TWISTED TRACES OF MODULAR FUNCTIONS ON HYPERBOLIC 3-SPACE

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Abstract. We compute analogues of twisted traces of CM values of harmonic modular functions on hyperbolic 3-space and show that they are essentially given by Fourier coefficients of the j-invariant. From this we deduce that the twisted traces of these harmonic modular functions are integers. Additionally, we compute the twisted traces of Eisenstein series on hyperbolic 3-space in terms of Dirichlet L-functions and divisor sums.

1. Introduction and statement of results

The values of the modular j-invariant at imaginary quadratic irrationalities are called *singular moduli*. By the theory of complex multiplication, the singular moduli are algebraic integers, and their traces are rational integers. A famous result of Zagier [16] states that the generating function of traces of singular moduli is a weakly holomorphic modular form of weight 3/2. This result has been extended in various directions, for example to traces of (weakly holomorphic and non-holomorphic) modular forms on congruence subgroups by Bruinier and Funke [1]. Mizuno [14] proved an analogue of Zagier's result for automorphic forms on hyperbolic 3-space $\mathbb{H}^3$. He showed that the "traces" of Niebur Poincaré series and Eisenstein series on $\mathbb{H}^3$ appear in the Fourier coefficients of certain linear combinations of non-holomorphic elliptic Poincaré series and Eisenstein series, respectively, of odd weight. Kumar [12] gave "twisted" versions of Mizuno's results. Similar results in the untwisted case were obtained by Matthes [13] on higher dimensional hyperbolic spaces.

In the present paper we restrict our attention to the special case of harmonic automorphic forms on $\mathbb{H}^3$ and their "twisted traces". The automorphic forms we consider here are constructed as special values of Niebur Poincaré series, which can be viewed as analogues on $\mathbb{H}^3$ of the modular j-invariant. We show that the twisted traces of these harmonic automorphic forms on $\mathbb{H}^3$ are Fourier coefficients of weakly holomorphic modular functions for $\mathrm{PSL}_2(\mathbb{Z})$ (by "Zagier duality", they are also Fourier coefficients of weight 2 weakly holomorphic modular forms). This allows us to deduce that the twisted traces are integers, which is not a priori clear since the theory of complex multiplication is not available in our setting. Using the same method we can also compute the twisted traces of weight 0 real-analytic Eisenstein series on $\mathbb{H}^3$.

In the following we describe our results in more detail. Let $\mathbb{Q}(\sqrt{D})$ be an imaginary quadratic field of discriminant $D < 0$, and let $\mathcal{O}_D$ be its ring of integers. The group

$$\Gamma = \mathrm{PSL}_2(\mathcal{O}_D)$$

acts on the hyperbolic 3-space

$$\mathbb{H}^3 = \{P = z + rj \, : \, z \in \mathbb{C}, r \in \mathbb{R}_{>0}\}$$

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(viewed as a subset of $\mathbb{R}[i,j,k]$ of Hamilton's quaternions) by fractional linear transformations. Let $\mathfrak{d}_D^{-1}$ denote the inverse different of $\mathbb{Q}(\sqrt{D})$. For $\nu \in \mathfrak{d}_D^{-1}$ with $\nu \neq 0$ and $s \in \mathbb{C}$ with $\mathrm{Re}(s) > 1$ we consider the Niebur Poincaré series

$$F_\nu(P,s) = 2\pi|\nu| \sum_{\gamma \in \Gamma_\infty \backslash \Gamma} r(\gamma P) I_s(4\pi|\nu| r(\gamma P)) e(\mathrm{tr}(\nu z(\gamma P))),$$

with the usual I-Bessel function. Here Γ_∞ denotes the subgroup of Γ consisting of the matrices $\pm\left(\begin{smallmatrix} 1 & \beta \\ 0 & 1 \end{smallmatrix}\right)$ with $\beta \in \mathcal{O}_D$, and we write $\gamma P = z(\gamma P) + r(\gamma P)j$. The Niebur Poincaré series converges for $\mathrm{Re}(s) > 1$ and satisfies the Laplace equation

$$(\Delta - (1 - s^2))F_\nu(P,s) = 0, \tag{1.1}$$

where Δ denotes the usual hyperbolic Laplace operator on $\mathbb{H}^3$. By analyzing the Fourier expansion, it was shown in [9, Proposition 4.4] that $F_\nu(P,s)$ has an analytic continuation to $\mathrm{Re}(s) > 1/2$ which is holomorphic at $s = 1$.

Definition 1.1. For $\nu \in \mathfrak{d}_D^{-1}$ with $\nu \neq 0$ we define the function

$$J_\nu(P) = F_\nu(P,1),$$

which is a harmonic Γ-invariant function on $\mathbb{H}^3$.

We may view the functions $J_\nu(P)$ as hyperbolic 3-space analogues of the elliptic modular functions $j_n(\tau)$ whose Fourier expansions are of the form $j_n(\tau) = q^{-n} + O(q)$. Indeed, $j_n(\tau)$ can be constructed as a Niebur Poincaré series in an analogous way, see Section 2. This inspired the notation $J_\nu(P)$.

