrals, or higher period polynomials, for any sequence of modular forms. The construction is simplified by exploiting the explicit universal covering spaces that we have at our disposal.

4.1. **Tangential base points and iterated integrals.** Let $\overline{C}$ be a smooth complex curve, $p \in \overline{C}$ a point, and $C = \overline{C} \backslash p$ the punctured curve. Let T_p denote the tangent space of $\overline{C}$ at the point p, and $T_p^\times = T_p \backslash \{0\}$ the punctured tangent space.

A tangential base point on C at the point p is an element $\vec{v} \in T_p^\times$ ([14], §15.3-15.12). A convenient way to think of the tangential base point is to choose a germ of an analytic isomorphism $\Phi : (T_p, 0) \rightarrow (\overline{C}, p)$ such that $d\Phi : T_p \rightarrow T_p$ is the identity. One can glue the space $T_p^\times$ to C along the map Φ to obtain a space

$$T_p^\times \cup_\Phi C$$

which is homotopy equivalent to C. The tangential base point $\vec{v}$ is simply an ordinary base point on this enlarged space. A path from a point $x \in \overline{C}$ to this tangential base point can be thought of as a path in $\overline{C}$ from x to a point $\Phi(\varepsilon)$ close to p, followed by a path from ε to $\vec{v}$ in the tangent space T_p. This is pictured below.

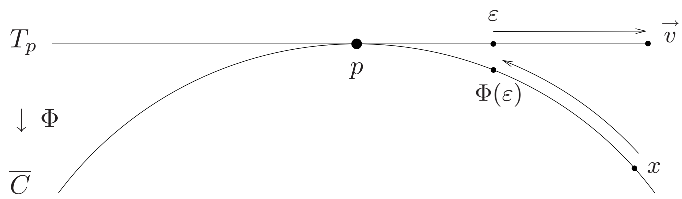

FIGURE 1

Now let ω be a meromorphic one-form on C with at most a logarithmic singularity at p. If we choose a linear function q on T_p, we can write

$$\Phi^*(\omega) = \sum_{n \geq 0} \alpha_n q^n \frac{dq}{q}$$

and define the polar part $P\Phi^*(\omega)$ to be the one-form $\alpha_0 \frac{dq}{q}$ on $T_p^\times$. It does not depend on the choice of function q. The line integral of ω along a path from x to $\overline{v}$ is defined to be

$$\int_x^{\vec{v}} \omega = \lim_{\varepsilon \rightarrow p} \Big(\int_x^{\Phi(\varepsilon)} \omega + \int_\varepsilon^{\vec{v}} P\Phi^*(\omega) \Big)$$

It is straightforward to verify that the limit is finite and does not depend on Φ. The analogue for iterated integrals is given by the composition of paths formula (3.1). If $\omega_1, \ldots, \omega_n$ are closed holomorphic one forms with logarithmic singularities at p, let

$$\int_x^{\vec{v}} \omega_1 \ldots \omega_n = \lim_{\varepsilon \rightarrow p} \Big(\sum_{k=0}^{n} \int_x^{\Phi(\varepsilon)} \omega_1 \ldots \omega_k \int_\varepsilon^{\vec{v}} P\Phi^*(\omega_{k+1}) \ldots P\Phi^*(\omega_n) \Big)$$

The iterated integral is finite and is independent of the choice of Φ. It only depends on x and $\vec{v}$ in the sense that homotopy equivalent paths from x to $\vec{v}$ give rise to the same integral (since $\omega_i \wedge \omega_j = 0$ for all i, j). The integrals in the right-hand factors of the right-hand side are performed on $T_p^\times$, those on the left on C.

We are interested in the case $C = \mathcal{M}_{1,1}^{an}$, $\overline{C} = \overline{\mathcal{M}}_{1,1}^{an}$ and p the cusp (image of $i\infty$). The punctured tangent space $T_p^\times$ is isomorphic to the punctured disc with coordinate q. The tangential base point corresponding to $1 \in T_p^\times$ is often denoted by $\frac{\partial}{\partial q}$.

Remark 4.1. There are many equivalent ways to think of tangential base points. A better way is to view $\overrightarrow{v}$ as a point on the exceptional locus of the real oriented blow-up of $\overline{C}$ at p. This makes the independence of Φ obvious. In our setting, however, we have a canonical map Φ (given by the q-disc) so the presentation above is more convenient.

A more general version of regularisation exists for vector bundles with flat connections, using Deligne's canonical extension ([14], §15.3-15.12). Instead of presenting this approach, we prefer to adapt the above construction for universal covering spaces, which gives a more direct route to the same answer.

4.2. **Universal covering space at $\frac{\partial}{\partial q}$.** The punctured tangent space $T_p^\times$ of $\overline{\mathcal{M}}_{1,1}^{an}$ is isomorphic to $\mathbb{C}^\times$. Its universal covering space is $(\mathbb{C}, 0)$ with the covering map

$$\tau \mapsto \exp(2\pi i\tau) : (\mathbb{C}, 0) \to (\mathbb{C}^\times, 1) \ .$$

We can therefore glue a copy of $\mathbb{C}$ to $\mathfrak{H}$ via the natural inclusion map $i_\infty : \mathfrak{H} \to \mathbb{C}$ to define a space $\mathfrak{H} \cup_{i_\infty} \mathbb{C}$ pictured below.

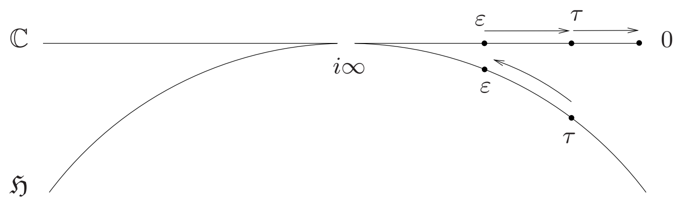

FIGURE 2

A path from $\tau \in \mathfrak{H}$ to $\overrightarrow{1}_\infty$ can be thought of as the compositum of the following two path segments on $\mathfrak{H} \cup_{i_\infty} \mathbb{C}$:

(i) a path from τ to a point $\varepsilon \in \mathfrak{H}$ infinitely close to $i\infty$,
(ii) a path from $i_\infty(\varepsilon)$ to the point 0 in $\mathbb{C}$.

As shown in the picture, the latter path can be divided into two segments, from ε to τ and from τ to 0. Recombining these three segments in a different way gives

(i)′ a path from τ to a point ε, followed by a path from $i_\infty(\varepsilon)$ to $i_\infty(\tau)$.
(ii)′ a path from $i_\infty(\tau)$ to the point 0 in $\mathbb{C}$.

Later we shall identify $\mathfrak{H}$ with its image in $\mathbb{C}$, which means that we drop all i_∞'s from the notation (as in figure 2 above) and compute all integrals on $\mathbb{C}$.

Remark 4.2. The space $(\mathfrak{H} \cup_{i_\infty} \mathbb{C}, 0)$ is the universal covering space of $(\mathcal{M}_{1,1}^{an} \cup_\Phi \mathbb{C}^\times, \frac{\partial}{\partial q})$, where Φ^{-1} is the germ of the map $\tau \mapsto \exp(2i\pi\tau)$, at the tangential base point $1 \in T_p^\times$. One can repeat this construction by gluing a copy of $\mathbb{C}$ at every cusp (rational point) along the boundary of $\mathfrak{H}$. This gives rise to a space $\mathfrak{H} \cup_{\mathbb{Q}\cup\{\infty\}} \mathbb{C}$, which now carries an action of Γ. Its orbifold quotient is $\mathcal{M}_{1,1}^{an} \cup_\Phi \mathbb{C}^\times$.

4.3. **Iterated integrals on the tangent space.** In §4.1, the divergent part of ω corresponded to the form $\frac{dq}{q}$ on $T_p^\times$. On a universal covering space of $T_p^\times$, the divergent parts correspond to iterated integrals in $\frac{dq}{q}$, namely, polynomials in τ times $d\tau$.

Definition 4.3. Let $f \in \mathcal{M}_{2k}(\Gamma)$, and denote the constant term in its Fourier expansion by $a_0(f)$. Define the tangential component of $\underline{f}(\tau)$ to be

$$\underline{f}^\infty(\tau) = (2\pi i)^{2k-1} a_0(f)(X - \tau Y)^{2k-2} d\tau \ . \quad (4.1)$$

It is to be viewed as a section of $\Omega^1(\mathbb{C}; V_{2k-2}\otimes\mathbb{C})$ on the tangent space $\mathbb{C}\subset\mathfrak{H}\cup_{i_\infty}\mathbb{C}$. Clearly, f is a cusp form if and only if $\underline{f}^\infty(\tau)$ vanishes.

One can repeat the discussion of §3.3 with the trivial bundle $\mathbb{C}\langle\langle M^\vee\rangle\rangle$ viewed this time over $\mathbb{C}$, and replacing ∇ with the connection $\nabla_\infty = d+\Omega^\infty(\tau)$, where

$$\Omega^\infty(\tau) = \sum_{f\in\mathcal{B}} \mathsf{A}_f\, \underline{f}^\infty(\tau)\ , \tag{4.2}$$

For any pair of points $a,b\in\mathbb{C}$, define $I^\infty(a;b)\in\mathbb{C}\langle\langle M^\vee\rangle\rangle$ to be the iterated integral

$$I^\infty(a;b) = 1+\int_\gamma \Omega^\infty + \int_\gamma \Omega^\infty\,\Omega^\infty + \ldots \tag{4.3}$$

along any piecewise smooth path $\gamma:[0,1]\to\mathbb{C}$ such that $\gamma(0)=a, \gamma(1)=b$. It only depends on the endpoints a,b for similar reasons to proposition 3.2. In particular, the composition of paths formula $I^\infty(a;c)=I^\infty(a;b)\,I^\infty(b;c)$ holds for all $a,b,c\in\mathbb{C}$, and $I^\infty(a;b)\in\Pi(\mathbb{C})$. We have a similar equivariance property

$$\Omega^\infty(\gamma(\tau))\big|_\gamma = \Omega^\infty(\tau) \qquad \text{for all } \gamma\in\Gamma_\infty\ .$$

4.4. **Iterated Eichler integrals.** As in figure 2, we integrate the form $\Omega(\tau)$ along the first path segment (i) on $\mathfrak{H}$, and integrate $\Omega^\infty(\tau)$ along the second segment (ii) on $\mathbb{C}$. Since composition of paths corresponds to the concatenation product of generating series of iterated integrals, one arrives at the following definition.

Definition 4.4. The iterated Eichler integral from $\tau\in\mathfrak{H}$ to $\vec{1}_\infty$ is

$$I(\tau;\infty) = \lim_{\varepsilon\to i\infty}\big(I(\tau;\varepsilon)\ I^\infty(i_\infty(\varepsilon);0)\big) \qquad \in\Pi(\mathbb{C})\subset\mathbb{C}\langle\langle M^\vee\rangle\rangle\ ,$$

where $i_\infty:\mathfrak{H}\to\mathbb{C}$ is the inclusion.

The right-hand integral I^∞ in the definition is viewed on the tangent space $\mathbb{C}$, the left-hand one on $\mathfrak{H}$. However, using the gluing map $i_\infty:\mathfrak{H}\to\mathbb{C}$, we can compute both kinds of iterated integral on a single copy of $\mathbb{C}$: in short we can drop all occurrences of i_∞ from the notation and henceforth work entirely on $\mathbb{C}$.

To verify the finiteness of the iterated Eichler integral, we first define, for $\tau_0,\tau_1\in\mathfrak{H}$, the regularized iterated integral to be

$$RI(\tau_0;\tau_1) = I(\tau_0;\tau_1)I^\infty(\tau_1;\tau_0)\ .$$

Lemma 4.5. *$RI(\tau;x)$ is finite as $x\to i\infty$ and converges like $O(e^{2\pi i x})$.*

Proof. From the differential equation for I (Proposition 3.2 i)), we check that

$$\frac{\partial}{\partial x}RI(\tau;x) = I(\tau_0;x)\Big(\Omega(x)-\Omega^\infty(x)\Big)I^\infty(x;\tau_0)\ .$$

For each $\omega\in\mathcal{M}_k(\Gamma)$, the form $\underline{\omega}(x)$ grows at most polynomially in x near ∞. Therefore each term in $I(\tau_0;x)$, and $I^\infty(x;\tau_0)$, is of polynomial growth in x. On the other hand

$$\Omega(x)-\Omega^\infty(x) = O(\exp(2\pi i x)) \qquad \text{as} \quad x\to i\infty\ ,$$

which follows from the Fourier expansion §2.1.3. This proves the lemma. □

As a consequence, we define

$$RI(\tau) = \lim_{x\to i\infty} RI(\tau;x)\ . \tag{4.4}$$

Recombining the paths in figure 2 into the two parts $(i)'$ and $(ii)'$ leads to the following formula for the generating series of iterated Eichler integrals.

Corollary 4.6. *The iterated Eichler integral is a product*

$$I(\tau;\infty) = RI(\tau)\, I^{\infty}(\tau;0)\ . \tag{4.5}$$

Proof. By the composition of paths formula for I^{∞}, we have

$$I(\tau;\infty) = \lim_{x\rightarrow i\infty} \big(I(\tau;x)\ I^{\infty}(x;\tau)\big) I^{\infty}(\tau;0) = RI(\tau)\, I^{\infty}(\tau,0)\ .$$

□

4.5. **Properties.** The following properties are almost immediate from definition 4.4.

Proposition 4.7. *The iterated Eichler integrals $I(\tau;\infty)$ have the following properties:*

i). (Differential equation).

$$\frac{d}{d\tau} I(\tau;\infty) = -\Omega(\tau)\, I(\tau;\infty)\ .$$

ii). (Composition of paths). For any $\tau_1,\tau_2\in\mathfrak{H}$,

$$I(\tau_1;\infty) = I(\tau_1;\tau_2)\, I(\tau_2;\infty)\ .$$

iii). (Shuffle product). $I(\tau;\infty)\in\Pi(\mathbb{C})$, or equivalently,

$$I(\tau;\infty)\in\mathbb{C}\langle\langle M^{\vee}\rangle\rangle \text{ is invertible and group-like}\ .$$

Proof. To verify i), observe that

$$\frac{\partial}{\partial\tau} I(\tau;x)\, I^{\infty}(i_{\infty}(x);0) = -\Omega(\tau)\, I(\tau;x)\, I^{\infty}(i_{\infty}(x);0)$$

and take the limit as $x\rightarrow i\infty$, according to definition 4.4. The remaining properties are straightforward and follow in a similar manner to the proof of proposition 3.2. □

4.6. **Explicit formulae.** Let $\omega\in\mathcal{M}_k(\Gamma)$, and write

$$\underline{\omega}^0(\tau) = \underline{\omega}(\tau) - \underline{\omega}^{\infty}(\tau)\ , \tag{4.6}$$

where $\underline{\omega}^0,\underline{\omega},\underline{\omega}^{\infty}$ are viewed as sections of $\Omega^1(\mathbb{C};V_{k-2}\otimes\mathbb{C})$. We have seen that $\underline{\omega}^0(\tau)$ tends to zero like $e^{2\pi i\tau}$, as τ tends to $i\infty$ along the imaginary axis. In order to write down compact formulae for iterated Eichler integrals as integrals of absolutely convergent forms, we use the following notation. Let W be a vector space together with an isomorphism

$$(\pi^0,\pi^{\infty}): W \overset{\sim}{\longrightarrow} W^0\oplus W^{\infty}\ .$$

We shall also write w^0, w^{∞} for $\pi^0(w),\pi^{\infty}(w)$. Consider the convolution product

$$R = ш\circ(\mathrm{id}\otimes\pi^{\infty}S)\circ\Delta : T^c(W)\longrightarrow T^c(W)$$

where S,Δ, were defined in §2.2.1, and ш is the shuffle multiplication on $T^c(V)$. Explicitly, the map R is given for $\omega_1,\ldots,\omega_n\in W$ by

$$R[\omega_1|\ldots|\omega_n] = \sum_{i=0}^{n}(-1)^{n-i}[\omega_1|\ldots|\omega_i]\,ш\,[\omega_n^{\infty}|\ldots|\omega_{i+1}^{\infty}]\ . \tag{4.7}$$

Lemma 4.8. *For any elements $\omega_1,\ldots,\omega_n\in W$ we have*

$$R[\omega_1|\ldots|\omega_n] = \sum_{i=1}^{n}(-1)^{n-i}\Big[[\omega_1|\ldots|\omega_{i-1}]\,ш\,[\omega_n^{\infty}|\ldots|\omega_{i+1}^{\infty}]\,\Big|\,\omega_i^0\Big]\ . \tag{4.8}$$

Proof. By replacing the final ω_i^0 in (4.8) by $\omega_i - \omega_i^\infty$, we can view both (4.7) and (4.8) as formal expressions inside $T^c(W \oplus W^\infty)$. They satisfy the formulae $R(1) = 1$ and

$$\begin{aligned} \partial_{\omega_i} R[\omega_1|\dots|\omega_n] &= \delta_{i1} R[\omega_2|\dots|\omega_n] \\ \partial_{\omega_i^\infty} R[\omega_1|\dots|\omega_n] &= -R[\omega_1|\dots|\omega_{n-1}]\delta_{in} \ , \end{aligned}$$

where ∂_a is the differential operator on $T^c(W \oplus W^\infty)$ defined by $\partial_{\omega_i}[\omega_1|\dots|\omega_n] = \delta_{i1}$, and δ is the Kronecker delta. These equations uniquely determine R. □

Example 4.9. In lengths 1 and 2,

$$\begin{aligned} R[\omega_1] &= [\omega_1] - [\omega_1^\infty] \\ &= [\omega_1^0] \ . \end{aligned} \tag{4.9}$$

$$\begin{aligned} R[\omega_1|\omega_2] &= [\omega_1|\omega_2] - [\omega_1] \text{ш} [\omega_2^\infty] + [\omega_2^\infty|\omega_1^\infty] \\ &= [\omega_1|\omega_2^0] - [\omega_2^\infty|\omega_1^0] \ . \end{aligned} \tag{4.10}$$

Applying the above to the subspace $W \subset \Gamma^1(\mathbb{C}; \Omega^1_{\mathbb{C}} \otimes V)$ spanned by $\underline{f}(\tau)$ (2.1) for $f \in \mathcal{M}(\Gamma) \otimes \mathbb{C}$, and combining with (4.5) leads to the following formula:

$$\begin{aligned} \int_\tau^{\vec{1}_\infty} [\omega_1|\dots|\omega_n] &= \sum_{i=0}^n \int_\tau^\infty R[\omega_1|\dots|\omega_i] \int_\tau^0 [\omega_{i+1}^\infty|\dots|\omega_n^\infty] \\ &= \sum_{i=0}^n (-1)^{n-i} \int_\tau^\infty R[\omega_1|\dots|\omega_i] \int_0^\tau [\omega_n^\infty|\dots|\omega_{i+1}^\infty] \end{aligned} \tag{4.11}$$

Each right-hand factor (the integral from 0 to τ) is simply a polynomial in τ, and each left-hand factor (the integral from τ to ∞) converges exponentially fast in τ. The second line of (4.11) follows from the first by the reversal of paths formula §3.1.

Example 4.10. In length 1, this gives for ω a modular form of weight k by (4.9),

$$\int_\tau^{\vec{1}_\infty} \underline{\omega}(\tau) = \int_\tau^\infty \omega^0(\tau)(X - \tau Y)^{k-2} d\tau - \int_0^\tau a_0(\omega)(X - \tau Y)^{k-2} \ . \tag{4.12}$$

In length 2, with $\omega_1, \omega_2 \in \mathcal{M}(\Gamma)$, formula (4.11) combined with (4.9), (4.10) gives the following four rapidly-convergent integrals, for any $\tau \in i\mathbb{R}^{>0}$:

$$\begin{aligned} &\int_{\tau \le \tau_1 \le \tau_2 \le \infty} \underline{\omega_1}(\tau_1)\underline{\omega_2^0}(\tau_2) - \underline{\omega_2^\infty}(\tau_1)\underline{\omega_1^0}(\tau_2) \\ &\qquad - \int_\tau^\infty \underline{\omega_1^0}(\tau) \int_0^\tau \underline{\omega_2^\infty}(\tau) + \int_{0 \le \tau_2 \le \tau_1 \le \tau} \underline{\omega_2^\infty}(\tau_2)\underline{\omega_1^\infty}(\tau_1) \end{aligned} \tag{4.13}$$

Because of the exponentially fast convergence of the integrals, these formulae lend themselves very well to numerical computations.

5. The canonical Γ-cocyle

5.1. **Definition.** Let $I(\tau; \infty)$ denote the non-commutative generating series of iterated Eichler integrals defined in §4.4.