We are interested in the values of $J_\nu(P)$ at special points in $\mathbb{H}^3$. For a positive integer $m > 0$ we let

$$L^+_{|D|m} = \left\{ X = \begin{pmatrix} a & b \\ \overline{b} & c \end{pmatrix} : a, c \in \mathbb{N},\, b \in \mathcal{O}_D,\, \det(X) = |D|m \right\}$$

be the set of positive definite integral binary hermitian forms of determinant $|D|m$ over $\mathbb{Q}(\sqrt{D})$. The group Γ acts on $L^+_{|D|m}$, with finitely many orbits. To $X = \left(\begin{smallmatrix} a & b \\ \overline{b} & c \end{smallmatrix}\right) \in L^+_{|D|m}$ we associate the *special point*

$$P_X = \frac{b}{c} + \frac{\sqrt{|D|m}}{c} j \in \mathbb{H}^3.$$

It can be viewed as an analogue of a CM point on $\mathbb{H}^3$. We refer to the book [5] for more on binary hermitian forms and the connection to the hyperbolic 3-space.

We now define twisted traces of special values of functions on $\mathbb{H}^3$. We can write $D = \prod_{p \mid D} p^*$ as a product of *prime discriminants* p^*, that is, for an odd prime p we have $p^* = (\frac{-1}{p})p$, and we have $2^* \in \{-4, \pm 8\}$. For $X \in L^+_{|D|m}$ we define the *twisting function*

$$\chi_D(X) = \prod_{p \mid D} \chi_{p^*}(X), \qquad \chi_{p^*}(X) = \begin{cases} \left(\frac{p^*}{a}\right), & \text{if } p \nmid a, \\ \left(\frac{p^*}{c}\right), & \text{if } p \nmid c, \\ 0, & \text{if } p \mid \text{g.c.d.}(a,c). \end{cases}$$

This function was considered by Bruinier and Yang [2] and Ehlen [4] for positive fundamental discriminants D, and it was used to study twisted Borcherds products on Hilbert modular surfaces.

As in [2], one can check that $\chi_D(X)$ is well-defined and Γ-invariant. For a Γ-invariant function f on $\mathbb{H}^3$ we define its *m-th twisted trace* by

$$\mathrm{tr}_{m,D}(f) = \sum_{X \in \Gamma \backslash L^+_{|D|m}} \frac{\chi_D(X)}{|\Gamma_X|} f(P_X),$$

where Γ_X denotes the stabilizer of X in Γ.

Remark 1.2. Note that we twist with the quadratic character associated to the discriminant D of the underlying imaginary quadratic field $\mathbb{Q}(\sqrt{D})$. In contrast, the classical traces of CM values of modular functions for $\mathrm{PSL}_2(\mathbb{Z})$ can be twisted by genus characters associated to arbitrary fundamental discriminants dividing the discriminant of the CM points (see [16], for example). It would be interesting to find an analogue of "twists by genus characters" of traces on $\mathbb{H}^3$.

Our main result is the following explicit evaluation of the twisted traces of the harmonic modular functions J_ν in terms of Fourier coefficients of the elliptic modular functions j_n.

Theorem 1.3. *For $\nu \in \mathfrak{d}_D^{-1}$ with $\nu \neq 0$ we have*

$$\mathrm{tr}_{m,D}(J_\nu) = m \sum_{d \mid \nu} \left(\frac{D}{d}\right) d\, c_{|D||\nu|^2/d^2}(m),$$

where $c_n(m)$ are the Fourier coefficients of $j_n(\tau)$, and $d \mid \nu$ means that $\nu/d \in \mathfrak{d}_D^{-1}$.

Remark 1.4.

(1) The above theorem implies that for every unit $u \in \mathcal{O}_D^\times$ and every $\nu \in \mathfrak{d}_D^{-1}$ with $\nu \neq 0$ we have $\mathrm{tr}_{m,D}(J_{u\nu}) = \mathrm{tr}_{m,D}(J_\nu)$. This can also be proved directly as follows. For every $P = z + rj \in \mathbb{H}^3$, we have the relation

$$J_{u\nu}(z + rj) = J_\nu(uz + rj).$$

Moreover, if $P = P_X$ is the special point associated to the positive definite hermitian form $X = \left(\begin{smallmatrix} a & b \\ \bar{b} & c \end{smallmatrix}\right)$, then $uz + j$ is the special point associated to $X_u = \left(\begin{smallmatrix} a & ub \\ \overline{ub} & c \end{smallmatrix}\right)$ and $\chi_D(X) = \chi_D(X_u)$. The equality of the traces is then a consequence of the fact that $X \mapsto X_u$ defines a bijection $L^+_{|D|m} \to L^+_{|D|m}$.

(2) The family $\{1\} \cup \{j_n\}_{n \geq 1}$ is a basis of the $\mathbb{C}$-vector space $M_0^!$ of weakly holomorphic modular functions for $\mathrm{PSL}_2(\mathbb{Z})$. Defining

$$S_n := -\frac{j_n'}{n} = \frac{1}{q^n} + \sum_{m=1}^{\infty} b_n(m) q^m,$$

where $j_n'(\tau) = \frac{1}{2\pi i}\frac{\partial}{\partial \tau} j_n(\tau)$, we get a family a functions $\{S_n\}_{n \geq 1}$ that is a basis of the space $M_2^!$ of weight 2 weakly holomorphic modular forms for the same group. The families $\{j_n\}_{n\geq 1}$ and $\{S_n\}_{n \geq 1}$ are *Zagier dual* in the sense that

$$c_m(n) = -b_n(m) \text{ for all integers } n, m \geq 1,$$

and the formula in Theorem 1.3 can be rewritten as

$$\mathrm{tr}_{m,D}(J_\nu) = -m \sum_{d \mid \nu} \left(\frac{D}{d}\right) d\, b_m\left(\frac{|D||\nu|^2}{d^2}\right).$$

The method we use for the proof of Theorem 1.3 is by now classical and has been employed in various previous works such as [17], [11], [10], [3], [14] and [12], among others. We write out the left-hand side as an infinite series involving an I-Bessel function and certain finite exponential sums. By writing j_n as a special value of a Niebur Poincaré series for $\mathrm{PSL}_2(\mathbb{Z})$, one obtains an expression for its coefficients $c_n(m)$ as an infinite series involving the same I-Bessel function and certain Kloosterman sums, see Section 2. Hence, the proof of the theorem boils down to an identity of finite exponential sums, see Section 3. The details of the proof will be given in Section 4.