Lemma 5.1. *For every $\gamma \in \Gamma$, there exists a series $\mathcal{C}_\gamma \in \Pi(\mathbb{C})$, such that*

$$I(\tau; \infty) = I(\gamma(\tau); \infty)\big|_\gamma \mathcal{C}_\gamma \tag{5.1}$$

It does not depend on τ. It satisfies the cocycle relation

$$\mathcal{C}_{gh} = \mathcal{C}_g\big|_h \mathcal{C}_h \qquad \textit{for all } g, h \in \Gamma \ . \tag{5.2}$$

Proof. Let $\gamma \in \Gamma$. It follows from the Γ-invariance of $\Omega(\tau)$ that $I(\tau;\infty)$ and $I(\gamma(\tau);\infty)|_\gamma$ are two solutions to the differential equation $\frac{\partial}{\partial \tau} L(\tau) = -\Omega(\tau)\, L(\tau)$ where $L(\tau) \in \Pi(\mathbb{C})$. They therefore differ by multiplication on the right by a constant series $C_\gamma \in \Pi(\mathbb{C})$ which does not depend on τ. The proof of (5.2) is standard. Put $\gamma = g$ in (5.1), replace τ with $h(\tau)$, and act on the right by h. This gives

$$I(h(\tau);\infty)\big|_h = I(gh(\tau);\infty)\big|_{gh}\mathcal{C}_g\big|_h \ .$$

Subsituting this equation into (5.1) with $\gamma = h$ gives

$$I(\tau;\infty) = I(gh(\tau);\infty)\big|_{gh}\mathcal{C}_g\big|_h\mathcal{C}_h \ .$$

The cocycle relation then follows from definition of $\mathcal{C}_{gh}$. □

Equation (5.2) follows without calculation from remark 5.3 below since the monodromy of $(\mathbb{C}\langle\langle M^\vee\rangle\rangle, \nabla)$ at $\frac{\partial}{\partial q}$ gives a homomorphism $\gamma \mapsto (\gamma, C_\gamma) : \Gamma \to \Gamma \ltimes \Pi(\mathbb{C})$.

Definition 5.2. Define the ring of multiple modular values $\mathcal{MMV}_\Gamma$ for Γ to be the $\mathbb{Q}$-algebra generated by the coefficients of (3.3) in $\mathcal{C}_\gamma$ for all $\gamma \in \Gamma$.

Setting $\tau = \gamma^{-1}(\infty)$ in equation (5.1) gives the following formula for $\mathcal{C}_\gamma$

$$\mathcal{C}_\gamma = I(\gamma^{-1}(\infty);\infty) \ . \tag{5.3}$$

To make sense of this formula, one must define iterated integrals $I(a;b)$ regularised with respect to two tangential base points a and b. But this follows easily from the previous construction using the formula $I(a;b) = I(\tau;a)^{-1}I(\tau;b)$, for any $\tau \in \mathfrak{H}$.

5.2. **Non-abelian cocycles.** Let G be a group, and let A be a group with a right G-action. This means that $ab|_g = a|_g b|_g$ for all $a, b \in A$ and $g \in G$, and

$$a|_{gh} = (a|_g)|_h$$

for all $a \in A$, and $g, h \in G$. The set of cocycles of G in A is defined by

$$Z^1(G,A) = \{C : G \to A \text{ such that } C_{gh} = C_g\big|_h C_h \text{ for all } g,h \in G\}$$

Two such cocycles C, C' differ by a coboundary if there exists a $B \in A$ such that

$$C'_g = B|_g C_g B^{-1}$$

This defines an equivalence relation on cocycles, and the set of equivalence classes is denoted by $H^1(G,A)$. It has a distinguished element $1 : g \mapsto 1$.

Remark 5.3. Let $\mathrm{Hom}_G(G, G \ltimes A)$ denote the set of group homomorphisms from G to $G \ltimes A$ whose composition with the projection $G \ltimes A \to G$ is the identity on $G \to G$. As is well known, there is a canonical bijection

$$\begin{array}{rcl} Z^1(G,A) & = & \mathrm{Hom}_G(G, G\ltimes A) \\ z & \mapsto & (g \mapsto (g, z_g)) \end{array}$$

The canonical cocycle $\mathcal{C}$ defines an element

$$\mathcal{C} \in Z^1(\Gamma;\Pi(\mathbb{C})) \ .$$

Since Γ is generated by S and T (§2.1.1), the cocycle $\mathcal{C}$ is completely determined by $\mathcal{C}_S$ and $\mathcal{C}_T$. Since $i \in \mathfrak{H}$ is fixed by S, formula (5.1) gives the following formula for $\mathcal{C}_S$:

$$\mathcal{C}_S = I(i;\infty)\big|_S^{-1} I(i;\infty) \ . \tag{5.4}$$

The series $\mathcal{C}_T$ will be computed explicitly in the next paragraph. Its coefficients are rational multiples of powers of $2\pi i$. Therefore the ring $\mathcal{MMV}$ is generated by the coefficients of $\mathcal{C}_S$ and $2\pi i$.

Remark 5.4. For every point $\tau_1 \in \mathfrak{H}$, one obtains a cocycle $C(\tau_1) \in Z^1(\Gamma;\Pi(\mathbb{C}))$ defined by $I(\tau;\tau_1) = I(\gamma(\tau);\tau_1)|_\gamma C_\gamma(\tau_1)$. The composition of paths formula for I implies that the cocyles $C_\gamma(\tau_1)$, for varying τ_1, define the same cohomology class. Manin called this class the non-commutative modular symbol in [32].

5.3. **Equations.** To simplify notations, let $Z^1(\Gamma;\Pi)$ denote the functor on commutative unitary $\mathbb{Q}$-algebras $R \mapsto Z^1(\Gamma;\Pi(R))$.

Lemma 5.5. *An element $C \in Z^1(\Gamma,\Pi)$ is uniquely determined by a pair $C_S, C_T \in \Pi$ satisfying the relations:*

$$\begin{aligned} 1 &= C_S\big|_S C_S \\ 1 &= C_U\big|_{U^2} C_U\big|_U C_U \end{aligned}$$

where $C_U = C_T\big|_S C_S$.

Proof. Since all modular forms for Γ have even weight, it follows from the definition of Π that the image of the maps (3.7) for any element of Π have even weight (-1 acts trivially). Therefore $C_{-1} = 1$ for any cocycle $C \in Z^1(\Gamma,\Pi)$ and thus

$$Z^1(\Gamma,\Pi) \overset{\sim}{\longrightarrow} Z^1(\Gamma/\{\pm 1\},\Pi) \ .$$

It is well-known (§2.1.1) that $\Gamma/\{\pm 1\} = \langle S,T,U : U = TS, U^3 = S^2 = 1\rangle$. Now simply apply remark 5.3. A computational proof was given in [32], §1.2.1. □

These equations can be made more explicit by the following observation. Consider $C \in Z^1(\Gamma,\Pi(R))$. Since $C_\gamma \in \Pi(R)$, its leading term is 1, and we can define

$$C' : \Gamma \longrightarrow R\langle\langle M^\vee\rangle\rangle$$

by the equation $C' = C - 1$. The element C' satisfies

$$C'_{gh} - C'_g\big|_h - C'_h = C'_g\big|_h C'_h$$

for all $g,h \in \Gamma$. Thinking now of C_γ as a morphism via (3.7), the previous equation can be written, for all $n \geq 1$, as a system of cochain equations (à la Massey)

$$\delta C[\mathsf{a}_1|\dots|\mathsf{a}_n] = \sum_{i=1}^{n-1} C[\mathsf{a}_1|\dots|\mathsf{a}_i] \cup C[\mathsf{a}_{i+1}|\dots|\mathsf{a}_n] \ , \tag{5.5}$$

where $\mathsf{a}_i \in M$ and where $\delta^1(C)(g,h) = C_{gh} - C_g\big|_h - C_h$ and $(A \cup B)(g,h) = A_g|_h \otimes B_h$ are the coboundary and cup product for Γ-cochains (see §2.3.1, §2.3.2).

Caveat 5.6. A cocycle C, viewed as a series of higher period polynomials (3.7) is completely determined by the shuffle equation (3.8), together with the equations (5.5) evaluated at the pairs (S,S), (T,S), (U,U^2) by lemma 5.5. They are unobstructed in the sense that they can be solved recursively in the length: the $C[\mathsf{a}_1]$ are ordinary abelian cocyles, and so on. This is because Γ has cohomological dimension 1.

However, we will need to constrain the value of C_T which leads to non-trivial obstructions to solving (5.5). These obstructions are the object of study of §8.

5.4. **Real structure.** The real Frobenius acts on $\Pi(\mathbb{C})$ as follows. Let

$$\epsilon = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{5.6}$$

It acts on the right on V_∞ via $(X,Y) \mapsto (X,-Y)$ and acts diagonally on $T(V_\infty)$. This defines an involution on $\Pi(\mathbb{C})$ by acting trivially on the elements a_f (respectively A_f).

Let c denote the action of complex conjugation on the coefficients of $\Pi(\mathbb{C})$. Let

$$(5.7)\qquad \begin{array}{rcl} F_\infty : \Pi(\mathbb{C}) & \longrightarrow & \Pi(\mathbb{C}) \\ S & \mapsto & c(S)\big|_\epsilon \end{array}$$

denote the involution obtained by composing them. Recall that complex conjugation on $\mathcal{M}^{an}_{1,1} \cup_\Phi T^*_\infty$ corresponds to the map $\tau \mapsto -\overline{\tau}$ on $\mathfrak{H} \cup_{i_\infty} \mathbb{C}$.

To justify the formula for F_∞, let $f \in \mathcal{M}(\Gamma)$ be a modular form with rational (and in particular, real) Fourier coefficients. Then it follows from the definition (2.1) that

$$\underline{f}(-\overline{\tau}) = \overline{\underline{f}(\tau)}\big|_\epsilon$$

and there is a similar equation on replacing $\underline{f}$ with $\underline{f}^\infty$. Thus the action of complex conjugation c_{dR} on differential forms $\underline{f}(\tau)$ is right action by ϵ, and the action of real Frobenius F_∞ indeed corresponds to (5.7).

On the other hand, complex conjugation acts on the space $\mathcal{M}^{an}_{1,1} \cup_\Phi \mathbb{C}^\times$ which induces an action on $\Gamma = \pi_1(\mathcal{M}^{an}_{1,1}, \frac{\partial}{\partial q})$. This is given by conjugation by ϵ, because

$$-\overline{\gamma(\tau)} = \epsilon\gamma\epsilon^{-1}(-\overline{\tau})$$

for all $\tau \in \mathfrak{H}, \gamma \in \Gamma$, and similarly for $\tau \in \mathbb{C}$ in the tangent space at the cusp, and $\gamma \in \Gamma_\infty$. The following lemma is an immediate corollary.

Lemma 5.7. *Let $\mathcal{C}$ denote the canonical cocycle. Then*

$$(5.8)\qquad F_\infty \mathcal{C}_\gamma = \mathcal{C}_{\epsilon\gamma\epsilon^{-1}} \ .$$

In particular, $\mathcal{C}_S$ is invariant under F_∞ and $F_\infty \mathcal{C}_T = \mathcal{C}_{T^{-1}}$.

One can also prove that $F_\infty \mathcal{C}_S = \mathcal{C}_S$ by direct computation using (5.4): $\mathcal{C}_S$ is obtained by integrating along the imaginary axis which is invariant under $\tau \mapsto -\overline{\tau}$. Likewise the path T corresponds to a simple loop around 0 in $\mathbb{C}^\times$ and is reversed under complex conjugation and a similar computation using (6.2) below gives $F_\infty \mathcal{C}_T = \mathcal{C}_{T^{-1}}$. Equation (5.8) can then be deduced from (5.2). Finally, observe that

$$(5.9)\qquad \partial^k(\varepsilon \otimes \varepsilon) = (-1)^k \varepsilon\, \partial^k \ .$$

which follows immediately from the definition of ∂^k, §2.4.1.

6. Cocycle at the cusp

It is straightforward to compute the image of the canonical cocycle $\mathcal{C}$ under the map

$$(6.1)\qquad Z^1(\Gamma; \Pi) \longrightarrow Z^1(\Gamma_\infty; \Pi) \ .$$

6.1. **Rational structure.** Since Γ_∞ is generated by -1 and T, and $\mathcal{C}_{-1} = 1$, the image of $\mathcal{C}$ under (6.1) is determined by $\mathcal{C}_T$.

Lemma 6.1. *We have the following formula for $\mathcal{C}_T$:*

$$(6.2)\qquad \mathcal{C}_T = I^\infty(-1; 0) \ .$$

In particular, $\mathcal{C}_T$ has coefficients in $\mathbb{Q}[2\pi i]$ (see below for an explicit formula).

Proof. It follows from setting $\gamma = T^{-1}$ in (5.1) that $\mathcal{C}_T$ can be computed by integrating along a path from the tangential base point $T^{-1}\overrightarrow{1}_\infty$ to $\overrightarrow{1}_\infty$. On the universal covering $\mathfrak{H} \cup_{i_\infty} \mathbb{C}$ this is simply the path from -1 to 0 on the tangent space $\mathbb{C}$. Formula (6.2) is immediate from the discussion of §4.4. The second statement follows from the observation that the coefficients of $\Omega^\infty(\tau)$ are given by the zeroth Fourier coefficients of Eisenstein series (multiplied by a power of $2\pi i$). By §2.1.3, the latter are rational. □

Remark 6.2. The map (6.1) can be interpreted as follows. The inclusion of the tangent space $T_p^\times \to \mathcal{M}_{1,1}^{an} \cup_\Phi T_p^\times$ gives rise to the local monodromy map

$$\pi_1(T_p^\times, 1) \longrightarrow \pi_1(\mathcal{M}_{1,1}^{an}, \partial/\partial q) \ ,$$

which is the inclusion of Γ_∞ into Γ. One can deduce that the coefficients of $\mathcal{C}_T$ are periods of the unipotent fundamental group of $T_\infty^\times \cong \mathbb{G}_m$, which are in $\mathbb{Q}[2\pi i]$.

If we view $\mathcal{C}_T \in \Pi(\mathbb{C})$ as a linear map from a sequence of modular forms to polynomials via (3.7), then it follows from the above discussion that

$$\mathcal{C}_T(\mathsf{a}_{f_1} \dots \mathsf{a}_{f_n}) = 0 \tag{6.3}$$

whenever any f_i is a cusp form (since $\underline{f}_i^\infty$ vanishes in that case). The only non-zero contributions to $\mathcal{C}_T$ come from iterated integrals of Eisenstein series only.

6.2. **Formula for $\mathcal{C}_T$.** In order to write down $\mathcal{C}_T$ it is convenient to rescale the Eisenstein series as follows. By comparing with §2.1.3, we define normalized letters

$$\widetilde{\mathbf{E}}_{2k} = \frac{1}{(2\pi i)^{2k-1}} \frac{-4k}{\mathsf{b}_{2k}(2k-2)!} \mathbf{E}_{2k} \ , \ \text{for } k \geq 2 \ .$$

The rational factor is chosen so that in this alphabet,

$$\Omega^\infty(\tau) = \sum_{k\geq 2} \frac{\widetilde{\mathbf{E}}_{2k}}{(2k-2)!}(X - Y\tau)^{2k-2} \ .$$

With this choice of normalisation, we can write down the cocycle explicitly as follows.

Lemma 6.3. *The coefficient of* $\widetilde{\mathbf{E}}_{2k_1} \dots \widetilde{\mathbf{E}}_{2k_n}$ *in* $\mathcal{C}_T$ *is equal to the coefficient of* $s_1^{2k_1-2} \dots s_n^{2k_n-2}$ *in the commutative generating series*

$$e^{s_1X_1+\dots+s_nX_n}\Big(\sum_{i=0}^n \frac{(-1)^{n-i}}{\pi^L(s_1Y_1,\dots,s_iY_i)} \frac{e^{s_1Y_1+\dots+s_iY_i}}{\pi^R(s_{i+1}Y_{i+1},\dots,s_nY_n)}\Big) \ . \tag{6.4}$$

Here we use the notation 'pile up on the left or right':

$$\begin{aligned} \pi^L(z_1,\dots,z_n) &= (z_1+\dots+z_n)\cdots(z_{n-1}+z_n)z_n \\ \pi^R(z_1,\dots,z_n) &= z_1(z_1+z_2)\cdots(z_1+\dots+z_n) \end{aligned}$$

For clarity, formula (6.4) in lengths 1 and 2, and with $s_1 = s_2 = 1$ reads

$$e^{X_1}\Big(\frac{e^{Y_1}}{Y_1} - \frac{1}{Y_1}\Big) \qquad \text{and} \qquad e^{X_1+X_2}\Big(\frac{e^{Y_1+Y_2}}{(Y_1+Y_2)Y_2} - \frac{e^{Y_1}}{Y_1Y_2} + \frac{1}{Y_1(Y_1+Y_2)}\Big)$$

Lemma 6.3 can be deduced from (6.2) but follows from the discussion below. Note that (6.4), despite appearances, has no poles. It is clearly defined over $\mathbb{Q}$.

6.3. **Trivialisation.** We can formally trivialise the restriction of $\mathcal{C}$ to $Z^1(\Gamma_\infty, \Pi(\mathbb{C}))$ by enlarging the space of coefficients in the following way. By (3.7), we can regard $\mathcal{C}_T$ as a map from sequences of modular forms into the space $T(V_\infty)$ of polynomials in infinitely many variables X_i, Y_i. Enlarge it by letting

$$\widehat{T(V_\infty)} = \mathbb{Q}[X_1, Y_1, X_2, Y_2, \dots]\Big[\frac{1}{Y_1}, \frac{1}{Y_1+Y_2}, \dots, \frac{1}{Y_i+\dots+Y_{i+r}}\Big]$$

denote the space of polynomials in X_i, Y_i with denominators in $Y_i + Y_{i+1} + \dots + Y_{i+r}$. Since the elements Y_i are fixed by T, this space inherits an action of Γ_∞ by §2.1.1.

Proposition 6.4. *There exists a series $\mathcal{V} \in \widehat{T(V_\infty)}\langle\langle \widetilde{\mathbf{E}}_{2n} \rangle\rangle$ which trivialises $\mathcal{C}_T$, i.e.,*

$$\mathcal{C}_T = \mathcal{V}|_T \, \mathcal{V}^{-1} \ . \tag{6.5}$$

It is not unique. A representative is given by the series whose coefficient of $\widetilde{\mathbf{E}}_{2k_1} \ldots \widetilde{\mathbf{E}}_{2k_n}$ is the coefficient of $s_1^{2k_1-2} \ldots s_n^{2k_n-2}$ in the commutative generating series

$$\frac{e^{s_1 X_1 + \ldots + s_n X_n}}{(s_1 Y_1 + \ldots + s_n Y_n) \ldots (s_{n-1} Y_{n-1} + s_n Y_n) s_n Y_n} . \tag{6.6}$$

expanded in the sector $0 \ll s_1 \ll \ldots \ll s_n$.

Proof. By (5.1), restricted to the tangent space $\mathbb{C}$ of $\mathfrak{H} \cup_{i_\infty} \mathbb{C}$, we have

$$I^\infty(\tau; 0) = I^\infty(\tau + 1; 0)\big|_T \mathcal{C}_T \ .$$

We wish to set $\mathcal{V} = \lim_{\tau \to \infty} I^\infty(\tau; 0)^{-1}$. For this, consider the series $I^\infty(0; \tau)$ in length n, and view it as a commutative formal power series by replacing the words $\widetilde{\mathbf{E}}_{2k_1} \ldots \widetilde{\mathbf{E}}_{2k_n}$ with $s_1^{2k_1-2} \ldots s_n^{2k_n-2}$, for $r \leq n$. Since $I^\infty(0; \tau)$ is the iterated integral of $\Omega^\infty(\tau)$ by (4.3), the coefficients of $I^\infty(0; \tau)$ are represented by the iterated integral

$$\int_0^\tau [e^{(X_1 - \tau Y_1) s_1} | \ldots | e^{(X_n - \tau Y_n) s_n}] d\tau \ .$$

Formally taking the limit as $\tau \to \infty$ (thinking of Y_n as positive real numbers) gives (6.6). From this we deduce that (6.5) holds, as a function of the parameters s_i. By transposing the concatenation and inversion of formal (non-commutative) power series into the language of commutative generating series, one readily sees that (6.5) implies (6.4). Finally, equation (6.6) is justified by expanding the expression $\mathcal{V}|_T \mathcal{V}^{-1}$ (which is well-defined as a power series in s_i) in the chosen sector. □

Expanding (6.6) in a different sector gives rise to a different choice of trivialisation for the restriction of $\mathcal{C}$ to Γ_∞. However, after projecting

$$\pi_d : \widehat{T(V_\infty)} \to \mathbb{Q}[X, Y, \frac{1}{Y}]$$

by sending (X_i, Y_i) to (X, Y), we obtain a canonical trivialisation from (6.6)

$$\frac{e^{(s_1 + \ldots + s_n) X}}{Y^n (s_1 + \ldots + s_n) \ldots (s_{n-1} + s_n) s_n}$$

which can be uniquely expanded as a Laurent power series in the s_i (in any sector).