Since the coefficients of j_n are integers, we obtain the following rationality result.

Corollary 1.5. *The twisted traces* $\mathrm{tr}_{m,D}(J_\nu)$ *are integers which are divisible by* m*.*

This is remarkable since the theory of complex multiplication is not available in the hyperbolic 3-space setting. We can rephrase the evaluation of $\mathrm{tr}_{m,D}(J_\nu)$ as a modularity result. Recall that $j_n'(\tau) = \frac{1}{2\pi i}\frac{\partial}{\partial\tau} j_n(\tau)$.

Corollary 1.6. *For* $\nu \in \mathfrak{d}_D^{-1}$ *with* $\nu \neq 0$*, let*

$$\mathscr{Z}_{\nu,D}(\tau) = -\sum_{d\mid\nu}\left(\frac{D}{d}\right)\frac{|D||\nu|^2}{d} q^{-|D||\nu|^2/d^2} + \sum_{m=1}^{\infty} \mathrm{tr}_{m,D}(J_\nu) q^m$$

be the generating function over m *for the twisted traces* $\mathrm{tr}_{m,D}(J_\nu)$*. Then*

$$\mathscr{Z}_{\nu,D}(\tau) = \sum_{d\mid\nu}\left(\frac{D}{d}\right) d\, j'_{|D||\nu|^2/d^2}(\tau). \tag{1.2}$$

In particular, it is a weakly holomorphic modular form of weight 2 *for* $\mathrm{PSL}_2(\mathbb{Z})$*.*

Example 1.7. Let $D = -4$, so $\mathbb{Q}(\sqrt{D}) = \mathbb{Q}(i)$. Then $\mathcal{O}_D = \mathbb{Z}[i]$ and $\mathfrak{d}_D^{-1} = \frac{1}{2}\mathbb{Z}[i]$. Take $\nu = \frac{1}{2}$, such that $|\nu|^2 = \frac{1}{4}$. Then for every $m \geq 1$ we have

$$\mathrm{tr}_{m,-4}(J_{1/2}) = m c_1(m),$$

where $c_1(m)$ is the m-th coefficient of the j-invariant. In particular, we have

$$-q^{-1} + \sum_{m=1}^{\infty} \mathrm{tr}_{m,-4}(J_{1/2}) q^m = j'(\tau).$$

For example, for $m = 1$ the set $\Gamma\backslash L_4^+$ consists of the three binary hermitian forms $X_1 = \left(\begin{smallmatrix} 4 & 0 \\ 0 & 1 \end{smallmatrix}\right), X_2 = \left(\begin{smallmatrix} 3 & 1+i \\ 1-i & 2 \end{smallmatrix}\right), X_3 = \left(\begin{smallmatrix} 2 & 0 \\ 0 & 2 \end{smallmatrix}\right)$, with corresponding special points $P_1 = 2j, P_2 = \frac{1+i}{2} + j, P_3 = j$, and stabilizers of orders $4, 4, 8$, respectively (see [5, p. 413]). Moreover, we have $\chi_D(X_1) = 1, \chi_D(X_2) = -1$, and $\chi_D(X_3) = 0$. By evaluating the defining series of $J_{1/2}$ numerically, we can now compute

$$\mathrm{tr}_{1,-4}(J_{1/2}) = \frac{1}{4}J_{1/2}(P_1) - \frac{1}{4}J_{1/2}(P_2) = \frac{1}{4}\cdot(786286.36\ldots) - \frac{1}{4}\cdot(-1249.60\ldots) = 196883.99\ldots$$

Up to rounding errors, this agrees with the coefficient $c_1(1) = 196884$.

Remark 1.8. Using the basis $\{S_n\}_{n\geq 1}$ from Remark 1.4(2) we can rewrite (1.2)

$$-\sum_{d\mid\nu}\left(\frac{D}{d}\right)\frac{|D||\nu|^2}{d} q^{-|D||\nu|^2/d^2} + \sum_{m=1}^{\infty}\mathrm{tr}_{m,D}(J_\nu)q^m = -\sum_{d\mid\nu}\left(\frac{D}{d}\right)\frac{|D||\nu|^2}{d} S_{|D||\nu|^2/d^2}(\tau).$$

This can be compared with Zagier's result [16] in the elliptic case. Indeed, in *loc. cit.* Zagier constructs a basis $\{g_D\}_{D>0,D\equiv 0,1(4)}$ for the space $M^{!,+}_{3/2}$ of weight 3/2 weakly holomorphic modular forms in the plus space, and for every integer $n \geq 1$ and every fundamental discriminant $D > 0$ he shows the equality

$$-\sum_{d|n}\left(\frac{D}{d}\right)\frac{\sqrt{D}n}{d}q^{-Dn^2/d^2}+\sum_{d=1}^{\infty}\mathrm{tr}_{-d,D}(j_n)q^d=-\sum_{d|n}\left(\frac{D}{d}\right)\frac{\sqrt{D}n}{d}\,g_{Dn^2/d^2}(\tau)$$

for the generating function of the twisted traces of the function j_n over CM points of discriminant $-dD$.

Remark 1.9. (1) On the one hand, the results of Mizuno [14] imply that the non-twisted traces of J_ν are Fourier coefficients of a *non-holomorphic* modular form of odd weight for $\Gamma_0(|D|)$ with character $\left(\frac{D}{\cdot}\right)$. Indeed, the form $\mathcal{G}(z,1)$ obtained from [14, Theorem 6] has weight k an odd integer, and it is an eigenfunction of the Laplace operator $\Delta_k = -v^2\left(\frac{\partial^2}{\partial_u^2}+\frac{\partial^2}{\partial_v^2}\right)+ikv\left(\frac{\partial}{\partial_u}+i\frac{\partial}{\partial_v}\right)$ with eigenvalue $(k^2-2k)/4 \neq 0$. Hence, it seems that the non-twisted traces of J_ν do not have good algebraic properties. On the other hand, using vector-valued modular forms and similar methods as in [14], one can prove some rationality results for the non-twisted traces of the *non-harmonic* function $F_\nu(P,k/2)$, by expressing them in terms of the Fourier coefficients of weakly holomorphic modular forms. For example, in the case $D=-4$ and $\nu=\frac{1}{2}$, noting that there is only one form in $\Gamma\backslash L_1^+$, corresponding to the special point $P=j$, with stabilizer of order 4, we numerically compute to get

$$\mathrm{tr}_1\left(F_{1/2}\left(\cdot,\tfrac{3}{2}\right)\right)=\frac{1}{4}F_{1/2}\left(j,\tfrac{3}{2}\right)=384.$$

(2) Kumar [12] gave twisted versions of Mizuno's results, but did not consider the relation to the j-invariant or the algebraic nature of the twisted traces of J_ν.

It is also possible to construct a generating function summing over ν for the twisted traces $\mathrm{tr}_{m,D}(J_\nu)$. This leads to a weight 2 automorphic form on $\mathbb{H}^3$ with singularities at the special points in $T_{m,D} = \{P_X : X \in L^+_{m|D|}, \chi_D(X) \neq 0\}$. In order to be more precise, let $m > 0$ be a fixed integer, and for $P = z + rj$ and $\ell \in \{0,1,2\}$ let us define

$$\mathcal{F}^{(\ell)}_{m,D}(z+rj)=\sum_{\substack{\nu\in\mathfrak{d}_D^{-1}\\ \nu\neq 0}}\mathrm{tr}_{m,D}(J_\nu)\xi(\nu)^{\ell-1}r\widetilde{K}_\ell(4\pi|\nu|r)e(\mathrm{tr}(\nu z)),\tag{1.3}$$

with $\xi(\nu)=\frac{\nu}{|\nu|}$ and special functions

$$\widetilde{K}_\ell(y)=\begin{cases}-K_1(y), & \ell=2,\\ 2iK_0(y), & \ell=1,\\ K_1(y), & \ell=0.\end{cases}$$

The series (1.3) converge for $r > \sqrt{m|D|}$, and in Section 6 we prove the following.

Theorem 1.10. *Let $m > 0$ be an integer. Then, for each $\ell \in \{0,1,2\}$ the function $\mathcal{F}^{(\ell)}_{m,D}$ given in* (1.3) *extends to a smooth function on $\mathbb{H}^3 \setminus T_{m,D}$, and $\mathcal{F}_{m,D} = (\mathcal{F}^{(2)}_{m,D}, \mathcal{F}^{(1)}_{m,D}, \mathcal{F}^{(0)}_{m,D})^t$ defines an automorphic form of weight* 2 *for Γ on $\mathbb{H}^3 \setminus T_{m,D}$.*

The proof of Theorem 1.10 is based on properties of the automorphic Green's function associated to $\Gamma = \mathrm{PSL}(\mathcal{O}_D)$ and properties of certain differential operators acting on automorphic forms on $\mathbb{H}^3$ studied by Friedberg in [6], see Section 6.

Remark 1.11. The form $\mathcal{F}_{m,D}$ in Theorem 1.10 is the analogue of the generating function

$$\mathrm{tr}_{-d,D}\left(\frac{j'(\tau)}{j(\cdot)-j(\tau)}\right) = \sum_{n=1}^{\infty} \mathrm{tr}_{-d,D}(j_n)q^n,$$

which is an elliptic modular form of weight 2 for $\mathrm{PSL}_2(\mathbb{Z})$ with a singularity at each CM point of discriminant $-dD$ whenever the twisting function does not vanish.

Finally, we compute the twisted trace of the weight 0 real-analytic Eisenstein series

$$E_0(P,s) = \sum_{\gamma \in \Gamma_\infty \backslash \Gamma} r(\gamma P)^{s+1}.$$

The Eisenstein series converges absolutely for $s \in \mathbb{C}$ with $\mathrm{Re}(s) > 1$, and has meromorphic continuation to $\mathbb{C}$ with a simple pole at $s = 1$, whose residue is independent of P. It also satisfies the Laplace equation (1.1). Moreover, it defines a Γ-invariant function on $\mathbb{H}^3$.