Remark 6.5. Zagier's 'extended period polynomials' for Eisenstein series are the coefficients of $\mathsf{A}_{E_{2k}}$ in the cocycle $\gamma \mapsto \mathcal{V}|_\gamma^{-1} \mathcal{C}_\gamma \mathcal{V}$ (viewed as a cocycle whose coefficients are in the field of rational functions in X_i, Y_i) applied to $\gamma = S$.

7. The abelianised cocycle and the Eichler-Shimura theorem

We compute the image of the canonical cocycle $\mathcal{C}$ under the map

$$Z^1(\Gamma; \Pi(\mathbb{C})) \longrightarrow Z^1(\Gamma; \Pi^{ab}(\mathbb{C})) \ .$$

The results of this section are well-known, but are recalled here for convenience.

7.1. **Abelianization of $\mathcal{C}$.** For any commutative $\mathbb{Q}$-algebra R we have §2.2.3

$$\Pi^{ab}(R) \cong \mathrm{Hom}(M,R) = \prod_k M_k^\vee \otimes V_{k-2} \otimes R \ .$$

The natural map $\Pi \rightarrow \Pi^{ab}$ therefore induces a map

$$Z^1(\Gamma,\Pi) \longrightarrow Z^1(\Gamma;\Pi^{ab}) \cong \prod_k M_k^\vee \otimes Z^1(\Gamma;V_{k-2}) \ .$$

This can be written

$$Z^1(\Gamma,\Pi) \longrightarrow \prod_k \mathrm{Hom}(M_k, Z^1(\Gamma;V_{k-2})) \ .$$

In particular, for $f \in \mathcal{B}_k$, the coefficient of A_f in $\mathcal{C}$, which is denoted by $\mathcal{C}(\mathsf{a}_f)$ (see (3.7)), is a Γ-cocycle in V_{k-2}. This defines a linear map

$$\mathsf{p} : \mathcal{M}_k(\Gamma) \longrightarrow Z^1(\Gamma;V_{k-2}) \otimes \mathbb{C}$$

which we call p for period. It is the abelianization of the canonical cocycle $\mathcal{C}$. Explicit formulae for p are obtained from (5.4) and (4.12).

7.2. **Periods of cusp forms.** For any cusp form $f \in S_{2k}(\Gamma)$ of weight $2k$,

$$\begin{aligned}\mathsf{p}(f)_T &= 0\\ \mathsf{p}(f)_S &= (2\pi i)^{2k-1}\int_0^{i\infty} f(\tau)(X-\tau Y)^{2k-2} d\tau \ .\end{aligned}$$

Performing a Fourier expansion of the second equation yields the formula

$$\mathsf{p}(f)_S = (2\pi i)^{2k-1}\sum_{r=1}^{2k-1}(-i)^{r-1}\binom{2k-2}{r-1}\Lambda(g,r)X^{2k-r-1}Y^{r-1}$$

In particular, we immediately deduce that the numbers $(2\pi i)^{2k-1} i^{r-1}\Lambda(g,r)$ are multiple modular values for all values of r inside the critical strip $1 \leq r \leq 2k-1$. If f is a normalised Hecke eigenform, Manin showed [30] that there exist two real numbers

$$\omega_f^+, \omega_f^- \in \mathbb{R} \ ,$$

called the periods of f, such that (extending scalars $\mathsf{p} : \mathcal{M}_k \otimes \mathbb{C} \rightarrow V_{2k-2} \otimes \mathbb{C}$),

$$\mathsf{p}(f)_S = \omega_f^+ P_f^+(X,Y) + i\, \omega_f^- P_f^-(X,Y)$$

where $P_f^\pm(X,Y) \in V_{k-2}^\pm \otimes K_f$, and K_f is the number field generated by the Fourier coefficients of f, and $\pm$ denotes the eigenspaces with respect to ε. In fact, we can assume that the coefficients $\omega_f^\pm$ are equivariant: $\sigma(\omega_f^\pm) = \omega_{\sigma(f)}^\pm$ for all $\sigma \in \mathrm{Aut}_{\mathbb{Q}}(K_f)$.

7.3. **Periods of Eisenstein series.** Let

$$c(x) = \frac{1}{e^x-1} + \frac{1}{2} - \frac{1}{x} \qquad (7.1)$$

Define a set of rational cocycles $e_{2k}^0 \in Z^1(\Gamma;V_{2k-2})$ via their generating series

$$e^0 = \sum_{k\geq 2} \frac{2}{(2k-2)!} e_{2k}^0$$

where e^0 is the unique cocycle defined on Γ by

$$\begin{aligned} e^0(S) &= c(X)c(Y)\\ e^0(T) &= \tfrac{1}{Y}(c(X+Y)-c(X)) - \tfrac{1}{12}\end{aligned} \qquad (7.2)$$

One easily verifies that the e_{2k}^0 do indeed satisfy the cocycle relations.

Lemma 7.1. *(Zagier). The cocycles of Eisenstein series are*

$$\mathsf{p}(E_{2k}) = (2i\pi)^{2k-1} e^0_{2k} - \frac{(2k-2)!}{2}\zeta(2k-1)\delta^0(Y^{2k-2}) \ ,$$

where δ^0 is the differential §2.3.1 and $k \geq 2$. The coboundary term $\delta^0(Y^{2k-2})$ is the cocycle which sends T to 0 and S to $X^{2k-2} - Y^{2k-2}$.

Proof. (Sketch). For any $f \in \mathcal{M}_k(\Gamma)$, the value of the cocycle $\mathcal{C}^{ab}(f)$ on S is given by:

$$\mathcal{C}^{ab}(f)_S = (2\pi i)^{2k-1}\Big(\int_i^{i\infty} f^0(X-\tau Y)^{k-2}d\tau - \int_0^{\tau} a_0(f)(X-\tau Y)^{k-2}d\tau\Big)\Big|_{S-1}$$

by (5.4) and (4.12), where f^0 is defined by (4.6). The left-hand integral can be expressed in terms of the L-function of E_{2k} which is a product of zeta functions §2.1.4; the right-hand integral is elementary. The value of $\mathsf{p}(E_{2k})$ on T follows from §6.2. □

The coefficients of the cocycle $\mathsf{p}(E_{2k})$ lie in $\zeta(2k-1)\mathbb{Q} + (2\pi i)^{2k-1}\mathbb{Q}$. We have

$$\begin{array}{rcl} [\mathsf{p}] : \mathcal{E}_k(\Gamma) & \longrightarrow & H^1(\Gamma; V_{k-2}) \otimes (2\pi i)^{2k-1}\mathbb{Q} \ . \\ E_{2k} & \mapsto & (2i\pi)^{2k-1}[e^0_{2k}] \end{array} \tag{7.3}$$

Thus the cohomology class of the Eisenstein cocycle is, up to a power of $2\pi i$, rational, although the cocycle itself is not, due to the presence of the odd zeta value. An explanation of this phenomenon will follow from the description of the motivic Galois action on cocycles to be given in §9.9.

7.4. **Eichler-Shimura isomorphism.** We clearly have $H^0(\Gamma; V_\infty) = V_\infty^\Gamma = \mathbb{Q}$, and furthermore, $H^i(\Gamma; V_n)$ vanishes for all $i \geq 2$, because $\mathcal{M}^{an}_{1,1}(\mathbb{C})$ is of real dimension 2 and non-compact. The group $H^1(\Gamma; V_n)$ is described by the Eichler-Shimura theorem.

By §5.4, complex conjugation acts on V_n by ϵ on the right, and the real Frobenius acts on Γ by conjugation by ϵ. This defines the following action on cochains:

$$\begin{array}{rcl} C^i(\Gamma; V_n) & \longrightarrow & C^i(\Gamma; V_n) \\ \phi & \mapsto & \big((g_1, \ldots, g_n) \mapsto \phi(\epsilon g_1 \epsilon^{-1}, \ldots, \epsilon g_n \epsilon^{-1})\big|_\epsilon\big) \end{array} \tag{7.4}$$

It is a morphism of complexes, and therefore induces an action on cohomology. Denote the eigenspaces of $H^1(\Gamma; V_n)$ for this action by $\pm$. Thus elements of $H^1(\Gamma; V_n)^\pm$ can be represented by cocycles satisfying

$$C_{\epsilon\gamma\epsilon^{-1}}\big|_\epsilon = \pm C_\gamma$$

For example, $C_S|_\varepsilon = C_S$ if and only if C_S is even in Y (an 'even period polynomial') and $C_S|_\varepsilon = -C_S$ if and only if C_S is odd in Y.

Theorem 7.2. *(Eichler-Shimura) For all $n \geq 2$, integration defines isomorphisms*

$$\begin{array}{rcccl} [\mathsf{p}^+] & : & S_n(\Gamma) & \stackrel{\sim}{\longrightarrow} & H^1(\Gamma; V_{n-2})^+ \otimes \mathbb{R} \ , \\ [\mathsf{p}^-] & : & \mathcal{M}_n(\Gamma) & \stackrel{\sim}{\longrightarrow} & H^1(\Gamma; V_{n-2})^- \otimes \mathbb{R} \ . \end{array}$$

where $\mathsf{p}^+ = \mathrm{Re}\,\mathsf{p}$ and $\mathsf{p}^- = \mathrm{Im}\,\mathsf{p}$. In particular, for all $n \geq 2$

$$\dim_\mathbb{Q} H^1(\Gamma; V_{n-2}) = \dim_\mathbb{Q} \mathcal{E}_n(\Gamma) + 2 \dim_\mathbb{Q} \mathcal{S}_n(\Gamma) \ .$$

The restriction map induced from the inclusion i of Γ_∞ in Γ is

$$i^* : H^1(\Gamma; V_n) \to H^1(\Gamma_\infty; V_n)$$

Denote the kernel of this map by $H^1_{\mathrm{cusp}}(\Gamma; V_n) \subset H^1(\Gamma; V_n)$.

7.5. **Hecke-equivariant splitting.** Let $k \geq 2$, and let

$$Z^1_{\mathrm{cusp}}(\Gamma; V_{2k}) = \ker(Z^1(\Gamma; V_{2k}) \longrightarrow Z^1(\Gamma_\infty; V_{2k}))$$

denote the subspace of cuspidal cocycles. The subspace of coboundaries in $Z^1_{\mathrm{cusp}}(\Gamma; V_{2k})$ is one-dimensional, spanned by $\delta^0 Y^{2k}$. This follows immediately from the following exact sequence of $\mathbb{Q}$-vector spaces:

$$0 \longrightarrow Y^{2k}\mathbb{Q} \longrightarrow V_{2k} \overset{T-1}{\longrightarrow} V_{2k} \longrightarrow X^{2k}\mathbb{Q} \longrightarrow 0 \ .$$

Since the cocycle of a cusp form vanishes on T, we have

$$\mathsf{p}^{\pm} : S_k(\Gamma) \longrightarrow Z^1_{\mathrm{cusp}}(\Gamma, V_{k-2})^{\pm} \otimes \mathbb{R} \longrightarrow H^1_{\mathrm{cusp}}(\Gamma, V_{k-2})^{\pm} \otimes \mathbb{R} \ .$$

Manin defined [30] the action of Hecke operators onto $Z^1_{\mathrm{cusp}}(\Gamma, V_{k-2})^{\pm}$ and proved that $\mathsf{p}^{\pm}$ commutes with this action. Linear algebra implies the following lemma.

Lemma 7.3. *There is a canonical splitting over* $\mathbb{Q}$

$$s : H^1_{\mathrm{cusp}}(\Gamma; V_{2k}) \to Z^1_{\mathrm{cusp}}(\Gamma; V_{2k})$$

which is equivariant for the action of Hecke operators. We have

$$Z^1_{\mathrm{cusp}}(\Gamma; V_{2k}) = \delta^0 Y^{2k}\mathbb{Q} \oplus s(H^1_{\mathrm{cusp}}(\Gamma; V_{2k})) \ .$$

Proof. The map s can be written explicitly by noting that the space $s(H^1_{\mathrm{cusp}}(\Gamma; V_{2k}))$ is orthogonal to the space of Eisenstein cocycles e^0_{2k} with respect to the inner product $\{\ ,\}$ defined in (2.8), which is equivariant for the action of Hecke operators [29, 34]. Since a cuspidal cocycle C (or its cohomology class) is uniquely determined by the polynomial $C_S \in V_{2k}$, we can simply define $s(C)_T = 0$ and

$$s(C)_S = C_S + \alpha(X^{2k} - Y^{2k})$$

where α is determined by $\{e^0_{2k}, C_S\} + \alpha\{e^0_{2k}, X^{2k} - Y^{2k}\} = 0$. The coefficient of α is non-zero by the following lemma. □

Lemma 7.4. *Let* e^0_{2k} *denote the rational cocycle defined above. Then*

$$\{e^0_{2k}, \delta^0 Y^{2k-2}\} = \frac{3\mathsf{b}_{2k}}{2k} \quad \textit{for} \quad k \geq 2 \ . \tag{7.5}$$

Proof. Applying definition (2.8) gives

$$\langle e^0_{2k}(S), (X-Y)^{2k-2} - (X+Y)^{2k-2}\rangle - 2\langle e^0_{2k}(T), (X^{2k-2} - Y^{2k-2})\big|_{1+T}\rangle$$

By §5.4, we have $F_\infty \mathcal{C}_T = \mathcal{C}_{T^{-1}}$. Since $\mathcal{C}$ is a cocycle, $0 = \mathcal{C}_T|_{T^{-1}} + \mathcal{C}_{T^{-1}}$ and hence $\mathcal{C}_T|_\epsilon = \mathcal{C}_T|_{T^{-1}}$. This implies that $e^0_{2k}(T)|_{T^{-1}} = e^0_{2k}(T)|_\epsilon$. Using the Γ, and ϵ-invariance of $\langle\ ,\ \rangle$, the previous expression therefore becomes

$$\langle e^0_{2k}(S), (X-Y)^{2k-2} - (X+Y)^{2k-2}\rangle \ - \ 4\langle e^0_{2k}(T), X^{2k-2} - Y^{2k-2}\rangle$$

Replacing e^0 with its generating series, and applying formula (2.7) proves that the expression (7.5) is $\frac{(2k-2)!}{2}$ times the coefficient of t^{2k-2} in

$$c(t)c(-t) - c(t)c(t) + 4\Big(c'(t) - \frac{c(t)}{t}\Big) = 6c'(t) - \frac{1}{2} \ .$$

The previous identity follows easily from the definition (7.1). □

In summary, the following diagram is commutative:

$$\begin{array}{ccc} H^1_{\mathrm{cusp}}(\Gamma; V_{2k})^+ \otimes \mathbb{R} & \overset{s\otimes\mathbb{R}}{\longrightarrow} & Z^1_{\mathrm{cusp}}(\Gamma; V_{2k})^+ \otimes \mathbb{R} \\ \uparrow_{[\mathsf{p}^+]} & & \| \\ S_{2k+2}(\Gamma) & \overset{\mathsf{p}^+}{\longrightarrow} & Z^1_{\mathrm{cusp}}(\Gamma; V_{2k})^+ \otimes \mathbb{R} \end{array}$$

By the above remarks, we can completely determine elements in $Z^1_{\mathrm{cusp}}(\Gamma; V_{2k})$ by pairing with the cocycles of cusp forms §7.2 and Eisenstein series §7.3 with respect to $\{\ \}$ (since it is well-known that the Haberlund-Peterssen inner product is non-degenerate).

8. Transference of periods

The non-vanishing of $H^2(\Gamma, \Gamma_\infty; \mathbb{Q})$ leads to non-trivial identities between periods of iterated Eichler integrals. It gives rise to a kind of 'transference principle' whereby periods of iterated integrals of certain modular forms are related to periods of iterated integrals of completely different modular forms.

8.1. **Relative H^2.** The group Γ is of cohomological dimension 1. The cohomology of Γ relative to Γ_∞ (§2.3.3), however, satisfies

$$H^2(\Gamma, \Gamma_\infty; V_n) = \begin{cases} \mathbb{Q} & \text{if } n = 0\ , \\ 0 & \text{if } n \text{ even} > 0\ . \end{cases} \tag{8.1}$$

corresponding to the compactly supported cohomology of $\mathcal{M}^{an}_{1,1}$. Equation (8.1) can also be easily verified using the long exact sequences of relative cohomology and the results of the previous section. We construct an isomorphism

$$h : H^2(\Gamma, \Gamma_\infty; \mathbb{Q}) \overset{\sim}{\longrightarrow} \mathbb{Q}$$

by standard arguments in homological algebra. An element in $H^2(\Gamma, \Gamma_\infty; \mathbb{Q})$ can be represented by a pair (α, β), where $\alpha \in Z^2(\Gamma; \mathbb{Q})$, $\beta \in C^1(\Gamma_\infty; \mathbb{Q})$ and $\alpha|_{\Gamma_\infty} = \delta^1\beta$.

Lemma 8.1. *Let $(\alpha, \beta) \in Z^2(\Gamma, \Gamma_\infty; \mathbb{Q})$ as above. Then*

$$h((\alpha, \beta)) = \beta_T + \frac{1}{6}\big(2\alpha_{(U,U)} + 2\alpha_{(U^2,U)} + 6\alpha_{(T,S)} - 3\alpha_{(S,S)}\big) \tag{8.2}$$

defines an isomorphism $h : H^2(\Gamma, \Gamma_\infty; \mathbb{Q}) \overset{\sim}{\to} \mathbb{Q}$.

Proof. The long exact cohomology sequence (2.5) implies that

$$H^1(\Gamma; \mathbb{Q}) \to H^1(\Gamma_\infty; \mathbb{Q}) \to H^2(\Gamma, \Gamma_\infty; \mathbb{Q}) \to H^2(\Gamma; \mathbb{Q}) = 0$$

and since $H^1(\Gamma; \mathbb{Q}) = 0$ this gives $H^1(\Gamma_\infty; \mathbb{Q}) \overset{\sim}{\to} H^2(\Gamma, \Gamma_\infty; \mathbb{Q})$. It is induced by the map $v \mapsto (0, v)$ on cocycles. Now $v \mapsto v_T$ gives an isomorphism $H^1(\Gamma_\infty; \mathbb{Q}) \cong \mathbb{Q}$ and we define h to be the compositum $H^2(\Gamma, \Gamma_\infty; \mathbb{Q}) \cong \mathbb{Q}$. In particular, $h([0, v]) = v_T$.

Since $H^2(\Gamma; \mathbb{Q}) = 0$ there exists $f \in C^1(\Gamma; \mathbb{Q})$ such that $\alpha = -\delta^1 f$. To compute f_T, evaluate the equation $\alpha = -\delta^1 f$ on pairs in Γ^2 using §2.3.1 to get:

$$\begin{array}{rclcrcl} \alpha_{(S,S)} & = & 2f_S & , & \alpha_{(T,S)} & = & f_S + f_T - f_U \\ \alpha_{(U,U)} & = & 2f_U - f_{U^2} & , & \alpha_{(U^2,U)} & = & f_U + f_{U^2}\ . \end{array}$$

Combining these equations gives

$$6f_T = 2\alpha_{(U,U)} + 2\alpha_{(U^2,U)} + 6\alpha_{(T,S)} - 3\alpha_{(S,S)}\ .$$

Now the element

$$(\alpha, \beta) + \delta(f, 0) = (0, \beta + i^* f)$$

represents the same cohomology class as (α, β) where $i : \Gamma_\infty \to \Gamma$. The value of $h([\alpha, \beta])$ is defined to be $\beta_T + f_T \in \mathbb{Q}$, which gives (8.2). $\square$

8.2. **Pairing and cup product.** There is a cup product

$$\begin{array}{rcl} Z^1(\Gamma;V_n)\times Z^1(\Gamma,\Gamma_\infty;V_n) & \overset{\cup}{\longrightarrow} & Z^2(\Gamma,\Gamma_\infty;V_n\otimes V_n) \\ \gamma\cup(\alpha,\beta) & = & (\gamma\cup\alpha,\gamma\cup\beta) \end{array}$$

Composing with the projection $V_n\otimes V_n\to V_0\cong\mathbb{Q}$ of §2.4.2, taking cohomology, and applying the map h of (8.2) yields a pairing between cocycles and relative cocycles. In particular, via tha map $\alpha\mapsto(\alpha,0):Z^1_{\mathrm{cusp}}(\Gamma;V_n)\to Z^1(\Gamma;\Gamma_\infty;V_n)$ it gives a pairing

$$\{\ ,\ \}:Z^1(\Gamma;V_n)\times Z^1_{\mathrm{cusp}}(\Gamma;V_n)\longrightarrow\mathbb{Q}$$

We can lift this formula to cochains (non-uniquely) by substituting §2.3.1 into (8.2).

Definition 8.2. Define a bilinear pairing

$$\mathfrak{h}:C^1(\Gamma;V_m)\otimes C^1(\Gamma;V_n)\longrightarrow V_m\otimes V_n \tag{8.3}$$

by the formula $\mathfrak{h}(\alpha\otimes\beta)=h(\alpha\cup\beta)$. Explicitly,

$$\mathfrak{h}(\alpha,\alpha')=\frac{1}{3}\big(\alpha'_U+\alpha'_{U^2}\big)\big|_U\otimes\alpha_U+\big(\alpha'_T-\frac{1}{2}\alpha'_S\big)\big|_S\otimes\alpha_S \tag{8.4}$$

The pairing $\mathfrak{h}$ is a precursor to the Peterssen-Haberlund inner product.