Theorem 1.12. *The m-th twisted trace of the Eisenstein series is given by*

$$\mathrm{tr}_{m,D}\left(E_0(\,\cdot\,,s)\right) = \frac{|D|^{\frac{s+1}{2}} L_D(s)}{\zeta(s+1)} m^{\frac{1-s}{2}} \sigma_s(m),$$

where $\sigma_s(m) = \sum_{d|m} d^s$ is a divisor sum and $L_D(s) = \sum_{n=1}^{\infty}\left(\frac{D}{n}\right) n^{-s}$ is a Dirichlet L-series. In particular, the twisted trace is holomorphic at $s = 1$, with

$$\mathrm{tr}_{m,D}\left(E_0(\,\cdot\,,s)\right)\big|_{s=1} = \frac{12}{\pi}\frac{\sqrt{|D|}h(D)}{w(D)}\sigma_1(m),$$

where $h(D)$ is the class number of $\mathbb{Q}(\sqrt{D})$ and $\omega(D) \in \{1,2,3\}$ is half the number of units of $\mathcal{O}_D$.

The proof of Theorem 1.12 is analogous to the proof of Theorem 1.3, compare Sections 4 and 5. The holomorphicity of the twisted traces of the Eisenstein series at $s = 1$ and the fact that the residue of the Eisenstein series does not depend on P together imply that the twisted traces of the constant 1 function vanish.

Corollary 1.13. *We have*

$$\mathrm{tr}_{m,D}(1) = 0.$$

Remark 1.14. An analogous vanishing result for twisted Hurwitz class numbers (that is, twisted traces of 1 over CM points of a fixed discriminant, twisted by a genus character) is well known, and follows from the fact that the classes of primitive binary quadratic forms of a fixed discriminant form a finite group, combined with classical ortogonality of characters. In our setting, classes of binary hermitian forms do not form a group. However, as explained in [8, Remark 5.9], one can express $\mathrm{tr}_{m,D}(1)$ as a multiple of an integral of a non-trivial adelic character on an adelic group, which implies the vanishing of $\mathrm{tr}_{m,D}(1)$, again by orthogonality of characters. Note that in [8] we worked with prime discriminants D, but the properties used in the remark about the vanishing of $\mathrm{tr}_{m,D}(1)$ extend easily to general fundamental discriminants.

This work is organized as follows. In Section 2 we recall the Fourier expansion of the Niebur Poincaré series for $\mathrm{PSL}_2(\mathbb{Z})$, which is given in terms of Bessel functions and Kloosterman sums. In Section 3 we give an identity between these Kloosterman sums and certain exponential sums occuring in the Fourier expansion of the Niebur Poincaré series $F_\nu(P,s)$ on hyperbolic 3-space. In Section 4 we put these two results together to prove our main result Theorem 1.3. The proof of Theorem 1.12 is presented in Section 5. Finally, in Section 6 we recall the properties of the automorphic Green's function for $\mathrm{PSL}_2(\mathcal{O}_D)$ and prove Theorem 1.10 by using a result of Friedberg [6] on raising operators for automorphic forms in $\mathbb{H}^3$.

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2. Niebur Poincaré series for $\mathrm{PSL}_2(\mathbb{Z})$

We recall some known results about Niebur Poincaré series for $\mathrm{PSL}_2(\mathbb{Z})$, following [2]. For a positive integer $n>0$ it is defined by ($\tau = u+iv \in \mathbb{H}^2$)

$$F_n(\tau,s) = \pi\sqrt{n} \sum_{M\in\Gamma'_\infty\backslash\Gamma'} \sqrt{v} I_{s-\frac{1}{2}}(2\pi n v) e(-nu)|_0 M,$$

with the usual I-Bessel function, $\Gamma' = \mathrm{PSL}_2(\mathbb{Z})$ and $\Gamma'_\infty = \{\pm\left(\begin{smallmatrix}1 & b\\ 0 & 1\end{smallmatrix}\right) : b\in\mathbb{Z}\}$. Niebur [15] showed that $F_n(\tau,s)$ can be analytically continued to $s=1$ via its Fourier expansion, which is given as follows.

Proposition 2.1. *The Fourier expansion of the Niebur Poincaré series $F_n(\tau,s)$ is given by*

$$\begin{aligned} F_n(\tau,s) &= (2\mathcal{I}_s(2\pi n v) + \mathcal{K}_s(2\pi n v)) e(-nu) \\ &\quad + c_n(0,s) v^{1-s} + \sum_{m\in\mathbb{Z}\setminus\{0\}} c_n(m,s)\mathcal{K}_s(2\pi m v) e(mu), \end{aligned}$$

with the Bessel functions $\mathcal{I}_s(y) = \sqrt{\frac{\pi|y|}{2}} I_{s-1/2}(|y|)$ and $\mathcal{K}_s(y) = \sqrt{\frac{2|y|}{\pi}} K_{s-1/2}(|y|)$, and coefficients

$$c_n(m,s) = \begin{cases} 2\pi\left|\dfrac{n}{m}\right|^{1/2} \displaystyle\sum_{c=1}^{\infty} H_c(m,n) I_{2s-1}\left(\frac{4\pi}{c}\sqrt{|mn|}\right), & m>0,\\[2ex] \dfrac{4\pi^{1+s} n^s}{(2s-1)\Gamma(s)} \displaystyle\sum_{c=1}^{\infty} c^{1-2s} H_c(n,0), & m=0,\\[2ex] -\delta_{-n,m} + 2\pi\left|\dfrac{n}{m}\right|^{1/2} \displaystyle\sum_{c=1}^{\infty} H_c(m,n) J_{2s-1}\left(\frac{4\pi}{c}\sqrt{|mn|}\right), & m<0, \end{cases}$$

with the Kloosterman sum

$$H_c(m,n) = \frac{1}{c}\sum_{d(c)^*} e\left(\frac{nd - md'}{c}\right), \tag{2.1}$$

where the sum runs over the multiplicative group $(\mathbb{Z}/c\mathbb{Z})^*$ *and* d' *denotes the inverse of* d *in that group.*

For $m = 0$ we have the more explicit formula

$$c_n(0,s) = \frac{4\pi}{(2s-1)} \frac{n^{1-s}\sigma_{2s-1}(n)}{\pi^{-s}\Gamma(s)\zeta(2s)}, \tag{2.2}$$

with the divisor sum $\sigma_s(n) = \sum_{d|n} d^s$, compare [2, Proposition 2.2]. Moreover, we have the special values

$$\mathcal{I}_1(y) = \sinh(|y|), \qquad \mathcal{K}_1(y) = e^{-|y|}, \qquad 2\mathcal{I}_1(y) + \mathcal{K}_1(y) = e^{|y|}.$$

Plugging in $s = 1$, we find that

$$F_n(\tau, 1) = j_n(\tau) + 24\sigma_1(n),$$

where $j_n(\tau)$ is the unique weakly holomorphic modular form of weight 0 for $\mathrm{PSL}_2(\mathbb{Z})$ with Fourier expansion of the form $j_n(\tau) = q^{-n} + O(q)$. In particular, we have

$$c_n(m,1) = \begin{cases} 24\sigma_1(n), & m = 0, \\ c_n(m), & m > 0, \\ 0, & m < 0, \end{cases} \tag{2.3}$$

where $c_n(m)$ denote the coefficients of j_n.

Remark 2.2. Niebur also defined $F_n(\tau, s)$ for negative index n. These functions are related by the equality $F_{-n}(\tau, s) = F_n(-\overline{\tau}, s)$. In particular, plugging $s = 1$ we get

$$F_n(\tau, 1) = j_{|n|}(-\overline{\tau}) + 24\sigma_1(|n|) \text{ when } n < 0,$$

which is an anti-holomorphic modular function for $\mathrm{PSL}_2(\mathbb{Z})$.

3. Exponential sums

Let $D < 0$ be a negative fundamental discriminant. For a natural number c we let $D_c \mid D$ be the fundamental discriminant dividing D which has the same prime divisors as g.c.d.(c, D), that is, D_c is the product of the prime discriminants p^* for $p \mid$ g.c.d.(c, D). Note that D/D_c is also a fundamental discriminant. Following [2], for $\nu \in \mathfrak{d}_D^{-1}$ we consider the finite exponential sum

$$\widetilde{G}_c(|D|m, \nu) = \left(\frac{D/D_c}{c}\right) \sum_{\substack{b \in \mathcal{O}_D/c\mathcal{O}_D \\ |b|^2 \equiv -|D|m(c)}} \left(\frac{D_c}{\frac{|D|m+|b|^2}{c}}\right) e\left(\mathrm{tr}(\nu b)/c\right). \tag{3.1}$$

We have the following relation with the Kloosterman sum $H_c(m, n)$ given in (2.1).

Lemma 3.1. *For* $c \in \mathbb{N}$, $m \in \mathbb{Z}$ *and* $\nu \in \mathfrak{d}_D^{-1}$ *we have*

$$\frac{1}{c}\widetilde{G}_c(|D|m, \nu) = \sum_{\substack{d|\nu \\ d|c}} \left(\frac{D}{d}\right) H_{c/d}(m, |D||\nu|^2/d^2).$$

Proof. This can be proved similarly as the Proposition in [17, Section 4]. We also refer to [2, Lemma 4.3] for the proof in the case that $D > 1$ is a positive odd prime discriminant, in which case one replaces $|b|^2$ with the norm $N(b) = bb'$ in $\mathbb{Q}(\sqrt{D})$. We leave the details to the reader. □

4. Twisted traces of Niebur Poincaré series - Proof of Theorem 1.3

Theorem 1.3 follows from the following evaluation of the twisted traces of the Niebur Poincaré series $F_\nu(P,s)$ on $\mathbb{H}^3$, by plugging in $s=1$ and using (2.3).

Proposition 4.1. *For $\nu \in \mathfrak{d}_D^{-1}$ with $\nu \neq 0$ we have*

$$\mathrm{tr}_{m,D}(F_\nu(\,\cdot\,,s)) = m\sum_{d\mid\nu}\left(\frac{D}{d}\right) d\, c_{|D||\nu|^2/d^2}(m,\tfrac{s+1}{2}),$$

where $c_n(m,s)$ are the coefficients of the Niebur Poincaré series $F_n(\tau,s)$ on $\mathrm{PSL}_2(\mathbb{Z})$ from Proposition 2.1.

Proof. We first write

$$\begin{aligned}\mathrm{tr}_{m,D}(F_\nu(\,\cdot\,,s)) &= 2\pi|\nu|\sum_{X\in\Gamma\backslash L^+_{|D|m}}\frac{\chi_D(X)}{|\Gamma_X|}\sum_{\gamma\in\Gamma_\infty\backslash\Gamma} r(\gamma P_X)I_s(4\pi|\nu|r(\gamma P_X))e(\mathrm{tr}(\nu z(\gamma P_X)))\\ &= 2\pi|\nu|\sum_{X\in\Gamma_\infty\backslash L^+_{|D|m}}\chi_D(X)r(P_X)I_s(4\pi|\nu|r(P_X))e(\mathrm{tr}(\nu z(P_X))).\end{aligned}$$