Lemma 8.3. *If $f\in Z^1(\Gamma;V_{2k})$ and $g\in Z^1_{\mathrm{cusp}}(\Gamma;V_{2k})$ then*

$$\{f,g\}=-6\langle\mathfrak{h}(g,f)\rangle$$

where the bracket $\{\ ,\}$ *was defined in* (2.8).

Proof. For any cocycle c, we have $0=c_U+c_{U^2}|_U$ since $U^3=1$, and also $c_U=c_S+c_T|_S$ since $U=TS$. Because $g_T=0$, we have furthermore $g_U=g_S$. Therefore

$$\langle h(g,f)\rangle=\frac{1}{3}\langle g_S\big|_{TS}-g_S,f_S+f_T\big|_S\rangle-\frac{1}{2}\langle g_S\big|_S,f_S\rangle\ .$$

Using the Γ-invariance of the inner-product, and the equation $c_S|_S=-c_S$ gives

$$6\langle h(g,f)\rangle=\langle g_S-2g_S|_T,f_S\rangle+2\langle g_S\big|_{1+T},f_T\rangle\ . \tag{8.5}$$

On the other hand, for any cocycle c we have $c_U+c_U|_U+c_U|_{U^{-1}}=0$, which, applied to g gives $g_S+g_S|_{TS}+g_S|_{ST^{-1}}=0$. Pairing with f_S leads to the equation

$$\langle g_S,f_S\rangle=\langle g_S\big|_T,f_S\rangle+\langle g_S\big|_{T^{-1}},f_S\rangle$$

Substituting into (8.5) and using the fact that $\langle\ ,\rangle$ is symmetric on $V_{2k}\otimes V_{2k}$ gives the required formula (2.8). ☐

8.3. **Transference principle.** Let $\mathcal{C}$ denote the canonical cocyle. By (3.7), we shall view $\mathcal{C}$ as a collection of cochains

$$\mathcal{C}:M_{k_1}\otimes\ldots\otimes M_{k_r}\longrightarrow C^1(\Gamma;V_{k_1-2}\otimes\ldots\otimes V_{k_r-2})$$

The vector space on the left has a basis given by words $w=\mathsf{a}_{f_1}\ldots\mathsf{a}_{f_r}$ where $f_i\in\mathcal{B}_{k_i}$. Let $\mathcal{C}(w)$ denote the corresponding Γ-cochain.

Theorem 8.4. *Let $\pi:V_{k_1-2}\otimes\ldots\otimes V_{k_r-2}\to V_0$ denote any SL_2-equivariant projection onto a copy of $V_0\cong\mathbb{Q}$. The coefficients of $\mathcal{C}$ satisfy an equation*

$$\pi\Big(\sum_{uv=w}\mathfrak{h}(\mathcal{C}(u),\mathcal{C}(v))+\mathcal{C}(w)_T\Big)=0 \tag{8.6}$$

for any word w in the a_f, where the sum is over strict factorisations of w. If w contains at least one letter a_f where f is a cusp form, then

$$\pi\sum_{uv=w}\mathfrak{h}(\mathcal{C}(u),\mathcal{C}(v))=0\ .$$

Proof. Denote the restriction of $\mathcal{C}_w$ to Γ_∞ by $i^*\mathcal{C}_w$. Then

$$\delta^1(\mathcal{C}(w),0) = (\sum_{w=uv} \mathcal{C}(u)\cup\mathcal{C}(v), i^*\mathcal{C}(w))$$

is a relative coboundary by (5.5), so its class in $H^2(\Gamma;\Gamma_\infty,\mathbb{Q})$ vanishes. Applying (8.2) to this coboundary leads to equation (8.6) via definition (8.4). The last equation follows immediately from (8.6) on applying (6.3). □

One can rewrite relation (8.6) as a certain pairing between non-abelian cochains. It states that $\mathcal{C}$ pairs with itself to give 0. Equation (8.6) implies relations between iterated Eichler integrals of length n coming from the existence of iterated Eichler integrals of length $n+1$.

8.4. **Length one.** Let $n \geq 2$ and let $\mathsf{a}_1, \mathsf{a}_2 \in M_{2n}$ where a_1 corresponds to a cusp form. Then $\mathcal{C}(\mathsf{a}_1\mathsf{a}_2)$ is cuspidal (vanishes on T), and we deduce that

$$\langle \mathfrak{h}(\mathcal{C}(\mathsf{a}_1), \mathcal{C}(\mathsf{a}_2))\rangle = 0\ ,$$

which implies by lemma 8.3 that $\{\mathcal{C}(\mathsf{a}_2), \mathcal{C}(\mathsf{a}_1)\} = 0$ since the $\mathcal{C}(\mathsf{a}_i)$ are cocycles. In particular, if f is a cusp form of weight $2n$, then $\mathcal{C}(\mathsf{a}_f)$ is $\mathsf{p}(f)$ and $\mathcal{C}(\mathbf{e}_{2n})$ is, by §7.3, a multiple of the rational cocycle e^0_{2n} plus a coboundary term. It follows immediately from lemma 8.3 that the cocycles of cusp forms satisfy

$$\{e^0_{2n}, \mathsf{p}(f)\} = 0\ . \tag{8.7}$$

This is of course well-known [29].

8.5. **Examples in length two.** Let $p, q, r \in \mathbb{N}$ be a triangle:

$$|p-q| \leq r \leq p+q$$

and let $\mathsf{a}_1 \in M_{2p+2}, \mathsf{a}_2 \in M_{2q+2}, \mathsf{a}_3 \in M_{2r+2}$. Then we have

$$\langle \mathfrak{h}(\mathcal{C}(\mathsf{a}_1), \partial^{q+r-p}\mathcal{C}(\mathsf{a}_2\mathsf{a}_3))\rangle + \langle \mathfrak{h}(\partial^{p+q-r}\mathcal{C}(\mathsf{a}_1\mathsf{a}_2), \mathcal{C}(\mathsf{a}_3))\rangle \quad \in \quad \mathbb{Q}(2i\pi)^{2p+2q+2r+3}\ .$$

The left-hand side vanishes if $\mathsf{a}_1, \mathsf{a}_2, \mathsf{a}_3$ are not all Eisenstein series.

On the other hand, when $r = p+q$, and $\mathsf{a}_1, \mathsf{a}_2, \mathsf{a}_3$ are Eisenstein series, we obtain:

$$\langle \partial^0\mathfrak{h}(\mathcal{C}(\mathbf{e}_m\mathbf{e}_n), \mathcal{C}(\mathbf{e}_{m+n-2}))\rangle + \langle \mathfrak{h}(\mathcal{C}(\mathbf{e}_m), \partial^{n-2}\mathcal{C}(\mathbf{e}_n\mathbf{e}_{m+n-2}))\rangle \quad \in \quad \mathbb{Q}(2i\pi)^{2m+2n-5}$$

from the previous formula with $m = 2p+2, n = 2q+2$. Since we know the cocycles $\mathcal{C}(\mathbf{e}_m)$ explicitly, this gives a relation between the highest-weight and lowest-weight parts of double Eisenstein cocycles

$$\partial^0\mathcal{C}(\mathbf{e}_m\mathbf{e}_n) \qquad \text{and} \qquad \partial^{n-2}\mathcal{C}(\mathbf{e}_n\mathbf{e}_{m+n-2})$$

This is significant because these are precisely the two places (see §12) where we obtain non-trivial multiple zeta value coefficients (as opposed to single zeta values).

More strikingly, if $\mathsf{a}_1, \mathsf{a}_2$ are Eisenstein series and a_3 corresponds to a cusp form, we find non-trivial relations between the periods of double Eisenstein integrals $\mathcal{C}(\mathbf{e}_m\mathbf{e}_n)$ and the iterated integral $\mathcal{C}(\mathbf{e}_n\mathsf{a}_f)$ of an Eisenstein series and a cusp form.

9. Cocycle structure and automorphisms

We define the Betti fundamental groupoid $\mathfrak{P}$ of $\Gamma\backslash\backslash\mathfrak{H}$ at cusps and compute its group of automorphisms. Many of the results of this section are valid for general relative Malcev completions, and will be studied in much greater detail in [5].

9.1. **Betti fundamental group.** Compare the discussion in §3.2. For all $k \geq 2$, define a $\mathbb{Q}$-vector space of rational cohomology classes by

$$P_k = H^1(\Gamma; V_{k-2}) \ .$$

Since the right-hand side admits an action of Hecke operators and also an action of ϵ §7.4 we have in particular a decomposition

$$P_k = P_k^{\mathrm{eis}} \oplus P_k^{\mathrm{cusp}} \qquad \text{and} \qquad P_k^{\mathrm{cusp}} = P_k^{\mathrm{cusp},+} \oplus P_k^{\mathrm{cusp},-}$$

The subspace P_k^{eis} is spanned by cocycles of Eisenstein series §7.3 and is anti-invariant with respect to ϵ. The subspace P_k^{cusp} is defined to be $H^1_{\mathrm{cusp}}(\Gamma, V_{k-2})$.

Now let $P_k^\vee$ denote the vector space dual to P_k, and define

$$P = \bigoplus_{k\geq 2} P_k \otimes V_{k-2}^\vee \qquad \text{and} \qquad P^\vee = \bigoplus_{k\geq 2} P_k^\vee \otimes V_{k-2} \ .$$

Then P is a graded left SL_2 module, and $P^\vee$ is a graded right SL_2-module.

Definition 9.1. Let $T^c(P)$ denote the tensor coalgebra §2.2.1 on P. It is a graded Hopf algebra over $\mathbb{Q}$ equipped with a left action of SL_2, and hence Γ. Define

$$\mathfrak{P} = \mathrm{Spec}\,(T^c(P)) \ .$$

It is a pro-unipotent affine group scheme over $\mathbb{Q}$, and its set of R-points is

$$\mathfrak{P}(R) = \{S \in R\langle\langle P^\vee \rangle\rangle^\times \text{ such that } S \text{ group-like}\} \ .$$

This is the set of group-like formal power series with respect to the coproduct for which elements of $P^\vee$ are primitive, where R is any commutative unitary $\mathbb{Q}$-algebra.

The group $\mathfrak{P}(R)$ admits a right action of SL_2, and hence Γ, satisfying

$$S\big|_\gamma T\big|_\gamma = ST\big|_\gamma \qquad \text{for all } S, T \in \mathfrak{P}(R) \ .$$

An element $S \in \mathfrak{P}(R)$ can be viewed as a collection of linear maps

$$S : P_{k_1} \otimes \ldots \otimes P_{k_r} \longrightarrow V_{k_1-2} \otimes \ldots \otimes V_{k_r-2} \otimes R$$

which satisfies the analogue of the shuffle equation (3.8).

Remark 9.2. The scheme $\mathfrak{P}$ is isomorphic to the pro-unipotent radical of the relative Malcev completion of Γ, graded for the lower central series filtration [22, 24].

9.2. **Cocycles tangent to the identity.** We describe a certain subspace of cycles in $Z^1(\Gamma; \mathfrak{P}(R))$ tangent to the identity. The general case will be discussed in [5].

For any commutative $\mathbb{Q}$-algebra R we have by §2.2.3

$$\mathfrak{P}^{ab}(R) \cong \mathrm{Hom}(P, R) \cong \prod_{k\geq 2} P_k^\vee \otimes V_{k-2} \otimes R \ .$$

The natural map $\mathfrak{P} \to \mathfrak{P}^{ab}$ therefore induces a map

$$Z^1(\Gamma; \mathfrak{P}) \longrightarrow Z^1(\Gamma; \mathfrak{P}^{ab}) \cong \prod_k P_k^\vee \otimes Z^1(\Gamma; V_{k-2}) \ .$$

Since $P_k = H^1(\Gamma; V_{k-2})$, this can be written

$$Z^1(\Gamma; \mathfrak{P}) \longrightarrow \prod_k \mathrm{Hom}(H^1(\Gamma; V_{k-2}), Z^1(\Gamma; V_{k-2})) \ . \tag{9.1}$$

Define the tangent map to be

$$t : Z^1(\Gamma; \mathfrak{P}) \longrightarrow \prod_k \mathrm{Hom}(H^1(\Gamma; V_{k-2}), H^1(\Gamma; V_{k-2})) \subset \mathrm{Hom}(P, P) \ .$$

In general, we are interested in the subset of cocycles of $Z^1(\Gamma;\mathfrak{P})$ which map to automorphisms of $H^1(\Gamma;V_{k-2})$ commuting with the action of Hecke operators [5]. For simplicity, here we shall only consider those mapping to the identity.

Definition 9.3. Define the subspace of cocycles tangent to the identity by

$$Z^1_t(\Gamma;\mathfrak{P}) = \{C \in Z^1(\Gamma;\mathfrak{P}) \text{ such that } t(C) = \mathrm{id}\} \ .$$

Since Γ is finitely-generated, $Z^1(\Gamma;\mathfrak{P})$ is defined by a finite number of equations defined over $\mathbb{Q}$ (lemma 5.5) and $Z^1_t(\Gamma;\mathfrak{P})$ is an affine scheme over $\mathbb{Q}$.

9.3. **Automorphisms.** The Lie algebra $\mathrm{Lie}\,\mathfrak{P}$ of $\mathfrak{P}$ is isomorphic to the completion of the free graded Lie algebra generated by

$$\bigoplus_{k\geq 2} P_k^\vee \otimes V_{k-2}$$

It admits a right action of SL_2. Let

$$\begin{aligned}(9.2)\quad \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2} = \{\phi : \mathrm{Lie}\,\mathfrak{P} \to \mathrm{Lie}\,\mathfrak{P} \text{ such that } \phi(x)|_g = \phi(x|_g) \text{ for all } g \in \mathrm{SL}_2 \\ \text{and such that } \phi^{ab} : \mathrm{Lie}\,\mathfrak{P}^{ab} \to \mathrm{Lie}\,\mathfrak{P}^{ab} \text{ is the identity}\} \ .\end{aligned}$$

The second condition means that any element $\phi \in \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}$ acts on generators $x \in P_k^\vee \otimes V_{k-2}$ by sending $x \mapsto x +$ commutators of length ≥ 2. Any element $\phi \in \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}(R)$ acts on formal power series by non-commutative substitutions:

$$\begin{array}{ccc} R\langle\langle P^\vee\rangle\rangle & \longrightarrow & R\langle\langle P^\vee\rangle\rangle \\ S & \mapsto & \phi(S) \end{array}$$

It clearly respects the actions of SL_2 and preserves the subspace of group-like formal power series. In particular, it preserves $\mathfrak{P}(R) \subset R\langle\langle P^\vee\rangle\rangle$.

The subspace of SL_2-invariants $\mathfrak{P}^{\mathrm{SL}_2} \leq \mathfrak{P}$ acts by conjugation on $\mathfrak{P}$. This defines a right action of $\mathfrak{P}^{\mathrm{SL}_2}$ on $\mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}$ which we denote by a subscript. It satisfies

$$(\phi_a)(S) = a^{-1}\phi(S)a \qquad \text{for all } S \in \mathfrak{P}, a \in \mathfrak{P}^{\mathrm{SL}_2} \ .$$

For every $a \in \mathfrak{P}^{\mathrm{SL}_2}$, the element ϕ_a is an automorphism of the Lie algebra $\mathrm{Lie}\,\mathfrak{P}$ because in any Hopf algebra, conjugation of a primitive element by a group-like element is primitive. For any $a \in \mathfrak{P}^{\mathrm{SL}_2}$, $\phi_a^{ab} = \mathrm{id}$ because conjugation by a is trivial on the abelianization, and ϕ_a is SL_2-invariant because a is.

Definition 9.4. Let $\mathcal{A}$ denote the semi-direct product

$$\mathcal{A} = \mathfrak{P} \rtimes_{\mathfrak{P}^{\mathrm{SL}_2}} \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2} \tag{9.3}$$

Elements of $\mathcal{A}$ are represented by $(B,\phi) \in \mathfrak{P} \times \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}$ modulo the equivalence

$$(Ba,\phi_a) \sim (B,\phi) \qquad \text{for all } a \in \mathfrak{P}^\Gamma \ . \tag{9.4}$$

Denote the equivalence class of (B,ϕ) by $[B,\phi]$.

One can show that $\mathcal{A}$ is an affine group scheme defined over $\mathbb{Q}$. It acts on the left on the subspace of cocyles $Z^1_t(\Gamma;\mathfrak{P}) \subset Z^1(\Gamma;\mathfrak{P})$ tangent to the identity as follows:

$$\begin{array}{ccc} \mathcal{A} \times Z^1_t(\Gamma;\mathfrak{P}) & \longrightarrow & Z^1_t(\Gamma;\mathfrak{P}) \\ {[B,\phi]} \circ C & = & \Big(\gamma \mapsto B\big|_\gamma\, \phi(C_\gamma)\, B^{-1}\Big) \end{array} \tag{9.5}$$

where $B \in \mathfrak{P}$ and $\phi \in \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}$. The element $[B,\phi]\circ C$ evidently satisfies the cocycle relations for C (§5.2) and is tangent to the identity because $\phi^{ab} = \mathrm{id}$. Note that (9.5) is well-defined: equivalent representatives (9.4) act in an identical way on $Z_t^1(\Gamma; \mathfrak{P})$. The group law is given by

$$[B_1, \phi_1] \circ [B_2, \phi_2] = [B_1 \phi_1(B_2), \phi_1 \phi_2] \ .$$

Remark 9.5. As observed in §9.1, an element $B \in \mathfrak{P}(R)$ can be viewed as a morphism. In order not to clutter the notation, we shall denote the image of $w \in P_{2k_1} \otimes \ldots \otimes P_{2k_r}$ under the map B by a subscript B_w. Thus

$$B_w \in V_{2k_1-2} \otimes \ldots \otimes V_{2k_r-2}$$

is a polynomial, and satisfies the analogue of the shuffle equations (3.8). On the other hand, an element $\phi \in \mathrm{Aut}_0(\mathrm{Lie}\,\mathfrak{P})^{\mathrm{SL}_2}$ can be viewed as a series of linear maps

$$\bigoplus_{k_1,\ldots,k_r} P_{2k_1} \otimes V_{2k_1-2}^\vee \otimes \cdots \otimes P_{2k_r} \otimes V_{2k_r-2}^\vee \longrightarrow \bigoplus_k P_{2k} \otimes V_{2k-2}^\vee$$

which are SL_2-equivariant and vanish on products. Thus we can view

$$\begin{aligned} \phi_w \quad &\in \quad \bigoplus_k P_{2k} \otimes \mathrm{Hom}_{\mathrm{SL}_2}(V_{2k-2}, V_{2k_1-2} \otimes \ldots \otimes V_{2k_r-2}) \\ &= \quad \bigoplus_k \mathrm{Hom}_{\mathrm{SL}_2}(P_{2k}^\vee \otimes V_{2k-2}, V_{2k_1-2} \otimes \ldots \otimes V_{2k_r-2}) \ . \end{aligned}$$

We will refer to B_w and ϕ_w as coefficients of B and ϕ, respectively.

9.4. **The space of cocycles as an $\mathcal{A}$-torsor.**

Theorem 9.6. *The space $Z_t^1(\Gamma; \mathfrak{P})$ is a principal $\mathcal{A}$-torsor.*

Proof. This is a special case of a more general theorem which will be proved in the context of relative Malcev completion [5], and follows easily from the universal property of relative completion via remark 5.3. In the meantime, I shall sketch an ad hoc proof here, which is heavy-handed but has the advantage of being constructive. Consider two cocycles $C^1, C^2 \in Z_t^1(\Gamma; \mathfrak{P})$. We wish to construct an $\alpha = [B, \phi] \in \mathcal{A}$ such that $\alpha \circ C^1 = C^2$. Suppose by induction that B and ϕ, viewed as morphisms as in remark 9.5, are defined on $P^{\otimes r}$ for $r \leq n-1$ such that

$$C^2 = \alpha \circ C^1 \pmod{\text{terms of length } \geq n} \ .$$

We wish to extend B and ϕ to pure tensors $w \in P^{\otimes n}$. Let $\{p\}$ denote a basis of $P^\vee$. By formula (9.5) for the action of $\mathcal{A}$, we have

$$(\alpha \circ C^1)_w = \delta^0 B_w + \sum_{\{p\}} \phi_w(p \otimes C_p^1) + (\alpha \,\widetilde{\circ}\, C^1)_w \tag{9.6}$$

where the right-most term consists of all terms in $(\alpha \circ C^1)_w$ which involve coefficients of B, ϕ of length $\leq n-1$ (which are known by the previous induction step). The middle sum is finite because ϕ has to be SL_2-invariant.

Now, by (5.5), we have the equation

$$\delta^1 C_w^i \equiv \sum_{uv=w} C_u^i \cup C_v^i$$

for $i = 1, 2$ where the sum is over strict factorisations of w. This implies that

$$\delta^1(\alpha \,\widetilde{\circ}\, C^1)_w = \delta^1(\alpha \circ C^1)_w = \sum_{uv=w} (\alpha \circ C^1)_u \cup (\alpha \circ C^1)_v = \sum_{uv=w} C_u^2 \cup C_v^2 = \delta^1 C_w^2$$

and the difference $\xi_w = C^2_w - (\alpha \,\widetilde{\circ}\, C^1)_w$ is closed hence a Γ-cocycle. The first equality follows from (9.6) using the fact that $\delta^1 C^1_p = 0$. The equation

$$\xi_w = \delta^0 B_w + \sum_{\{p\}} \phi_w(p \otimes C^1_p) \qquad (9.7)$$

can always be solved in B_w and $\phi(p)_w$, because C^1 is tangent to the identity and so the C^1_p are a basis for the cohomology of Γ. The first step in the induction $n = 1$ is guaranteed because C^2 is tangent to the identity, and so ϕ^{ab} is the identity. One can ensure that B is group-like and ϕ is a Lie algebra homomorphism using the fact that C^1, C^2 are group-like (solve (9.7) for algebra generators w; the remaining coefficients of B, ϕ are determined by multiplicativity). Note that the element B_w is uniquely defined up to addition of a Γ-invariant element and hence B is unique up to multiplication by an element of $\mathfrak{P}^{\Gamma} = \mathfrak{P}^{\mathrm{SL}_2}$. Hence $\alpha = [B, \phi] \in \mathcal{A}$ is unique.

Finally, the existence of a rational point on $Z^1_t(\Gamma; \mathfrak{P})$ is equivalent, by remarks 5.3 and 9.2, to the fact that the unipotent radical of the relative Malcev completion of Γ admits a splitting over $\mathbb{Q}$. This follows from a variant of Levi's theorem (see for example [24], proposition 3.1 for a proof of such a splitting). □

9.5. **Betti cocycle.** Recall from §7.4 that integration defines a linear map:

$$\mathsf{p} : M_k \longrightarrow P_k \otimes \mathbb{C} \ , \qquad (9.8)$$

from modular forms to cohomology classes. It defines a canonical morphism of affine group schemes over $\mathbb{C}$

$$\mathsf{p}^* : \mathfrak{P} \times \mathbb{C} \longrightarrow \Pi \times \mathbb{C} \qquad (9.9)$$

In particular, this induces a morphism

$$Z^1(\Gamma; \mathfrak{P})(\mathbb{C}) \longrightarrow Z^1(\Gamma; \Pi)(\mathbb{C}) \ . \qquad (9.10)$$

Let us denote, by abuse of notation, elements

$$\mathbf{e}_{2k} \in P_{2k} \qquad \text{and} \qquad \mathbf{E}_{2k} \in P^{\vee}_{2k}$$

for all $k \geq 2$, where $\mathbf{e}_{2k} = [e^0_{2k}] \in P^{\mathrm{eis}}_{2k}$ is cohomology class of the rational Eisenstein cocycle of §7.3 and $\mathbf{E}_{2k}$ is the dual element in $(P^{\mathrm{eis}}_{2k})^{\vee}$. They correspond to (3.2) via the map p. The Eisenstein series of weight $2k$ therefore defines elements $\mathbf{e}_{2k}, \mathbf{E}_{2k}$ without ambiguity in both M_{2k}, P_{2k} and their duals.

Theorem 9.7. *There exists a cocycle $z \in Z^1_t(\Gamma; \mathfrak{P})(\mathbb{C})$ whose image under the previous map is the canonical cocycle $\mathcal{C} \in Z^1(\Gamma; \Pi)(\mathbb{C})$. Its restriction to Γ_∞ is rational, i.e.,*

$$z_T \in \mathfrak{P}(\mathbb{Q}) \ .$$

Proof. (Sketch) This can be proved using Chen's formal power series connections [22], §9. One can choose a (de Rham rational) formal power series connection form

$$\widetilde{\Omega} \in \Omega^1(\mathfrak{H}, \mathfrak{P}(\mathbb{C}))$$

such that its image under the map (9.9) is Ω defined in (3.4). By [22], §9, this defines a splitting of the relative Malcev completion of Γ, and hence a cocycle $z \in Z^1(\Gamma; \mathfrak{P})(\mathbb{C})$ by remarks 5.3 and 9.2. The restriction of $\widetilde{\Omega}$ to the punctured tangent space at the cusp is Betti rational, because the motivic fundamental group of $\mathbb{G}_m$ at the unit tangent vector based at 0 is simply $\mathbb{Q}(-1)$. Therefore z_T is rational. □

Let us choose such an element z and denote by

$$\kappa = z_T \in \mathfrak{P}(\mathbb{Q})$$

By abuse of notation, we shall sometimes denote the restriction of z to Γ_∞ by $\kappa \in Z^1(\Gamma_\infty; \mathfrak{P})(\mathbb{Q})$ also. The image of κ under the map (9.9) is $\mathcal{C}_T$. It is unlikely that an element z can be chosen canonically, but it is an interesting problem to determine the coefficients of κ as explicitly as possible. For example, we can easily show that

$$\kappa_p = 0 \qquad \text{for all } p \in P^{\mathrm{cusp}} \ . \tag{9.11}$$

This is because, for all cusp forms f, we have $\mathsf{p}(f)_T = 0$ and hence $\mathsf{p}(f)^+_T = \mathsf{p}(f)^-_T = 0$. By the Eichler-Shimura isomorphism this implies (9.11). On the other hand,

$$\kappa_{\mathbf{e}_{2k}} = \frac{\mathsf{b}_{2k}}{4k(2k-1)} \frac{1}{Y}\big((X+Y)^{2k-1} - X^{2k-1}\big) = \frac{\mathsf{b}_{2k}}{4k(2k-1)} \frac{X^{2k-1}}{Y}\Big|_{T-1} \tag{9.12}$$

by the results of §6, since $\kappa_{\mathbf{e}_{2k}} = (2\pi i)^{1-2k} C_{\mathbf{e}_{2k}}$. Similar arguments imply that the coefficient of *ep* in κ also vanishes. These results can also be deduced by purely Hodge-theoretic arguments, but this is outside the scope of this paper.

9.6. **A scheme of cocycles.** We can define a certain scheme of non-abelian cocycles as follows. It will be studied in greater detail in [5].

Definition 9.8. Fix a κ as above, and let

$$i^* : Z^1(\Gamma; \mathfrak{P}) \longrightarrow Z^1(\Gamma_\infty; \mathfrak{P})$$

denote the restriction map. For R a $\mathbb{Q}$-algebra, define a space of cocycles

$$\mathcal{Z}_\kappa(R) = \{z \in Z^1_t(\Gamma; \mathfrak{P})(R) : i^*(z) = \kappa\}$$

Because κ is rational, one can show that $\mathcal{Z}$ is representable and defines an affine scheme over $\mathbb{Q}$.

Remark 9.9. We could dispense with a choice of κ by defining a space of cocycles $\mathcal{Z} \subset Z^1_t(\Gamma; \mathfrak{P})$ which have the property that their images under the composition

$$Z^1(\Gamma; \mathfrak{P}) \xrightarrow{i^*} Z^1(\Gamma_\infty; \mathfrak{P}) \xrightarrow{\mathsf{p}^*} Z^1(\Gamma_\infty; \Pi \times \mathbb{C}) \ ,$$

This weaker construction actually suffices for almost all the results of the present paper, where we are only considering holomorphic iterated integrals. However it is convenient, both notationally, and psychologically to do computations with a chosen rational element κ.

9.7. **Group of 'motivic' automorphisms.** With a fixed κ as above define a group of automorphisms of $\mathcal{Z}_\kappa$ as follows.

Definition 9.10. For any such κ, define $G_\kappa \leq \mathcal{A}$ to be the stabiliser of κ. More precisely, G_κ is the set of $[B, \phi] \in \mathcal{A}$ satisfying the equation:

$$B\big|_T^{-1} \phi(\kappa)\, B = \kappa \ . \tag{9.13}$$

By theorems 9.6 and theorem 9.7, $\mathcal{Z}_\kappa(\mathbb{C})$ is a torsor over the group $G_\kappa(\mathbb{C})$. It follows from standard arguments about torsors over unipotent groups that $\mathcal{Z}_\kappa$ contains a rational point. We shall see that the seemingly innocuous equation (9.13) actually contains a lot of arithmetic information, although we shall only scratch the surface here.

Choose a rational point $z^0 \in \mathcal{Z}_\kappa(\mathbb{Q})$ as above. Let $z \in \mathcal{Z}_\kappa(\mathbb{C})$ be a complex point whose image in $Z^1(\Gamma;\Pi)(\mathbb{C})$ is $\mathcal{C}$, as provided by theorem 9.7. Since $\mathcal{Z}_\kappa$ is a torsor over G_κ, there exists $[B,\phi] \in G_\kappa(\mathbb{C})$ such that

$$z = [B,\phi] \circ z^0$$

Corollary 9.11. *By applying the map* (9.10) *we obtain the following formula:*

$$\mathcal{C} = \mathsf{p}^*([B,\phi] \circ z^0) \ . \tag{9.14}$$

This equation enables us to tease out the coefficients of $\mathcal{C}$, and also describes the action of the corresponding motivic Galois group. More precisely, the coefficients of (3.3) in $\mathcal{C}$ involve periods of very different types superposed in a complicated way. Equation (9.14) enables us to separate them out.

9.8. **Transference and higher Petersson-Haberlund products.** By following the identical argument to theorem 8.4, we have an analogue for $\mathcal{Z}_\kappa$.

Theorem 9.12. *For all $z \in \mathcal{Z}_\kappa$, and all SL_2-invariant projections π onto the trivial representation $V_0 = \mathbb{Q}$, we have an equation*

$$\pi\Big(\sum_{uv=w} \mathfrak{h}(z(u), z(v))\Big) = -\pi(\kappa(w)) \ . \tag{9.15}$$

where the sum is over strict factorisations of w a word in elements of P.

We wish to view the left-hand side as a generalisation of the inner product $\{,\}$, via lemma 8.3. The action of the automorphism group G_κ fixes the right-hand side, and therefore fixes the left hand side also. Thus, for all $g \in G_\kappa$, we have

$$\pi\Big(\sum_{uv=w} \mathfrak{h}(g\circ z(u), g\circ z(v))\Big) = -\pi(\kappa(w)) \ . \tag{9.16}$$

Thus we can think of G_κ as preserving 'higher inner products'. In this way we see that the non-vanishing of $H^2(\Gamma,\Gamma_\infty;\mathbb{Q})$ leads to non-trivial constraints on κ. For example, take two elements $p,q \in P_k^{\mathrm{cusp}}$. Then (9.15) applied to the word $w = pq$ implies that

$$\{z_p, z_q\} = -6\kappa_{pq}$$

by lemma 8.3. Since $[z_p] = p$ and $[z_q] = q$, we deduce that $\kappa_{pq} \neq 0$ whenever the Petersson-Haberlund inner product $\{p,q\}$ is non-zero. In this respect, the non-vanishing components in V_0 of κ encode the non-vanishing higher inner products.

9.9. **Example: action of automorphisms in length 1.** We illustrate how to unravel the inertia equation (9.13) with some simple computations in length one. This gives the action of the motivic Galois group on multiple modular values of length one.

By definition of the tangential condition, every $[B,\phi] \in G_\kappa$, has the property that ϕ is the identity in length one. Therefore

$$B_p\big|_{T-1} = 0 \quad \text{for all } p \in P_k \tag{9.17}$$

which follows on taking the coefficient of p on both sides of (9.13). Thus

$$B_p = \alpha_p Y^{k-2} \quad \text{where } \alpha_p \in \mathbb{Q} \ , \quad \text{for all } p \in P_k \ . \tag{9.18}$$

Lemma 9.13. *Let $[B,\phi] \in G_\kappa$. Then $B_f = 0$ if $f \in P^{\mathrm{cusp}}$.*

Proof. Let $f \in P_{2k}^{\mathrm{cusp}}$ be cuspidal of degree $2k$ and let e denote the rational Eisenstein cocycle of the same degree. Take the coefficient of ef in (9.13) to obtain

$$B_{ef}\big|_{T-1} + B_e\kappa_f - \kappa_e B_f + ((\phi - \mathrm{id})\kappa)_{ef} = 0 \ , \tag{9.19}$$

using (9.17) and $B_{ef}^{-1} = B_e B_f - B_{ef}$. This equation is in $V_{2k} \otimes V_{2k}$. Project onto the component $V_0 = \mathbb{Q}$ as in §2.4.1. Since T acts trivially on V_0, the image of the left most term vanishes. The third term vanishes by (9.11). Finally, $\phi - \mathrm{id}$ is equivariant for the action of SL_2, and there is no coefficient of κ in length one with a non-trivial component in V_0, since $P_0 = 0$. Thus the final term vanishes also, leaving

$$\langle \kappa_e, B_f \rangle = 0 \ .$$

Since $B_f = \alpha_f Y^{2k-2}$, a simple application of (2.7) shows that $\alpha_f = 0$ since we know that κ_e is given explicitly by (9.12) and does not vanish at $Y = 0$. □

The type of argument of this lemma can be substantially generalised. A simpler way to prove the same result, using (9.15), is as follows. Apply equation (9.16) in the case $w = ef$, where e and f are as in the previous lemma and $g = [B, \phi] \in G_\kappa$. Since $\phi \equiv \mathrm{id}$ modulo terms of length ≥ 2, we have

$$(g \circ z)_p = z_p + \delta^0 B_p \ .$$

and therefore

$$\begin{aligned} \kappa_{ef} + \{z_e, z_f\} &= 0 \\ \kappa_{ef} + \{z_e + \delta^0 B_e, z_f + \delta^0 B_f\} &= 0 \ , \end{aligned} \tag{9.20}$$

By (9.17), $\delta^0 B_p = \alpha_p (X^{2k-2} - Y^{2k-2})$ for some α_p. Since the inner product of a coboundary with a cuspidal cocycle vanishes, we have $\{\delta^0 B_e, \delta^0 B_f\} = \{\delta^0 B_e, z_f\} = 0$. The equations (9.20) imply that $\{z_e, \delta^0 B_f\} = 0$ which, by (7.5) implies that $\alpha_f = 0$, since z_e is an Eisenstein cocycle.

In conclusion, every cocycle $z \in \mathcal{Z}_\kappa(\mathbb{Q})$ defines a collection of maps from P_{2k} to $Z^1(\Gamma; V_{2k-2})$. In length one, we have for all $p \in P_{2k}$,

$$z_p = s(p) + \alpha_p (X^{2k-2} - Y^{2k-2}) \qquad \text{for some } \alpha_p \in \mathbb{Q} \tag{9.21}$$

where s is the Hecke-equivariant splitting of §7.5, and α_p is zero if p is cuspidal. In other words, only the Eisenstein cocycles admit a non-trivial action of the automorphism group G_κ. This corresponds to the fact that the period polynomials of cusp forms have coefficients which are periods of pure motives (and therefore fixed under the action of the unipotent part of the motivic Galois group). On the other hand, periods of Eisenstein series have a single zeta value as the coefficient of $X^{2k} - Y^{2k}$, which is moved non-trivially by the unipotent radical of the motivic Galois group of $\mathcal{MT}(\mathbb{Z})$. This is precisely what the formulae above are telling us.

10. Action of automorphisms in length 2

We specialise the general description given in the previous section to write down closed formulae for the structure of double Eisenstein integrals in length 2.

10.1. **Determination of ϕ in length 2.** Using the equation (9.13), we can completely compute the action of ϕ on Eisenstein elements in length two. Let $[B, \phi] \in G_\kappa(R)$. Let $\mathbf{e}_{2m} \in P_{2m}^{\mathrm{eis}}$ denote the rational Eisenstein cocycle, and let $\mathbf{E}_{2m}$ denote the dual element in $(P_{2m}^{\mathrm{eis}})^\vee \subset P_{2m}^\vee$. We have

$$B_{\mathbf{e}_{2m}} = \alpha_{2m} Y^{2m-2} \qquad \text{for some } \alpha_{2m} \in R \ .$$

The following theorem completely describes the action of ϕ on Eisenstein elements up to length two. For every $|m-n| \leq k \leq m+n$, let us denote by

$$\iota_k^{m,n} : V_{2k} \to V_{2m} \otimes V_{2n}$$

the SL_2-equivariant map which is the inverse of ∂^{m+n-k} described in §2.4.1.

Theorem 10.1. *Let $[B,\phi] \in G_\kappa(R)$ as above. Then ϕ satisfies*

$$\phi(\mathbf{E}_{2k} \otimes v) = \mathbf{E}_{2k} \otimes v + \sum_{m<n} \lambda_k^{m,n} (\mathbf{E}_{2m}\mathbf{E}_{2n}\iota_k^{m,n} v + (-1)^{k-1}\mathbf{E}_{2n}\mathbf{E}_{2m}\iota_k^{n,m} v) \tag{10.1}$$
$$+ \text{ terms of length } \geq 3$$

for all $v \in V_{2k-2}$, and where all coefficients $\lambda_k^{m,n}$ vanish if $k \neq n-m+1$. In the remaining case $k = n-m+1$ and $m<n$, they are given explicitly by

$$\lambda_{n-m+1}^{m,n} = \frac{(n-m+1)}{n} \binom{2n-2}{2n-2m} \frac{\mathsf{b}_{2n}}{\mathsf{b}_{2n-2m+2}} \alpha_{2m} \tag{10.2}$$

where $\alpha_{2m} Y^{2m-2}$ is the coefficient of $\mathbf{e}_{2m}$ in B as above.

Proof. Taking the coefficient $\mathbf{e}_{2m}\mathbf{e}_{2n}$ in equation (9.13) gives

$$B_{\mathbf{e}_{2m}\mathbf{e}_{2n}}\big|_{T-1} + B_{\mathbf{e}_{2m}}\kappa_{\mathbf{e}_{2n}} - \kappa_{\mathbf{e}_{2m}}B_{\mathbf{e}_{2n}} + \sum_k \lambda_k^{m,n}\iota_k^{m,n}(\kappa_{\mathbf{e}_{2k}}) = 0$$

in $V_{2m-2} \otimes V_{2n-2}$. Here we have used the fact that B is T-invariant in length one. Applying ∂^r for each r, this splits into a series of equations in $V_{2m+2n-4-2r}$:

$$\partial^r B_{\mathbf{e}_{2m}\mathbf{e}_{2n}}\big|_{T-1} = \partial^r(\kappa_{\mathbf{e}_{2m}}B_{\mathbf{e}_{2n}} - B_{\mathbf{e}_{2m}}\kappa_{\mathbf{e}_{2n}}) - \lambda_{m+n-r-1}^{m,n}\kappa_{\mathbf{e}_{2m+2n-2r-2}} \tag{10.3}$$

This can be viewed as an equation between Γ_∞-cocycles. Concretely, consider the short exact sequence

$$0 \longrightarrow Y^{2k}\mathbb{Q} \longrightarrow V_{2k} \overset{T-1}{\longrightarrow} V_{2k} \overset{c_X}{\longrightarrow} X^{2k}\mathbb{Q} \longrightarrow 0$$

where c_X is the map $Y \mapsto 0$. Since the left-hand side of (10.3) is in the image of $T-1$, the right-hand side must be in the kernel of c_X.

By (9.12), $c_X(\kappa_{\mathbf{e}_{2k}}) = \frac{\mathsf{b}_{2k}}{4k}X^{2n-2}$. Since the Bernoulli number b_{2n} is non-zero, the numbers $\lambda_{m+n-r}^{m,n}$ are completely determined by applying c_X to the right-hand side of (10.3). A completely elementary calculation gives

$$c_X\partial^r B_{\mathbf{e}_{2m}}\kappa_{\mathbf{e}_{2n}} = \alpha_{2m}\frac{\mathsf{b}_{2n}}{2n}\binom{2n-2}{2n-2m}\delta_{r,2m-2}X^{2n-2m}$$

if $n \geq m$, and is zero if $n < m$. From this we deduce for $n > m$ that:

$$\lambda_{n-m+1}^{m,n} = \frac{(n-m+1)}{n}\binom{2n-2}{2n-2m}\frac{\mathsf{b}_{2n}}{\mathsf{b}_{2n-2m+2}}\alpha_{2m} \ .$$

Finally we need to show that $\phi(\mathbf{E}_{2k} \otimes v)$ has no cuspidal components. Let $e, f \in P$ be an Eisenstein and cuspidal cocycle, respectively. Returning to equation (9.19), and using the fact (from lemma 9.13) that $\kappa_f = B_f = 0$, we have

$$B_{ef}\big|_{T-1} + ((\phi - \mathrm{id})\kappa)_{ef} = 0 \ .$$

As above, we can view this as an equation of Γ_∞-cochains. By repeating a similar argument we deduce that the cohomology class of $((\phi-\mathrm{id})\kappa)_{ef}$ vanishes. The other case (coefficient of fg where $f, g \in P^{\mathrm{cusp}}$) is similar. □

The coefficients $\lambda_{n-1}^{2,n}$, up to a normalisation of the generators $\mathbf{e}_{2r}$, agree with the computations due to Pollack ([35], §5.3) of the action of the generator σ_3 in degree 3 of the Lie algebra of mixed Tate motives over $\mathbb{Z}$ on the derivations of the unipotent fundamental group of the Tate curve. He guessed correctly that the quadratic coefficients are a quotient of two Bernoulli numbers $\mathsf{b}_{2n}/\mathsf{b}_{2n-2}$. The connection between the previous theorem and his computations will be discussed in a joint work with Hain.