For $X = \left(\begin{smallmatrix} a & b\\ \bar{b} & c\end{smallmatrix}\right) \in L^+_{m|D|}$ we have $r(P_X) = \frac{\sqrt{|D|m}}{c}$ and $z(P_X) = \frac{b}{c}$. Moreover, note that $\left(\begin{smallmatrix} 1 & \beta\\ 0 & 1\end{smallmatrix}\right) \in \Gamma_\infty$ changes b to $b + a\beta$, but does not change c. Hence, a system of representatives for $\Gamma_\infty\backslash L^+_{|D|m}$ is given by the matrices $\left(\begin{smallmatrix} a & b\\ \bar{b} & c\end{smallmatrix}\right)$ where c runs through all positive integers, b runs through $\mathcal{O}_D/c\mathcal{O}_D$ with $|b|^2 \equiv -|D|m \pmod{c}$, and a is determined by $a = \frac{|D|m+|b|^2}{c}$. Then we have

$$\chi_D\left(\begin{pmatrix} a & b\\ \bar{b} & c\end{pmatrix}\right) = \left(\frac{D/D_c}{c}\right)\left(\frac{D_c}{a}\right) = \left(\frac{D/D_c}{c}\right)\left(\frac{D_c}{\frac{|D|m+|b|^2}{c}}\right).$$

Hence we get

$$\begin{aligned}&\mathrm{tr}_{m,D}(F_\nu(\,\cdot\,,s))\\ &\quad= 2\pi|\nu|\sum_{c>0}\sum_{\substack{b\in\mathcal{O}_D/c\mathcal{O}_D\\ |b|^2\equiv-|D|m(c)}}\left(\frac{D/D_c}{c}\right)\left(\frac{D_c}{\frac{|D|m+|b|^2}{c}}\right)\frac{\sqrt{|D|m}}{c}I_s\left(4\pi|\nu|\frac{\sqrt{|D|m}}{c}\right)e(\mathrm{tr}(\nu b)/c)\\ &\quad= 2\pi|\nu|\sqrt{|D|m}\sum_{c>0}\frac{1}{c}\widetilde{G}_c(|D|m,\nu)I_s\left(4\pi|\nu|\frac{\sqrt{|D|m}}{c}\right),\end{aligned}$$

with the exponential sum $\widetilde{G}_c(|D|m,\nu)$ defined in (3.1). Using Lemma 3.1 we can further compute

$$\begin{aligned}\mathrm{tr}_{m,D}(F_\nu(\,\cdot\,,s)) &= 2\pi|\nu|\sqrt{|D|m}\sum_{c>0}\sum_{\substack{d\mid\nu\\ d\mid c}}\left(\frac{D}{d}\right)H_{c/d}(m,|D||\nu|^2/d^2)I_s\left(4\pi|\nu|\frac{\sqrt{|D|m}}{c}\right)\\ &= 2\pi|\nu|\sqrt{|D|m}\sum_{d\mid\nu}\left(\frac{D}{d}\right)\sum_{c>0}H_c(m,|D||\nu|^2/d^2)I_s\left(4\pi|\nu|\frac{\sqrt{|D|m}}{cd}\right).\end{aligned}$$

Comparing the series over $c>0$ to the coefficients of the Niebur Poincaré series from Proposition 2.1, we obtain

$$\mathrm{tr}_{m,D}(F_\nu(\,\cdot\,,s)) = m\sum_{d|\nu}\left(\frac{D}{d}\right) d\, c_{|D||\nu|^2/d^2}(m, \tfrac{s+1}{2}).$$

This gives the stated formula. □

5. Twisted traces of Eisenstein series - Proof of Theorem 1.12

Replicating the first steps from the proof of Proposition 4.1 in Section 4 we arrive at

$$\begin{aligned}\mathrm{tr}_{m,D}(E_0(\,\cdot\,,s)) &= \sum_{c>0}\sum_{\substack{b\in\mathcal{O}_F/c\mathcal{O}_F\\ |b|^2\equiv -|D|m(c)}}\left(\frac{D/D_c}{c}\right)\left(\frac{D_c}{\frac{|D|m+|b|^2}{c}}\right)\left(\frac{\sqrt{|D|m}}{c}\right)^{s+1}\\ &= \left(\sqrt{|D|m}\right)^{s+1}\sum_{c>0}c^{-s-1}\widetilde{G}_c(|D|m,0).\end{aligned}$$

Using Lemma 3.1 we get

$$\begin{aligned}\mathrm{tr}_{m,D}(E_0(\,\cdot\,,s)) &= \left(\sqrt{|D|m}\right)^{s+1}\sum_{c>0}c^{-s}\sum_{r|c}\left(\frac{D}{r}\right)H_{c/r}(m,0)\\ &= \left(\sqrt{|D|m}\right)^{s+1}\sum_{t>0}\sum_{r>0}(tr)^{-s}\left(\frac{D}{r}\right)H_t(m,0)\\ &= \left(\sqrt{|D|m}\right)^{s+1}L_D(s)\sum_{t>0}t^{-s}H_t(m,0).\end{aligned}$$

Comparing the series on the right-hand side to the coefficient $c_m(0,s)$ of the Niebur Poincaré series $F_m(\tau,s)$ from Proposition 2.1, and using (2.2), we get

$$\begin{aligned}\mathrm{tr}_{m,D}(E_0(\,\cdot\,,s)) &= \left(\sqrt{|D|m}\right)^{s+1}L_D(s)\frac{s\Gamma(\frac{s+1}{2})}{4\pi^{\frac{s+3}{2}}m^{\frac{s+1}{2}}}c_m(0,\tfrac{s+1}{2})\\ &= \left(\sqrt{|D|m}\right)^{s+1}L_D(s)\frac{s\Gamma(\frac{s+1}{2})}{4\pi^{\frac{s+3}{2}}m^{\frac{s+1}{2}}}\frac{4\pi}{s}\frac{m^{\frac{1-s}{2}}\sigma_s(m)}{\pi^{-\frac{s+1}{2}}\Gamma(\frac{s+1}{2})\zeta(s+1)}\\ &= \frac{|D|^{\frac{s+1}{2}}L_D(s)}{\zeta(s+1)}m^{\frac{1-s}{2}}\sigma_s(m).\end{aligned}$$

This proves the stated formula. At $s=1$ using Dirichlet's class number formula, $L_D(1) = \frac{2\pi h(D)}{\sqrt{|D|}w(D)}$ and $\zeta(2)=\frac{\pi^2}{6}$ we complete the proof of Theorem 1.12.