10.2. **Remark on the top slice quotient.** Define the top slice of $\mathfrak{P}$ to be

$$\mathfrak{P}^{\mathrm{top}} = \pi_d \mathfrak{P}$$

where π_d is the map defined in (2.6) which retains the top slice of a tensor product of SL_2 representations. There is a natural map $\mathfrak{P} \to \mathfrak{P}^{\mathrm{top}}$. Elements of $\mathfrak{P}^{\mathrm{top}}(R)$ can be represented, via a version of (3.7), as morphisms

$$P_{k_1} \otimes \ldots \otimes P_{k_r} \longrightarrow \pi_d(V_{k_1-2} \otimes \ldots \otimes V_{k_r-2}) \otimes R = V_{k_1+\ldots+k_r-2r} \otimes R \ .$$

In particular, we have a morphism $Z^1(\Gamma;\mathfrak{P}) \to Z^1(\Gamma;\mathfrak{P}^{\mathrm{top}})$, and one checks that the group G_κ acts upon $Z^1_t(\Gamma;\mathfrak{P}^{\mathrm{top}})$ because in the definition 9.4 automorphisms are required to be SL_2-equivariant. One of the main advantages of looking at $\mathfrak{P}^{\mathrm{top}}$ is that $\mathcal{O}(\mathfrak{P}^{\mathrm{top}})$ contains a unique copy of the trivial representation $V_0 \cong \mathbb{Q}$, and therefore $H^2(\Gamma;\mathcal{O}(\mathfrak{P}^{\mathrm{top}})_{>0})$ vanishes. The argument in the previous section can be substantially generalised, and suggests that for every $[B,\phi] \in G_\kappa$, the image of $\pi_d\phi(\mathbf{E}_{2n})$ consists of words in Eisenstein series (this is true at least modulo terms of high *length*, of the order of about 10 corresponding to the fact that the first non-trivial cusp form for $\mathrm{SL}_2(\mathbb{Z})$ has *weight* 12). If the image of the Tannaka group of mixed Hodge structures (not discussed here) in G_κ consists of elements ϕ preserving the subspace of $\mathfrak{P}^{\mathrm{top}}$ generated by the Eisenstein cocycles $P^{\mathrm{eis}} \subset P$, then the action on this subspace defines a natural quotient whose underlying Lie algebra should be isomorphic, by the previous computations, to a free Lie algebra with one generator in every odd degree ≥ 3. This is isomorphic to the fundamental Lie algebra of $\mathcal{MT}(\mathbb{Z})$. This should give a purely geometric construction of the category $\mathcal{MT}(\mathbb{Z})$, and justifies the comments in the introduction which suggest that multiple modular values should give a natural construction of the category of mixed Tate motives over $\mathbb{Z}$.

10.3. **Double Eisenstein integrals.** Given a rational point $z^0 \in \mathcal{Z}(\mathbb{Q})$, there exists $[B,\phi] \in G_\kappa$ such that the element z of theorem 9.7 can be written in the form

$$z_\gamma = B\big|_\gamma \phi(z^0) B^{-1} \ . \tag{10.4}$$

We can assume the coefficients $z^0(\mathbf{e}_{2m})$ are the cocycles e^0_{2n} defined in proposition 7.1. Denote the coefficients $z^0(\mathbf{e}_{2m}\mathbf{e}_{2n})$ by $e^0_{2m,2n}$. They satisfy

$$\begin{aligned} e^0_{2m,2n} &\in C^1(\Gamma; V_{2m-2} \otimes V_{2n-2}) \\ \delta^1 e^0_{2m,2n} &= e^0_{2m} \cup e^0_{2n} \\ \left(e^0_{2m,2n}\right)_T &= (\kappa_{\mathbf{e}_{2m}\mathbf{e}_{2n}})_T \end{aligned}$$

together with the shuffle equation

$$e^0_{2m,2n}(X_1,Y_1,X_2,Y_2) + e^0_{2n,2m}(X_2,Y_2,X_1,Y_1) = e^0_{2m}(X_1,Y_1) e^0_{2n}(X_2,Y_2) \ .$$

These cochains are well-defined up to $Z^1_{\mathrm{cusp}}(\Gamma; V_{2m-2} \otimes V_{2n-2})$, i.e., rational cocycles which vanish on T. Furthermore, since the cocycles e^0_{2m} are odd with respect to ϵ, the middle equation above implies that the odd part $(\mathrm{id} - \epsilon) e^0_{2m,2n}$ is a cocycle, and we can assume it is zero. Therefore, we can assume that $e^0_{2m,2n}$ is ϵ-invariant.

The general formula (10.4) gives the following equation

$$z_{\mathbf{e}_{2m}\mathbf{e}_{2n}} = e^0_{2m,2n} + B_{\mathbf{e}_{2m}} \cup e^0_{2n} - e^0_{2m} \cup B_{\mathbf{e}_{2n}} + \delta^0 B_{\mathbf{e}_{2m}\mathbf{e}_{2n}} + \Phi \tag{10.5}$$

where the final term of (10.5) is a cochain

$$\Phi = ((\phi - \mathrm{id}) z_0)_{\mathbf{e}_{2m}\mathbf{e}_{2n}} \quad \in \quad Z^1(\Gamma; V_{2m-2} \otimes V_{2n-2})$$

and can be written explicitly

$$\Phi = \lambda^{m,n}_{n-m+1}\iota^{m,n}_{n-m+1}(e^0_{n-m+1}) + \sum_{p_i^+\in P_{2k}^{\mathrm{cusp},+}} \lambda^{m,n}_{i,+}\iota^{m,n}_k(sp_i^+) + \sum_{p_i^-\in P_{2k}^{\mathrm{cusp},-}} \lambda^{m,n}_{i,-}\iota^{m,n}_k(sp_i^-)$$

where the $p_i^\pm$ range over a basis in $P^\pm_{2k} = H^1_{\mathrm{cusp}}(\Gamma; V_{2k})^\pm$, s is the canonical Hecke-equivariant splitting of §7.5 (this follows from (9.21)) and where $\lambda^{m,n}_{n-m+1}$ is given in theorem 10.1. A formula for $\mathcal{C}_{\mathbf{e}_{2m}\mathbf{e}_{2n}}$ is deduced from (10.5) by applying the period map (9.8). Half of the coefficients $\lambda^{m,n}_{i,\pm}$ will be determined in the next paragraph and related to special values of L-functions of cusp forms.

Finally, the element $B_{\mathbf{e}_{2m}\mathbf{e}_{2n}} \in V_{2m-2}\otimes V_{2n-2}$ can be written down by solving equation (10.3) and using the trivialisation of κ in terms of $\mathcal{V}$ (6.5). This gives

$$\begin{aligned}(10.6)\quad \partial^r B_{\mathbf{e}_{2m}\mathbf{e}_{2n}} = f^{(r)}_{2m,2n}Y^{2m+2n-2r-2} &+ \partial^r(v_{2m}\cup B_{\mathbf{e}_{2n}} - B_{\mathbf{e}_{2n}}\cup v_{2m})\\ &- \partial^r B_{\mathbf{e}_{2m}}\cup B_{\mathbf{e}_{2n}} + \lambda^{m,n}_{n-m+1}v_{2m+2n-2r-2}\delta_{r,m-2}\end{aligned}$$

where $f^{(r)}_{2m,2n}$ is a new indeterminate, and

$$(10.7)\quad B_{\mathbf{e}_{2m}} = \frac{(2m-2)!}{2}f_{2m-1}Y^{2m-2} \quad \text{and} \quad v_{2n} = -\frac{\mathsf{b}_{2n}}{4n(2n-1)}\frac{X^{2n-1}}{Y}$$

Elements such as $v_{2m}\cup B_{\mathbf{e}_{2n}}$ in the right-hand side of (10.6) have poles, but the operators ∂^r make sense nonetheless. Formula (10.6) describes the shape of double Eisenstein integrals. All the interesting information is contained in the coefficients λ of Φ, and a single complex number $f^{(r)}_{2m,2n}$ for each $0\leq r\leq |m-n|$ (see §12).

11. Double Eisenstein Integrals and L-values

We can determine the imaginary part of the regularised iterated integrals of two Eisenstein series. It involves special values of L-functions of modular forms outside the critical strip and proves that the latter are periods.

11.1. **Statement.** Let $a, b\geq 2$. For all $k\geq 0$, define

$$(11.1)\qquad I^k_{2a,2b} = \partial^k \mathrm{Im}\big(\mathcal{C}_{\mathbf{e}_{2a}\mathbf{e}_{2b}} + \overline{b}_{2a}\cup \overline{e}^0_{2b} - \overline{e}^0_{2a}\cup\overline{b}_{2b}\big)$$

where $\mathcal{C}_{\mathbf{e}_{2a}\mathbf{e}_{2b}}$ is the coefficient of $\mathbf{e}_{2a}\mathbf{e}_{2b}$ in the canonical cocycle $\mathcal{C}$, and for $k\geq 2$,

$$(11.2)\qquad \begin{aligned}\overline{b}_{2k} &= -\frac{(2k-2)!}{2}\zeta(2k-1)Y^{2k-2}\\ \overline{e}^0_{2k} &= (2\pi i)^{2k-1}e^0_{2k}\ .\end{aligned}$$

It follows from the explicit description of the cocycle structure of double Eisenstein integrals in the previous section, and also the calculations below, that $I^k_{2a,2b}$ is a cocycle, and furthermore, that its cohomology class is cuspidal:

$$[I^k_{2a,2b}]\in H^1_{\mathrm{cusp}}(\Gamma, V_{2a+2b-4-2k})\ .$$

The cocycle $I^k_{2a,2b}$ is $(-1)^k$ invariant with respect to ϵ, and the shuffle product (3.8) for iterated integrals implies the symmetry $I^k_{2a,2b} = (-1)^{k-1}I^k_{2b,2a}$. The cohomology class $[I^k_{2a,2b}]$ is therefore completely determined by pairing with the cocycles of Hecke eigenforms via the Peterssen-Haberlund inner product $\{,\}$ defined in (2.8).

Theorem 11.1. *Let $k\geq 0$ and let g be a Hecke normalised cusp eigenform for Γ of weight $w = 2a+2b-2k-2$, and let C_g denote the corresponding cocycle. Then*

$$(11.3)\qquad \{I^k_{2a,2b}, C_g\} = 3A^k_{a,b}(2\pi i)^{w+k-1}\Lambda(g, 2a-k-1)\Lambda(g, w+k)$$

where $\Lambda(s) = (2\pi)^{-s}\Gamma(s)L(g,s)$ *and*

$$A^k_{a,b} = (-1)^a \binom{2a-2}{k}\binom{2b-2}{k}(k!)^3 \ .$$

Note that the functional equation of the L-series of g implies that formula (11.3) is compatible with the symmetry $I^k_{2a,2b} = (-1)^{k-1} I^k_{2b,2a}$.

The strategy of proof is the following: first we relate the coefficient of $\mathbf{E}_{2a}\mathbf{E}_{2b}$ in the indefinite iterated integral $\mathrm{Im}(I(\tau;\infty))$ to the product of a holomorphic Eisenstein series with a certain real analytic Eisenstein series. Then the Petersson inner product of its cocycle with that of an arbitrary cusp form g can be expressed as an integral over a fundamental domain via a generalisation of Haberlund's formula. This can in turn be computed using a version of the Rankin-Selberg method. When g is a Hecke eigenform, the final answer is a convolution L-function.

Corollary 11.2. *For every* a, b, k *as above, we can write*

$$I^k_{2a,2b}(S) \equiv \sum_{\{g\}} (2\pi i)^k \Lambda(g, w+k) P^{\pm}_g \pmod{\delta^0 (V_{w-2}\otimes \mathbb{C})_S} \qquad (11.4)$$

where the sum ranges over a basis of Hecke normalised cusp eigenforms of weight w*, and* $P^{\pm}_g \in P_{w-2}\otimes K_g$ *are Hecke-invariant period polynomials §7.2. Here,* $\pm$ *denotes* ϵ*-invariants if* k *is odd, and* ϵ*-anti-invariants if* k *is even, and* K_g *is the field generated by the Fourier coefficients of* g*. We can can assume* $\sigma(P^{\pm}_g) = P^{\pm}_{\sigma(g)}$ *for* $\sigma \in Aut_{\mathbb{Q}}(K_g)$*.*

Proof. By §7.2, we can choose the period $\omega^{\mp}_g$ (opposite parity to $\pm$ in the statement) to be the quantity $(2\pi i)^{w-1}\Lambda(g, 2a-k-1)$. The polynomials $P^{\pm}_g \in P^{\pm}_{w-2}\otimes K_g$ can be assumed to be $Aut_{\mathbb{Q}}(K_g)$ equivariant. Now write $I^k_{2a,2b} = \sum_{\{g\}} \alpha_g P^{\pm}_g$. Plugging into the formula of the previous theorem implies that

$$\{P^+_g, P^-_g\}\alpha_g \in (2i\pi)^k \Lambda(g, w+k)\mathbb{Q}$$

Rescaling $P^{\pm}_g$ by $\{P^+_g, P^-_g\}^{-1}$ gives the required statement. □

Let g be a cusp Hecke eigenform $g \in S_w(\Gamma)$. By pairing (11.4) with $P^{\mp}_g$ with respect to $\{,\}$, we deduce using $\Lambda(g,s) = (2\pi)^{-s}\Gamma(s)L(g,s)$ that the L-values

$$(2i\pi)^{-w} L(g,n) \quad \text{for all} \quad n \geq w$$

can be expressed as $\overline{\mathbb{Q}}$-linear combinations of double integrals of Eisenstein series.

11.2. **Double Eisenstein integrals.**

11.2.1. *Real analytic Eisenstein series.*

Definition 11.3. For any integers $i, j \geq 0$, and $s \in \mathbb{C}$ such that $i + j + 2\mathrm{Re}(s) > 2$, define a real analytic Eisenstein series for $z = x + iy \in \mathfrak{H}$ by

$$\mathcal{E}^s_{ij}(z) = \frac{1}{2}\sum_{(m,n)} \frac{y^s}{(mz+n)^{i+s}(m\overline{z}+n)^{j+s}} \qquad (11.5)$$

where the sum is over pairs (m, n) of coprime integers such that $(m, n) \neq (0, 0)$.

Clearly $\mathcal{E}^s_{ij}(z) = \mathcal{E}^s_{ji}(\overline{z})$. If $i = j + k$, where $k \geq 0$, then

$$2y^j \zeta(i+j+2s)\mathcal{E}^s_{ij}(z) = \sum_{m,n\in\mathbb{Z}^2\setminus\{(0,0)\}} \frac{y^{j+s}}{(mz+n)^k |mz+n|^{2j+2s}}$$

is the series considered in [38], (9.1), and has a meromorphic continuation with respect to s to the entire complex plane ([38], 9.7). The same is therefore true of $\mathcal{E}^s_{ij}(z)$.

For any element $\gamma \in \Gamma$, we have the transformation formula

$$\mathcal{E}^s_{ij}(\gamma(z)) = (cz+d)^i (c\overline{z}+d)^j \, \mathcal{E}^s_{ij}(\gamma(z)) \ . \tag{11.6}$$

It can be useful to think of $\mathcal{E}^s_{ij}$ as a modular form of 'weights' (i,j).

11.2.2. *Primitives of Eisenstein series.* Let $w \geq 4$ and consider the following real analytic function on $\mathfrak{H}$ taking values in $V_{w-2} \otimes \mathbb{C}$:

$$\underline{\mathcal{E}}_w(z) = \pi^{-1}\zeta(w)(w-2)! \sum_{i+j=w-2} \mathcal{E}^1_{i,j}(z)(X-zY)^i (X-\overline{z}Y)^j \tag{11.7}$$

where the sum is over $i,j \geq 0$. It is modular invariant.

$$\underline{\mathcal{E}}_w(\gamma(z))|_\gamma = \underline{\mathcal{E}}_w(z)|_\gamma \text{ for } \gamma \in \Gamma \ .$$

Lemma 11.4. $d\underline{\mathcal{E}}_w(z) = \frac{1}{2}(\underline{E_w}(z) - \underline{E_w}(\overline{z}))$

Proof. Writing out the definition of $\underline{\mathcal{E}}_w(z)$ gives

$$\underline{\mathcal{E}}_w(z) = \frac{(w-1)!}{4\pi i (w-1)} \sideset{}{'}\sum_{m,n\in\mathbb{Z}} \sum_{i+j=w-2} \frac{(z-\overline{z})(X-zY)^i(X-\overline{z}Y)^j}{(mz+n)^{i+1}(m\overline{z}+n)^{j+1}}$$

where the first sum is over $(m,n) \in \mathbb{Z}^2$ such that $(m,n) \neq (0,0)$. The lemma follows from the following elementary identity, and its complex conjugate:

$$\frac{\partial}{\partial z}\Big(\sum_{i+j=w-2} \frac{(z-\overline{z})(X-zY)^i(X-\overline{z}Y)^j}{(mz+n)^{i+1}(m\overline{z}+n)^{j+1}}\Big) = (w-1)\frac{(X-zY)^{w-2}}{(mz+n)^w}$$

The formula follows from the definition of $\underline{E}_w(z)$:

$$\underline{E}_w(z) = \frac{(w-1)!}{2\pi i} \sideset{}{'}\sum_{m,n\in\mathbb{Z}} \frac{(X-zY)^{w-2}}{(mz+n)^w}\, dz \ ,$$

which is verified by observing that the constant term of the inner sum at $z = i\infty$ is $2\zeta(w)$, which, by Euler's formula, is $-(2\pi i)^w \mathsf{b}_w (w!)^{-1}$. $\square$

Hereafter we use the following simplified notation for the iterated integrals

$$[\underline{E}_{2a}](z) = \int_z^{\vec{1}_\infty} \underline{E}_{2a}(\tau)$$

$$[\underline{E}_{2a}|\underline{E}_{2b}](z) = \int_z^{\vec{1}_\infty} \underline{E}_{2a}(\tau)\underline{E}_{2b}(\tau)$$

Lemma 11.5. *For all $a, b \geq 2$, we have the identities*

$$\mathrm{Re}\big([\underline{E}_{2a}](z)\big) = \underline{\mathcal{E}}_{2a}(z) - \overline{b}_{2a}$$

where $\overline{b}$ is defined in (11.2), *and*

$$\begin{aligned} d\left(\mathrm{Im}[\underline{E}_{2a}|\underline{E}_{2b}] - \mathrm{Re}[\underline{E}_{2a}]\mathrm{Im}[\underline{E}_{2b}]\right) = \ & \big(\underline{\mathcal{E}}_{2a}(z) - \overline{b}_{2a}\big)(X_1,Y_1)\,\mathrm{Im}(\underline{E}_{2b}(z)(X_2,Y_2)) \\ & - \mathrm{Im}(\underline{E}_{2a}(z)(X_1,Y_1))\,\big(\underline{\mathcal{E}}_{2b}(z) - \overline{b}_{2b}\big)(X_2,Y_2) \end{aligned} \tag{11.8}$$

Proof. Recall that $C_{e_{2a}}$ denotes the Γ-cocyle associated to $[\underline{E}_{2a}](z)$. Since $E_{2a}(q)$ has real Fourier coefficients, the previous lemma gives

$$\mathrm{Re}[\underline{E}_{2a}](z) = \underline{\mathcal{E}}_w(z) + P_{2a}$$

for some constant polynomial $P_{2a} \in V_{2a-2} \otimes \mathbb{C}$. By (11.6), the real analytic Eisenstein series is modular invariant $\underline{\mathcal{E}}_w(\gamma(z))|_\gamma = \underline{\mathcal{E}}_w(z)$. It follows that

$$\mathrm{Re}(C_{\mathbf{e}_{2a}})_\gamma = P_{2a}\big|_\gamma - P_{2a} \ .$$

Now since Γ acts without fixed points on V_{2a-2}, this uniquely determines P_{2a} from $\mathrm{Re}(C_{\mathbf{e}_{2a}})$. From lemma 7.1, it follows that $P_{2a} = -\overline{b}_{2a}$. The second equation follows from the general identity, for iterated integrals $[\omega_1|\omega_2]$ of two closed 1-forms ω_1, ω_2

$$d\big(\mathrm{Im}\,[\omega_1|\omega_2] - \mathrm{Re}\,[\omega_1]\mathrm{Im}\,[\omega_2]\big)\big) = \mathrm{Re}\,[\omega_1]\mathrm{Im}\,[\omega_2] - \mathrm{Im}\,[\omega_1]\mathrm{Re}\,[\omega_2]$$

which follows from $d[\omega_1|\omega_2] = -\omega_1[\omega_2]$ and $d[\omega_i] = -\omega_i$ for $i = 1, 2$. Applying it to $\omega_1 = \underline{E}_{2a}(z)(X_1, Y_1)$, and $\omega_2 = \underline{E}_{2b}(z)(X_2, Y_2)$ gives the required identity. □

11.2.3. *Double Eisenstein cocyle.* For all $a, b \geq 2$ define a 1-form

$$\mathcal{F}_{2a,2b}(z) = \mathrm{Im}(\underline{e_{2a}}(X_1, Y_1))\,\underline{\mathcal{E}_{2b}}(z)(X_2, Y_2) - \mathrm{Im}(\underline{e_{2b}}(X_2, Y_2))\,\underline{\mathcal{E}_{2a}}(z)(X_1, Y_1)$$

It is modular invariant: $\mathcal{F}_{2a,2b}(\gamma(z))|_\gamma = \mathcal{F}_{2a,2b}(z)$ for all $\gamma \in \Gamma$. Furthermore, it has at most logarithmic singularities (with respect to the coordinate $q = e^{2\pi i z}$) at the cusp and therefore we can define the regularised integral

$$[\mathcal{F}_{2a,2b}](z) = \int_z^{\vec{1}_\infty} \mathcal{F}_{2a,2b}(z)$$

Since $\mathcal{F}_{2a,2b}(z)$ is a closed 1-form, the integral only depends on z and not the choice of path. Denote the corresponding Γ-cocyle by

$$\begin{array}{rcl} \mathcal{D}_{2a,2b} : \Gamma & \longrightarrow & \mathbb{C}[X_1, Y_1, X_2, Y_2] \\ \mathcal{D}_{2a,2b}(\gamma) & = & [\mathcal{F}_{2a,2b}](\gamma(z))|_\gamma - [\mathcal{F}_{2a,2b}](z) \ . \end{array}$$

It follows from equation (11.8) and lemma 7.1 that

$$\mathcal{D}_{2a,2b} = \mathrm{Im}\big(\mathcal{C}_{[e_{2a}|e_{2b}]} + \overline{b}_{2a} \cup e^0_{2b} - e^0_{2a} \cup \overline{b}_{2b}\big) \ .$$

Our goal is to determine the cohomology class of this cochain.

11.3. **Haberlund's formula.**

11.3.1. Let $k \geq 0$ and $a, b \geq 4$ as above. Define two differential forms

$$\begin{array}{rcl} \omega_1(z, w) & = & \langle \partial^k \mathcal{F}_{2a,2b}(z), (X_1 - \overline{w} Y_1)^{2a+2b-2k-4} \rangle \\ \omega_2(w) & = & \overline{g(w)} d\overline{w} \end{array} \tag{11.9}$$

where g is any cusp form of weight $2a + 2b - 2k - 2$. The differential form ω_1 is a polynomial in $\overline{w}$ whose coefficients are closed 1-forms in dz and $d\overline{z}$. Then

$$\omega_1(z, w) \wedge \omega_2(w) = \langle \partial^k \mathcal{F}_{2a,2b}(z)\,,\, \overline{g(w)}(X_1 - \overline{w} Y_1)^{2a+2b-2k-4} d\overline{w} \rangle$$

is Γ-invariant for the diagonal action of Γ on $(w, z) \in \mathfrak{H} \times \mathfrak{H}$, by the Γ-invariance of the inner product. Since g vanishes at the cusp, the 2-form $\omega_1(z, z) \wedge \omega_2(z)$ is clearly integrable on the standard fundamental domain for Γ on $\mathfrak{H}$.

The following result is a corollary of a version of Haberlund's theorem.

Corollary 11.6. *Let C_g be the Γ-cocycle corresponding to the cusp form g. Then*

$$\{\partial^k \mathcal{D}_{2a,2b}, C_g\} = 6 \int_{\mathcal{D}} \omega_1(z, z) \wedge \omega_2(z)$$

where $\mathcal{D}$ is the standard fundamental domain for Γ in $\mathfrak{H}$.

The right-hand side can be interpreted as a kind of Petersson product.

Lemma 11.7. *With the above notations*

$$\omega_1(z,z)\wedge\omega_2(z) = J_{2a,2b} - (-1)^k J_{2b,2a}$$

where $J_{2a,2b}$ *is given explicitly by*

$$J_{2a,2b} = \frac{1}{2i}(2\pi i)^{2a-1}\frac{(2a-2)!k!}{(2a-2-k)!}\left(\pi^{-1}\zeta(2b)(2b-2)!\right) \times \Big((z-\overline{z})^{2a+2b-k-4}E_{2a}(z)\mathcal{E}^1_{2b-2-k,k}(z)\overline{g(z)}\Big)dz\wedge d\overline{z} \tag{11.10}$$

Proof. First check that for any $r,i,j,k\in\mathbb{Z}$, we have

$$\partial^k\Big[(aX_1+bY_1)^r(aX_2+bY_2)^i(cX_2+dY_2)^j\Big] = \frac{r!j!(ad-bc)^k}{(r-k)!(j-k)!}(aX_1+bY_1)^{r+i-k}(cX_1+dY_1)^{j-k} \tag{11.11}$$

To see this, simply apply the definition of ∂^k to both sides of the expression

$$\Big((\lambda aX_1+\lambda bY_1+(\mu a+\nu c)X_2+(\mu b+\nu d)Y_2\Big)^N = \sum_{\alpha+\beta+\gamma=N}\frac{(\alpha+\beta+\gamma)!}{\alpha!\beta!\gamma!}\lambda^\alpha\mu^\beta\nu^\gamma(aX_1+bY_1)^\alpha(aX_2+bY_2)^\beta(cX_2+dY_2)^\gamma$$

and read off the coefficients of $\lambda^r\mu^i\nu^j$. Suppose that $m=r+i+j-k\geq 0$. For any $P\in V_m$ we have

$$\langle P(X_1,Y_1),(X_1-tY_1)^m\rangle = P(t,1)$$

by definition of the inner product. Now apply the identity (11.11) to the expression $\partial^k\big((X_1-zY_1)^r(X_2-zY_2)^i(X_2-\overline{z}Y_2)^j\big)$ and put $X_1=\overline{z}$, $Y_1=1$. This gives

$$\langle\partial^k\big((X_1-zY_1)^r(X_2-zY_2)^i(X_2-\overline{z}Y_2)^j\big),(X_1-\overline{z}Y_1)^m\rangle = \delta_{j,k}\frac{(-1)^m r!k!}{(r-k)!}(z-\overline{z})^{m+k}$$

where $\delta_{j,k}$ is the Kronecker delta. Applying this identity to the definition of $\mathcal{F}_{2a,2b}$ and keeping track of the factors (using (11.7)) gives the required expression. □

11.3.2. *Haberlund's formula.* Suppose, as above, that we have two differential forms

$$\omega_1(z,w)\ ,\ \omega_2(w)$$

where ω_1 is a polynomial in $\overline{w}$ whose coefficients are closed 1-forms in z and $\overline{z}$ and $\omega_2(w)$ is closed and vanishes at the cusp $w=i\infty$. Suppose furthermore that

$$\gamma^*(\omega_1\wedge\omega_2)=\omega_1\wedge\omega_2$$

for all $\gamma\in\Gamma$, where γ acts on $(z,w)\in\mathfrak{H}\times\mathfrak{H}$ diagonally. We also assume that $\omega_1(z,w)$ has, for all $w\in\mathfrak{H}$, at most logarithmic singularities in $q=\exp(2\pi iz)$ at $z=i\infty$ (and likewise for all cusps $\gamma(i\infty)$, for $\gamma\in\Gamma$.). Therefore the following integral with respect to z exists

$$F(w)=\int_w^{\overrightarrow{1}_\infty}\omega_1(z,w)\ ,$$

and defines a real analytic function of $w\in\mathfrak{H}$. Since ω_1 is closed, it only depends on w and not the choice of path from w to $\overrightarrow{1}_\infty$. For all $\gamma\in\Gamma$, denote by

$$C^F_\gamma(w)=\int_{\gamma\overrightarrow{1}_\infty}^{\overrightarrow{1}_\infty}\omega_1(z,w)\ ,$$

where the integral is with respect to z and regularised with respect to the tangential base points at the cusps. It exists by the previous assumptions on $\omega_1(z,w)$.

Lemma 11.8. *For all* $\alpha, \beta \in \mathfrak{H} \cup \mathbb{Q} \cup \{i\infty\}$*, and* $\gamma \in \Gamma$*,*

$$\int_{\alpha}^{\beta} F\omega_2 = \int_{\gamma(\alpha)}^{\gamma(\beta)} F\omega_2 - \int_{\gamma(\alpha)}^{\gamma(\beta)} C_{\gamma}^{F}\,\omega_2\ . \tag{11.12}$$

Proof. First of all, there is the following identity (of 1-forms in w):

$$\gamma^*(F\omega_2) = F\omega_2 - C_{\gamma^{-1}}^{F}\,\omega_2 \tag{11.13}$$

To see this, note that the left-hand side is equal to

$$F(\gamma(w)) \wedge \gamma^*(\omega_2) = \int_{\gamma(w)}^{\vec{1}_\infty} \omega_1(z,\gamma(w)) \ \wedge\ \gamma^*(\omega_2) = \int_{w}^{\gamma^{-1}\vec{1}_\infty} \gamma^*(\omega_1 \wedge \omega_2)$$

by changing variables in z. But $\omega_1 \wedge \omega_2$ is Γ-invariant, and the domain of integration on the right-hand side can be written as a composition of paths:

$$\int_{w}^{\gamma^{-1}\vec{1}_\infty} \omega_1 \wedge \omega_2 = \int_{w}^{\vec{1}_\infty} \omega_1 \wedge \omega_2 - \int_{\gamma^{-1}\vec{1}_\infty}^{\vec{1}_\infty} \omega_1 \wedge \omega_2$$

where all integrals are with respect to z. This gives (11.13). Replacing γ with γ^{-1} in (11.13) and integrating from α to β in the w plane gives (11.12). □

Proposition 11.9. *Let* $\mathcal{D} \subset \mathfrak{H}$ *denote the standard fundamental domain for* Γ*. Then with the above assumptions on* ω_1, ω_2*,*

$$6\int_{\mathcal{D}} \omega_1(z,z) \wedge \omega_2(z) = \int_{T^{-1}p - Tp} C_S^F \omega_2 + 2\int_p (C_T^F - C_{T^{-1}}^F)\omega_2$$

where p *denotes the geodesic path from* $S(\vec{1}_\infty)$ *to* $\vec{1}_\infty$*.*

Proof. Consider the domain $\mathcal{D}'$ enclosed by the geodesic square with corners $-1, 0, 1, \infty$. We also shall denote the following tangential base points

$$\vec{1}_\infty \quad , \quad S(\vec{1}_\infty) \quad , \quad TS(\vec{1}_\infty) \quad , \quad T^{-1}S(\vec{1}_\infty)$$

by $\infty, 0, 1, -1$, respectively. The beautiful idea for taking the domain $\mathcal{D}'$, as opposed to $\mathcal{D}$, is due to Pasol and Popa [34]. It is covered by exactly 6 copies of $\mathcal{D}$. Applying Stokes' formula to $\mathcal{D}'$ gives

$$\int_{\mathcal{D}'} \omega_1(w,w) \wedge \omega_2(w) = \int_{\mathcal{D}'} d(F \wedge \omega_2) = \int_{\partial\mathcal{D}'} F\omega_2\ .$$

All integrals converge because $\omega_2(w)$ was assumed to vanish at the cusp. The boundary of $\mathcal{D}'$ consists of four geodesic path segments, from ∞ to -1 to 0 to 1 and back to ∞. Denote the geodesic path from 0 to ∞ by p. Each side of the square is a path γp for some $\gamma \in \Gamma$. Writing $-p$ for Sp, we have

$$\int_{\partial\mathcal{D}'} F\omega_2 = \Big(\int_{-T^{-1}p} + \int_{STp} + \int_{-ST^{-1}p} + \int_{Tp}\Big) F\omega_2$$

Applying (11.12) to each term gives, for example

$$\int_{T^{-1}p} F\omega_2 = \int_p F\omega_2 - \int_p C_T^F \omega_2$$

and applying it twice to the second term gives (since $S^2 = 1$),

$$\int_{STp} F\omega_2 = \int_{Tp} F\omega_2 - \int_{Tp} C_S^F \omega_2 = \int_p F\omega_2 - \int_p C_{T^{-1}}^F \omega_2 - \int_{Tp} C_S^F \omega_2\ .$$

Adding all four contributions together gives

$$\int_{\partial \mathcal{D}'} F\omega_2 = \int_{T^{-1}p - Tp} C_S^F \omega_2 + 2\int_p (C_T^F - C_{T^{-1}}^F)\omega_2$$

as required. □

In order to prove corollary 11.6, substitute the values (11.9) for ω_1, ω_2 into the previous formula. For example,

$$\begin{aligned}\int_{Tp} C_S^F \omega_2 &= \int_p \int_{Tp} \langle \partial^k \mathcal{F}_{2a,2b}(z), \overline{g(w)}(X_1 - \overline{w}Y_1)^m d\overline{w}\rangle \\ &= \langle \int_p \partial^k \mathcal{F}_{2a,2b}(z), \int_{Tp} \overline{g(w)}(X_1 - \overline{w}Y_1)^m d\overline{w}\rangle \\ &= -\langle \partial^k \mathcal{D}^S_{2a,2b}, (C_g)_S\big|_{T^{-1}}\rangle\end{aligned}$$

In the third line we used the Γ-invariance of $\overline{g(w)}(X_1 - \overline{w}Y_1)^m d\overline{w}$ and the formula

$$\mathcal{D}^\gamma_{2a,2b} = -\int_{\gamma^{-1}(\vec{1}_\infty)}^{\vec{1}_\infty} \partial^k \mathcal{F}_{2a,2b}(z)$$

which follows from the definition of $\mathcal{D}$. The other terms similarly give a total of

$$\langle P^S, Q^S\big|_T - Q^S\big|_{T^{-1}}\rangle + 2\langle P^{T^{-1}} - P^T, Q^S\rangle$$

where $P = \partial^k \mathcal{D}_{2a,2b}$ and $Q = C_g$. Since P is a Γ-cocyle, $P^{T^{-1}} + P^T\big|_{T^{-1}} = 0$, and the previous expression reduces to $\{P, Q\}$ by the Γ-equivariance of $\langle\ ,\ \rangle$.

Remark 11.10. The identical argument, applied in the case $\omega_1 = f(z)(z - \overline{w})^{k-2}dz$ and $\omega_2 = \overline{g(w)}d\overline{w}$ where f is a modular form of weight k, and g a cusp form of weight k, gives the generalisation of Haberlund's formula of Kohnen and Zagier [29].

11.4. **Rankin-Selberg Method.** Let $f \in M_k(\Gamma)$ be a modular form of weight k and let $g \in S_\ell(\Gamma)$ be a cusp form of weight ℓ. Let $m \geq \max(k, \ell)$ and $\mathrm{Re}\, s$ large. Then

$$f(z)\mathcal{E}^s_{m-k,m-\ell}(z)\overline{g(z)}\, y^{m-2} dxdy$$

is invariant under Γ and the integral

$$\langle f\mathcal{E}^s_{m-k,m-\ell}, g\rangle = \int_{\mathcal{D}} f(z)\mathcal{E}^s_{m-k,m-\ell}(z)\overline{g(z)} y^{m-2} dxdy$$

where $\mathcal{D} \subset \mathfrak{H}$ is the standard fundamental domain for Γ, converges. This is because, as $y \to \infty$, $g(z)$ is exponentially small in y, whereas $\mathcal{E}^s_{ij}(z)$ and $f(z)$ are of polynomial growth in y. In particular, it admits a meromorphic continuation to $\mathbb{C}$.

Proposition 11.11. *If* $f(z) = \sum_{n\geq 0} a_n e^{2\pi i n z}$ *and* $g(z) = \sum_{n \geq 1} b_n e^{2\pi i n z}$ *then*

$$\langle f\mathcal{E}^s_{m-k,m-\ell}, g\rangle = (4\pi)^{-(s+m-1)}\Gamma(s+m-1)\sum_{n\geq 1} \frac{a_n \overline{b_n}}{n^{s+m-1}}$$

for all Re(s) sufficiently large, and hence for all $s \in \mathbb{C}$*, by meromorphic continuation.*

Proof. The proof is a standard application of the Rankin-Selberg method. For the convenience of the reader, we sketch the argument here. Let

$$\phi^s(z) = f(z)\overline{g(z)} y^{s+m}\ .$$

It is invariant under Γ_∞. When $\mathrm{Re}(s)$ is sufficiently large, unfolding gives

$$\int_{\Gamma_\infty \backslash \mathfrak{H}} \phi^s(z) \frac{dxdy}{y^2} = \int_{\Gamma\backslash \mathfrak{H}} \sum_{\gamma \in \Gamma_\infty \backslash \Gamma} \phi^s(\gamma(z)) \frac{dxdy}{y^2}$$

and the right-hand integral reduces to $\langle f\mathcal{E}^s_{m-k,m-\ell}, g\rangle$. A fundamental domain for $\Gamma_\infty\backslash\mathfrak{H}$ is given by $(x,y) \in [0,1] \times \mathbb{R}^{>0}$ and the left-hand integral gives

$$\sum_{p\geq 0, q\geq 1} a_p \overline{b_q} \int_{0\leq x\leq 1} e^{2i\pi(p-q)x} dx \int_0^\infty e^{-2\pi(p+q)y} y^{s+m-2} dy$$

It converges for $\mathrm{Re}(s)$ large. After doing the x integral, only the terms with $p = q$ survive, and the previous expression reduces to

$$(4\pi)^{-(s+m-1)} \Gamma(s+m-1) \sum_{n\geq 1} \frac{a_n \overline{b_n}}{n^{s+m-1}} \ .$$

□

Corollary 11.12. *Suppose that $f = E_{2a}$ is the Hecke normalised Eisenstein series of weight $2a$ and g is a Hecke normalised cusp form of weight $2c$. Then, for any $m \geq 2a, 2c$, and writing $s' = s+m$, we have*

$$\zeta(2s'-2a-2c)\langle f\mathcal{E}^s_{m-2a,m-2c}, g\rangle = (4\pi)^{-(s'-1)}\Gamma(s'-1) \times L(g,s'-1)L(g,s'-2a) \ . \tag{11.14}$$

Proof. Assume $\mathrm{Re}(s)$ is large. For any Hecke eigenform f of weight k, let us write

$$L(f,s) = \sum_{n\geq 1} \frac{a_n(f)}{n^s} = \prod_p \frac{1}{(1-\alpha_p^f p^{-s})(1-\beta_p^f p^{-s})}$$

where $\{\alpha_p^f, \beta_p^f\}$ are solutions to the equations: $\alpha_p^f + \beta_p^f = a_p^f$ and $\alpha_p^f\beta_p^f = p^{k-1}$. It is well-known that for f, g Hecke normalised eigenfunctions of weights k, ℓ,

$$\sum_{n\geq 1} \frac{a_n(f)a_n(g)}{n^s} = \zeta(2s+2-k-\ell)^{-1} L(f\otimes g, s)$$

where the tensor product L-function is defined by

$$L(f\otimes g, s) = \prod_p \frac{1}{(1-\alpha_p^f\alpha_p^g p^{-s})(1-\alpha_p^f\beta_p^g p^{-s})(1-\beta_p^f\alpha_p^g p^{-s})(1-\beta_p^f\beta_g^f p^{-s})}$$

On the other hand, for an Eisenstein series of weight $2a$, we have:

$$L(E_{2a}, s) = \zeta(s)\zeta(s-2a+1) = \prod_p \frac{1}{(1-p^{-s})(1-p^{2a-1}p^{-s})} \ .$$

In particular,

$$L(E_{2a}\otimes g, s) = L(g,s)L(g,s-2a+1)$$

Therefore if $f = E_{2a}$ and g has weight $2c$, we have

$$\sum_{n\geq 1} \frac{a_n(f)a_n(g)}{n^s} = \zeta(2s+2-2a-2c)^{-1} L(g,s)L(g,s-2a+1)$$

Since a Hecke eigenfunction has real Fourier coefficients, applying this formula to the conclusion of the previous proposition gives the statement of the corollary. □

11.4.1. *Proof of theorem 11.1.* Putting all the pieces together, we let a, b, k and g be as in the statement of theorem 11.1. Then $I^k_{2a,2b} = \partial^k \mathcal{D}_{2a,2b}$ and so

$$\{I^k_{2a,2b}, \mathcal{C}_g\} = 6 \int_{\mathcal{D}} J_{2a,2b} - (-1)^k J_{2b,2a}$$

by corollary 11.6 and lemma 11.7, where $J_{2a,2b}$ is given by

$$J_{2a,2b} = (2\pi i)^{2a-1} \frac{(2a-2)!k!}{(2a-2-k)!} \left(\pi^{-1}\zeta(2b)(2b-2)!\right) \times (2i)^{2a+2b-k-4} \Big(y^{2a+2b-k-4} E_{2a}(z)\mathcal{E}^1_{2b-k-2,k}(z)\overline{g(z)}\Big) dxdy \quad (11.15)$$

using (11.10). Now plug $m = 2a + 2b - k - 2$, $2c = 2a + 2b - 2k - 2$, and $s = 1$, into the statement of corollary 11.12. It gives

$$\zeta(2b) \langle f\mathcal{E}^1_{2b-k-2,k}, g\rangle = 2^{-m}\Lambda(g, m)L(g, 2b - k - 1)$$

using the fact that $\Lambda(g, s) = (2\pi)^{-s}\Gamma(s)L(g, s)$. Using this same expression to replace $L(g, 2b - k - 1)$ with $\Lambda(g, 2b - k - 1)$ and combining with the above gives

$$J_{2a,2b} = (2\pi i)^{m-1} \frac{(2a-2)!k!(2b-2)!}{(2a-2-k)!(2b-2-k)!} \times \Lambda(g, m)\Lambda(g, 2b - k - 1)$$

Finally, writing $m = w + k$, and using the functional equation

$$\Lambda(g, 2b - k - 1) = (-1)^{a+b-k-1}\Lambda(g, 2a - k - 1)$$

since g is of weight $w = 2a + 2b - 2k - 2$, gives

$$J_{2a,2b} = \frac{1}{2}(2\pi i)^{w+k-1} A^k_{a,b}\Lambda(g, m)\Lambda(g, 2a - k - 1)$$

By the remark following theorem 11.1, the quantity $(-1)^{k-1}J_{2b,2a}$ gives an identical contribution.