6. Generating function over ν - Proof of Theorem 1.10

Corollary 1.6 gives the modularity of the generating function for the twisted traces $\mathrm{tr}_{m,D}(J_\nu)$ when summed over m, for fixed $\nu\in\mathfrak{d}_D^{-1}$ with $\nu\neq 0$. Instead in this section we fix m, and summing over ν we prove Theorem 1.10, which gives a weight 2 automorphic form $\mathcal{F}_{m,D} = (\mathcal{F}^{(2)}_{m,D},\mathcal{F}^{(1)}_{m,D},\mathcal{F}^{(0)}_{m,D})^t$ on $\mathbb{H}^3\setminus T_{m,D}$, whose Fourier coefficients are given in terms of $\mathrm{tr}_{m,D}(J_\nu)$.

We start by recalling the construction of the automorphic Green's function for Γ. It is defined by[1]

$$G_s(P_1, P_2) = \pi \sum_{\gamma\in\Gamma} \varphi_s\big(\cosh(d(P_1, \gamma P_2))\big),$$

for $P_1, P_2 \in \mathbb{H}^3, P_1 \not\equiv P_2 \pmod \Gamma$ and $s \in \mathbb{C}$ with $\mathrm{Re}(s) > 1$. Here

$$\varphi_s(t) = \left(t + \sqrt{t^2-1}\right)^{-s} (t^2-1)^{-1/2} \qquad \text{for } t > 1.$$

The Green's function is Γ-invariant in each variable and symmetric in P_1, P_2. It defines a smooth function on $(\Gamma\backslash\mathbb{H}^3) \times (\Gamma\backslash\mathbb{H}^3)$ away from the diagonal, with a singularity of the form

$$G_s(P, Q) = \frac{\pi|\Gamma_Q|}{d(P, Q)} + O_Q(1) \text{ as } P \to Q,$$

where $d(\cdot, \cdot)$ denotes the hyperbolic distance. Moreover, it satisfies

$$(\Delta_{P_1} - (1-s^2))G_s(P_1, P_2) = 0.$$

As a function of s it has meromorphic continuation to $\mathbb{C}$ with $s = 1$ a simple pole with constant residue (independent of P_1 and P_2).

The Fourier expansion of the Green's function in the variable $P_2 = z_2 + r_2 j$, for $r_2 > r(\gamma P_1)$ for all $\gamma \in \Gamma$, is given by

$$G_s(P_1, P_2) = \frac{4\pi^2}{\sqrt{|D|}}\left(\frac{r_2^{1-s}}{s}E_0(P_1, s) + \frac{1}{\pi}\sum_{\substack{\nu\in\mathfrak{d}_D^{-1}\\ \nu\neq 0}} F_{-\nu}(P_1, s)|\nu|^{-1} r_2 K_s(4\pi|\nu|r_2)e(\mathrm{tr}(\nu z_2))\right).$$

This Fourier expansion has analytic continuation to $\mathrm{Re}(s) > \frac{1}{2}, s \neq 1$. See [5] and [9] for proofs.

It follows from the properties of the Green's function described above that the function

$$\mathcal{L}_{m,D}(P) = \lim_{s\to 1} \mathrm{tr}_{m,D}\left(\frac{\sqrt{|D|}}{4\pi}G_s(\cdot, P) - \frac{\pi r(P)^{1-s}}{s}E_0(\cdot, s)\right),$$

for $P \in \mathbb{H}^3 \setminus T_{m,D}$, is Γ-invariant, harmonic, and has Fourier expansion

$$\mathcal{L}_{m,D}(z + rj) = \sum_{\substack{\nu\in\mathfrak{d}_D^{-1}\\ \nu\neq 0}} \mathrm{tr}_{m,D}(J_\nu)|\nu|^{-1} r K_1(4\pi|\nu|r)e(\mathrm{tr}(\nu z)), \tag{6.1}$$

valid when $r > r(Q)$ for all $Q \in T_{m,D}$ (in particular, when $r > \sqrt{m|D|}$). Finally, by [6, Proposition 1.2], the function $\mathfrak{D}_0\mathcal{L}_{m,D}$, where $\mathfrak{D}_0$ denotes the raising operator

$$\mathfrak{D}_0 = \frac{1}{2\pi i}(-\partial_z, \partial_r, \partial_{\overline{z}})^t,$$

is a smooth automorphic form of weight 2 for Γ on $\mathbb{H}^3 \setminus T_{m,D}$. Finally, applying $\mathfrak{D}_0$ to (6.1), using the identity

$$\frac{\partial}{\partial y}K_1(y) = -K_0 - \frac{1}{y}K_1(y)$$

(see, e.g., [7, Formula 8.472(1)]) and comparing the result with (1.3), we conclude that $\mathcal{F}_{m,D} = \mathfrak{D}_0\mathcal{L}_{m,D}$. This proves Theorem 1.10.

[1] Here we follow [8] where we used a different normalization than [5] and [9].

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