12. Examples and the depth-defect for double zeta values

The following highly schematic picture may give an intuitive picture of the periods which occur as coefficients of double Eisenstein integrals. By equation (10.5), a double Eisenstein integral of E_{2m} and E_{2n} can be written using notation (11.2) as an uninteresting part (which depends on a choice of rational cochain $e^0_{2m,2n}$):

$$\overline{e}^0_{2m,2n} - \overline{b}_{2m} \cup \overline{e}^0_{2n} + \overline{e}^0_{2m} \cup \overline{b}_{2n}$$

plus further terms corresponding to the right-hand side of (10.6), whose coefficients are $\mathbb{Q}$-linear combinations of $(2i\pi)^{2m+2n-2}$, $(2i\pi)^{2n-1}\zeta(2m-1)$, $(2i\pi)^{2m-1}\zeta(2n-1)$, and $\zeta(2m-1)\zeta(2n-1)$ plus a cocycle in

$$Z^1_{\mathrm{cusp}}(\Gamma; V_{2m-2} \otimes V_{2n-2} \otimes \mathbb{C}) \ .$$

Break up the latter group into its various pieces via the isomorphism

$$V_{2m-2} \otimes V_{2n-2} \cong V_{2m+2n-4} \oplus \ldots \oplus V_{2m-2n} \quad (12.1)$$

and use the fact that the Hecke-equivariant splitting §7.5 gives an isomorphism

$$Z^1_{\mathrm{cusp}}(\Gamma; V_{2r}) = \delta^0 Y^{2r}\mathbb{Q} \oplus H^1_{\mathrm{cusp}}(\Gamma; V_{2r}) \ .$$

Thus for every piece of the decomposition (12.1) we obtain a single 'coboundary period' (right-most column below) corresponding to the coefficient of $\delta^0 Y^{2r}$, and a pair of periods (in the columns λ^+_g, λ^-_g) for each Hecke-eigenclass $g \in H^1_{\mathrm{cusp}}(\Gamma; V_{2r})^{\pm}$.

These periods (ignoring powers of $2\pi i$ and rational pre-factors to avoid clutter) are schematically depicted in the table below. Explanations follow below.

r	$\partial^r(V_{2m-2}\otimes V_{2n-2})$	λ_g^+	λ_g^-	$f^{(r)}$
0	$V_{2m+2n-4}$	c_{g,w_g}	$L(g,w_g)$	$\boxed{f_{2m-1}f_{2n-1}}$
1	$V_{2m+2n-6}$	$L(g,w_g+1)$	c_{g,w_g+1}	$f_{2m+2n-3}$
2	$V_{2m+2n-8}$	c_{g,w_g+2}	$L(g,w_g+2)$	0
3	$V_{2m+2n-10}$	$L(g,w_g+3)$	c_{g,w_g+3}	$f_{2m+2n-5}$
4	$V_{2m+2n-12}$	c_{g,w_g+4}	$L(g,w_g+4)$	0
$\vdots$		$\vdots$	$\vdots$	$\vdots$
$2m-4$	$V_{2n-2m+4}$	c_{g,w_g+2m-4}	$L(g,w_g+2m-4)$	0
$2m-3$	$V_{2n-2m+2}$	$L(g,w_g+2m-3)$	c_{g,w_g+2m-3}	f_{2n+1}
$2m-2$	V_{2n-2m}	c_{g,w_g+2m-2}	$L(g,w_g+2m-2)$	$\boxed{f_{2m-1}f_{2n-2m+1}}$

FIGURE 3. A schematic depiction of the 'non-trivial' periods occurring as coefficients of double Eisenstein integrals.

Using the action of the real Frobenius §5.4 the periods in the λ_g^+ and $f^{(r)}$ columns are real (resp. imaginary) for r even (resp. r odd), and the opposite is true for the λ_g^- column. The imaginary periods are canonical, the real periods depend on the choice of cochain $e^0_{2m,2n}$ and hence lie in $\mathbb{R}/(2\pi\mathbb{Q})^t$ for appropriate t.

In the middle columns we find all special values of L-functions of cusp forms g at the edge, or to the right of the critical strip. The weight w_g of the cusp form in the r^{th} row is $2m+2n-2r$. The L-value is the regulator of an extension of $\mathbb{Q}$ by the motive $h(g)(w_g+r)$ of the corresponding modular form twisted by w_g+r; the number c_{g,w_g+r} is an ill-defined 'extended regulator' and is a different period of the same extension.

We expect the periods of the right-hand column to be periods of mixed Tate motives unramified over $\mathbb{Z}$. Our description of G_κ and the computations of §10.1 give the action of the Tannaka group of a category of Betti-de Rham realisations on the Betti-motivic periods of double Eisenstein integrals. Dualizing gives a formula for the coproduct: for example in the top row it is simply given by deconcatenation. In this way we expect that the periods in rows $r=1,\ldots,r=2m-2$ to correspond to elements of $\mathrm{Ext}^1_{\mathcal{MT}(\mathbb{Z})}(\mathbb{Q},\mathbb{Q}(2m+2n-r-2))$, which are odd or even single Riemann zeta values. The even zeta values are rational up to powers of $2\pi i$ and can be absorbed into the choice of element $e^0_{2m,2n}$. For this reason they are simply denoted by 0 in the table.

The top and bottom entries, which are boxed, correspond to biextensions and should also be periods of mixed Tate motives. Using the results of [6], there is a canonical isomorphism of the ring $\mathcal{H}$ of motivic multiple zeta values with a shuffle algebra

$$\mathcal{H} \xrightarrow{\sim} \mathbb{Q}\langle f_3, f_5, \ldots\rangle \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)] \tag{12.2}$$

which is compatible with the action of the motivic Galois group. In particular

$$\zeta^{\mathfrak{m}}(2n+1) \text{ corresponds to } f_{2n+1}\ .$$

The elements in the two boxed entries in the table are the periods for the elements in $\mathcal{H}$ corresponding to $f_{2m-1}f_{2n-1}+\zeta^{\mathfrak{m}}(2)^{m+n-1}\mathbb{Q}$ and $f_{2m-1}f_{2n-2m+1}+\zeta^{\mathfrak{m}}(2)^n\mathbb{Q}$ respectively. The rational pre-factors are determined by our computations of the group G_κ: for example, the top right-hand boxed entry occurs with a coefficient $\frac{(2m-2)!}{2}\frac{(2n-2)!}{2}$, the bottom right boxed entry involves the coefficient $\lambda_k^{m,n}$ of theorem 10.1.

Finally, the transference principle for double Eisenstein integrals relates, in particular, the bottom right boxed entry for the iterated integral $\partial^{2m-2}\mathcal{C}_{\mathbf{e}_{2m}\mathbf{e}_{2n}}$ to the top right boxed entry of a different iterated integral, namely $\partial^{0}\mathcal{C}_{\mathbf{e}_{2m}\mathbf{e}_{2n-2m}}$.

The above structure for the periods was checked numerically for all double Eisenstein integrals $\mathcal{C}_{\mathbf{e}_{2m}\mathbf{e}_{2n}}$ where $2m+2n \leq 18$ to between 50 and 100 digits. However, I did not find any mention in the literature for the extended regulators c_{g,w_g+k}, so it was not possible to compare these periods with any previously known quantities.

12.1. **Modular depth defect for double zeta values.** Let $\mathcal{S} = \bigoplus_n \mathcal{S}_n$ and $\mathcal{E} = \bigoplus_n \mathcal{E}_n$ denote the graded vector spaces of cusp and Eisenstein forms as in §2. For every $k \geq 0$, the Rankin-Selberg computation of §11 defines a surjective map

$$\begin{array}{rcl} \mu_2^k : \mathcal{E}\otimes\mathcal{E} & \longrightarrow\!\!\!\!\rightarrow & \mathrm{Hom}\,(\mathcal{S},\mathbb{C}) \\ E_{2a}\otimes E_{2b} & \mapsto & \big(g \mapsto \{I^k_{a,b}, C_g\}\big) \end{array}$$

which sends pairs of Eisenstein series of total weight N to $\mathcal{S}^\vee_{N-2k-2}\otimes\mathbb{C}$. This map is antisymmetric for k even, and symmetric for k odd. The surjectivity follows from theorem 11.1 and the non-vanishing of the special values of the L-function of g outside the critical strip. The case $k=0$ is the most interesting.

It gives rise to an exact sequence of graded vector spaces

$$0 \longrightarrow K\otimes\mathbb{C} \longrightarrow (\textstyle\bigwedge^2\mathcal{E})\otimes\mathbb{C} \overset{\mu_2^0}{\longrightarrow} \mathcal{S}^\vee\otimes\mathbb{C} \longrightarrow 0 \qquad (12.3)$$

where $K \subset \bigwedge^2\mathcal{E}$ is a rational subspace we shall describe presently.

12.1.1. *Reminders on depth-graded double zeta values* [8]. Consider the map

$$Z^1_{\mathrm{cusp}}(\Gamma;V_n) \longrightarrow V_n \longrightarrow XY\mathbb{Q}[X,Y] \qquad (12.4)$$

where the first map is evaluation of a cocycle on $S\in\Gamma$, and the second map is the inclusion $V_n \subset \mathbb{Q}[X,Y]$ followed by $f(X,Y)\mapsto f(X,Y)-f(0,Y)-f(X,0)$. The composite (12.4) has the effect of sending $\delta^0 Y^{2k}$ to zero and gives an embedding

$$P^{\mathrm{cusp}} = H^1_{\mathrm{cusp}}(\Gamma;V_\infty) \overset{s}{\longrightarrow} Z^1_{\mathrm{cusp}}(\Gamma;V_n) \overset{(12.4)}{\longrightarrow} XY\mathbb{Q}[X,Y]$$

where s is the splitting of lemma 7.3. The image of this map is the space of period polynomials. These are homogeneous polynomials P satisfying

$$P(X,Y)+P(X-Y,X)+P(-Y,X-Y)=0\ .$$

and we retrieve the well-known fact that cuspidal cohomology classes for Γ can be identified with period polynomials.

Since the previous maps are equivariant with respect to ϵ, we obtain an embedding of $P^{\mathrm{cusp},+}$ into the space of even period polynomials:

$$P^{\mathrm{cusp},+} \longrightarrow X^2Y^2\mathbb{Q}[X^2,Y^2]\ . \qquad (12.5)$$

The latter are antisymmetric with respect to $S\epsilon : (X,Y)\to(Y,X)$.

Now let $\mathrm{gr}^{\mathcal{D}}\mathcal{H}$ be the space of depth-graded motivic multiple zeta values [8].

Lemma 12.1. *There is an exact sequence of graded vector spaces*

$$0 \longrightarrow \mathrm{gr}^{\mathcal{D}}_2\mathcal{H}/(\mathrm{gr}^{\mathcal{D}}_1\mathcal{H})^2 \longrightarrow \textstyle\bigwedge^2\big(\bigoplus_{m\geq 1} f_{2m+1}\mathbb{Q}\big) \longrightarrow (P^{\mathrm{cusp},+})^\vee \longrightarrow 0$$

where the second map is induced by (12.2)*, and the third map is the dual of* (12.5)*, where we identify the dual of* $\bigoplus_{a,b\geq 1} X^{2a}Y^{2b}\mathbb{Q}$ *with* $\bigoplus_{a,b\geq1} f_{2a+1}\otimes f_{2b+1}\mathbb{Q}$ *via*

$$\langle X^{2r}Y^{2s}, f_{2a+1}\otimes f_{2b+1}\rangle = \delta_{r,a}\delta_{s,b}$$

Proof. This is the dual of the exact sequence (where $D_1 \cong X^2\mathbb{Q}[X^2]$),

$$0 \longrightarrow P^{\mathrm{cusp},+} \longrightarrow \bigwedge^2 D_1 \longrightarrow D_2 \longrightarrow 0$$

for the depth-graded motivic Lie algebra stated in [8], equation (7.8). □

12.1.2. *Ihara-Takao relations from multiple modular values.* Consider the isomorphism $\bigwedge^2\mathcal{E} \cong \bigwedge^2\big(\bigoplus_{m\geq 1} f_{2m+1}\mathbb{Q}\big)$ induced by the following isomorphism:

$$\begin{array}{rcll} \mathcal{E} & \overset{\sim}{\longrightarrow} & \displaystyle\bigoplus_{n\geq 1} f_{2n+1}\mathbb{Q} & \\ E_{2n} & \mapsto & \displaystyle\frac{2}{(2n-2)!} f_{2n-1} & \text{for } n \geq 2 \end{array} \tag{12.6}$$

By the previous lemma, $\mathrm{gr}^{\mathcal{D}}_2\mathcal{H}/(\mathrm{gr}^{\mathcal{D}}_1\mathcal{H})^2$ is isomorphic to the vector space

$$K' = \ker\Big(\bigwedge^2\big(\bigoplus_{m\geq 1} f_{2m+1}\mathbb{Q}\big) \longrightarrow (P^{\mathrm{cusp},+})^\vee\Big)$$

of linear relations between coefficients of even period polynomials. Define

$$K \subset \bigwedge^2\mathcal{E}$$

such that $K' \cong K$ via (12.6). One has to verify that $K \otimes \mathbb{C}$ is contained in the kernel of μ^0_2. This follows from the explicit formula (11.3) since, by §7.2, the appropriate generating function of $\Lambda(g, 2a-1)$ is proportional to an even period polynomial.

Corollary 12.2. *The kernel of μ^0_2 is equal to $K\otimes\mathbb{C}$, and K is isomorphic to the space of indecomposable depth-graded motivic double zeta values:*

$$K \cong \mathrm{gr}^{\mathcal{D}}_2\mathcal{H}/(\mathrm{gr}^{\mathcal{D}}_1\mathcal{H})^2\ .$$

Proof. Count dimensions using the previous lemma. By Eichler-Shimura $\dim_{\mathbb{Q}} \mathcal{S}_w = \dim_{\mathbb{Q}} P^{\mathrm{cusp},+}_w$. Since μ^0_2 is surjective, we deduce that $\dim_{\mathbb{C}} K\otimes\mathbb{C} = \dim_{\mathbb{C}} \mu^0_2$. □

Example 12.3. In weight 12, the image of the space of indecomposable double motivic zeta values in $\bigwedge^2\big(\bigoplus_{m\geq 1} f_{2m+1}\mathbb{Q}\big)$ is 1-dimensional, spanned by

$$3f_3 \wedge f_9 + f_5 \wedge f_7 \tag{12.7}$$

For example, $\zeta^{\mathfrak{m}}(3,9) \mapsto -9(3f_3\wedge f_9 + f_5\wedge f_7)$ and $\zeta^{\mathfrak{m}}(4,8) \mapsto 16(3f_3\wedge f_9 + f_5 \wedge f_7)$ under the map (12.2). The equation (12.7) is dual to the well-known relation found by Ihara and Takao in the depth-graded motivic Lie algebra of $\mathcal{MT}(\mathbb{Z})$.

On the other hand, (12.7) corresponds via (12.6) to a multiple of

$$9E_4 \wedge E_{10} + 14E_6 \wedge E_8$$

which spans $\ker \mu^0_2$. In other words, the L-value $L(\Delta, 12)$ of the cusp form Δ of weight 12 cancels out of the linear combination of iterated integrals $\partial^0(9\,\mathcal{C}_{\mathbf{e}_4\mathbf{e}_{10}} + 14\,\mathcal{C}_{\mathbf{e}_6\mathbf{e}_8})$.

In this way, double motivic multiple zeta values are isomorphic to the subspace of double Eisenstein integrals which are orthogonal to all cusp forms. This precisely explains the cuspidal defect [20, 8] for double zeta values in depth 2.

These calculations suggest that it is possible to read off the motivic version of the Broadhurst-Kreimer conjecture [8] from the structure of Hodge-motivic versions of multiple modular values, as mentioned in the introduction. I hope to return to this question shortly.

Remark 12.4. The kernel K can be interpreted as the length two component of the affine ring of the Lie algebra called $\mathfrak{u}^{\mathrm{eis}}$ of [26]. There is a direct way to relate it to double zeta values as follows. The double elliptic polylogarithms defined in [10] can be restricted to the zero section of the universal elliptic curve to obtain certain functions called double elliptic zeta values, which are functions on the punctured q-disc. They can be expressed as certain linear combinations of double iterated integrals of Eisenstein series which correspond exactly to the subspace K. Their regularised limit at $q = 0$ can be computed in terms of iterated integrals on $\mathbb{P}^1\backslash\{0, 1, \infty\}$ of depth 2, and hence evaluate to double zeta values. This is a joint project with A. Levin.

12.2. **Final remarks.** Multiple modular values for $\mathrm{SL}_2(\mathbb{Z})$ should simultaneously give a new construction of the periods of $\mathcal{MT}(\mathbb{Z})$ as certain coefficients of iterated integrals of Eisenstein series, and also explain the vagaries of the modular relations which are visible on multiple zeta values when graded by depth. It remains to study in greater detail the relation between the action of our automorphism group on cocycles and the mixed Hodge structure on relative unipotent completion. I hope that one can construct a genuine mixed Tate motive over $\mathbb{Z}$ (in the technical sense of [16]) out of this relative completion (for example, by some relative variant of a simplicial construction as in [39]) and deduce a new construction of $\mathcal{MT}(\mathbb{Z})$. The question of determining which mixed modular (i.e. non-Tate) motives are generated by $\mathrm{SL}_2(\mathbb{Z})$ is a fascinating one.

One wonders if there is a direct analytic method to compute information about the boundary periods (coefficients of $B_{\mathbf{e}_{2m_1}\ldots\mathbf{e}_{2m_r}}$ in (9.14)) of iterated integrals of Eisenstein series. One interesting possibility is to try to generalise the Rankin-Selberg method of §11 to work for multiple versions of Eisenstein series. Another way to achieve this could be with the following extension of remark 12.4. There is a natural morphism [25] from the Lie algebra of the relative Malcev completion of Γ, via $\mathfrak{u}^{\mathrm{eis}}$, to the stable derivations of the Lie algebra of the fundamental group of the Tate curve. Accordingly, the image of the cocycle $\mathcal{C} \in Z^1(\Gamma, \Pi)$ under a similar map should be related explicitly to the Drinfeld associator. This will give an evaluation of certain combinations of coefficients of $\mathcal{C}$ in terms of multiple zeta values, which, combined with the transference principle, should yield quite a lot of information about periods. There is also a Hodge-theoretic analogue of this idea, which will yield information on the image of the motivic Galois group in G_κ. All this needs to be incorporated into the present framework.

As a final comment to amplify the discussion in the last section of [9], it seems that the fundamental reason why the $\mathrm{SL}_2(\mathbb{Z})$ story is in some sense simpler than the projective line minus three points, is is that there are too many iterated integrals on $\mathbb{P}^1\backslash\{0, 1, \infty\}$ and hence a vast number of relations between them. A multiple zeta value, expressed as an iterated integral on $\mathbb{P}^1\backslash\{0, 1, \infty\}$, has length equal to its weight, which explains why the action of the motivic Galois group upon it is so complicated. On the other hand, multiple zeta values should be expressible as iterated integrals of Eisenstein series of length equal to their coradical degree and so the action of the motivic Galois group on the latter is essentially as simple as it can be.

It is humbling, having reached this point, to read the words of Grothendieck [19], $\frac{16}{17}$, $\frac{17}{18}$ and footnote 4, although he is no doubt referring to the profinite completion of $\mathrm{SL}_2(\mathbb{Z})$, as opposed to the relative unipotent completion considered here.

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