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Exotic approximate identities and Maass forms

by

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1. Introduction. There are many approximate identities coming from the theory of modular forms. Probably the most known is the result that the so-called Ramanujan constant $e^{\pi\sqrt{163}}$ differs from $744 + 640320^3$ by less than 10^{-12}.

The common point in most of these approximate identities, when appearing in number theory, is that they exploit a rapidly converging Fourier expansion of a quantity with some arithmetical meaning. In the case of Ramanujan constant (which, by the way, is due to Hermite and does not appear in Ramanujan's work, although there are some allied quantities in [14]), what is employed is the Fourier expansions of the j-invariant and the interpretation of special values of j as roots of the class equation (see [7] for a self-contained explanation). The integral approximation of the Ramanujan constant corresponds to taking two terms in the Fourier expansion.

We obtain here some approximate identities that are "exotic" in the sense that they are not associated to the Euclidean harmonic analysis but to the spectral resolution of the Laplace–Beltrami operator on Riemann surfaces (spectral theory of automorphic forms). The arithmetical quantities to be expanded here are series involving the number of representations as a sum of two squares. In comparison with the approximations derived from classical Fourier expansions, the role of positive integers is played by the discrete spectrum. The continuous spectrum, when it exists, contributes as a finite sum of integral terms.

To catch a glimpse of our approximate identities, we mention here two examples.

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Consider the series (that can be seen as a special value of the L-function associated to a shifted convolution) and the integral given by

$$S=\sum_{n=0}^{\infty}(3+(-1)^n)\frac{r(n)r(n+4)}{2(n+4)^2}\quad\text{and}\quad I=\int_{-\infty}^{\infty}\frac{1/4+t^2}{\cosh(\pi t)}|f(t)|^2\,dt,$$

where $r(n)=\#\{(a,b)\in\mathbb{Z}^2 : a^2+b^2=n\}$ and $f(t)=\zeta(s)L(s,\chi)/\zeta(2s)$, $s=1/2+it$, with $L(s,\chi)$ the Dirichlet L-function for the non-principal character χ modulo 4 (note that f is easily related to the Epstein zeta function for x^2+y^2). There are efficient numerical methods to approximate $f(t)$ (see for instance [5]) and I. Using several millions of terms in S one can check that

$$\frac{S-3}{I}=3.141592\ldots.$$

We shall prove that this number is not π but exceeds π by an amount less than $4\cdot 10^{-14}$. This accuracy is related to the size of the third eigenvalue of the Laplace–Beltrami operator on $\mathrm{PSL}_2(\mathbb{Z})\backslash\mathbb{H}$ and to a special value of the corresponding eigenfunction. In fact this is a two-sided relation: the value of $\pi-(S-3)/I$ gives an approximation for a certain expression involving these spectral quantities.

Our second example is the series

$$S=\sum_{n=1}^{\infty}r(n)r(3n+2)\sqrt{n}\,e^{-(\log(n)/4)^2}.$$

It turns out that S is very close to $72e^9\sqrt{\pi}$. In fact we shall prove that the relative error is not zero but is less than $3\cdot 10^{-7}$. This figure is related to the size of the first non-trivial eigenvalue of the Laplace–Beltrami operator on the simplest Shimura curve, $X(6,1)$ in the notation of [1], the one corresponding to a quaternion algebra with smallest discriminant. By an instance of Jacquet–Langlands correspondence that is explicit in this case (see [3], [15] and [11]), and is the same as the smallest eigenvalue for $\Gamma_0(6)\backslash\mathbb{H}$.

2. Some auxiliary results. We start by giving a brief overview of the spectral theory of automorphic forms to fix some notation. For more details, see [12]. We consider the Poincaré half-plane, i.e., the upper complex half-plane, $\mathbb{H}$, endowed with the metric $ds=y^{-2}(dx^2+dy^2)$. The induced distance ρ is given implicitly by $\cosh\rho(z,w)=1+2u(z,w)$, where

$$u(z,w)=\frac{|z-w|^2}{4\Im z\Im w}.$$

The usual group action of $G=\mathrm{SL}_2(\mathbb{R})$ on $\mathbb{H}$ gives rise to all the direct isometries of the Poincaré half-plane. This action is not faithful, so we will often think of G as $\mathrm{PSL}_2(\mathbb{R})=\mathrm{SL}_2(\mathbb{R})/\{\pm I\}$. We also consider Fuchsian groups F that we assume to be of the first kind, i.e., discrete subgroups of G having the extended real line as limit set.

We can associate with every cusp $\mathfrak{a}$ (point at the infinity) of a Fuchsian group F a *scaling matrix*. This is an element $\sigma_{\mathfrak{a}}$ of G such that $\sigma_{\mathfrak{a}}\infty = \mathfrak{a}$ and $\sigma_{\mathfrak{a}} F_{\mathfrak{a}} \sigma_{\mathfrak{a}}^{-1}$ is generated by the unit translation, where $F_{\mathfrak{a}} = \{g \in F : g\mathfrak{a} = \mathfrak{a}\}$.

Given a function $k : [0, \infty) \to \mathbb{C}$, and a Fuchsian group F acting on $\mathbb{H}$, we define the *automorphic kernel*

$$K(z, w) = \sum_{g \in F} k(u(gz, w)).$$

Under suitable regularity and decay conditions on k (as in [12, (1.63)]), which we implicitly assume along this paper, the previous definition makes sense and the spectral resolution of the Laplace–Beltrami operator $\Delta = y^2(\partial_x^2 + \partial_y^2)$ gives the spectral expansion of automorphic kernels

$$K(z, w) = \sum_{j=0}^{\infty} h(t_j) u_j(z) \overline{u_j(w)} + \frac{1}{4\pi} \sum_{\mathfrak{a}} \int_{-\infty}^{\infty} h(t) E_{\mathfrak{a}}(z, 1/2 + it) \overline{E_{\mathfrak{a}}(w, 1/2 + it)}\, dt, \tag{2.1}$$

where h is the *Selberg transform* of the function k,

$$h(t) = \int_0^{\infty} \int_{-\infty}^{\infty} k\left(\frac{x^2 + (y-1)^2}{4y}\right) y^{-3/2+it}\, dx\, dy;$$

$u_j(z)$ are the normalized Maass cusp forms with ordered eigenvalues $\lambda_j = -(1/4 + t_j^2)$ completed with the constant function u_0; and $E_{\mathfrak{a}}(z, s)$ are the Eisenstein series associated with the cusps $\mathfrak{a}$ of F. These series are defined for $s \in \mathbb{C}$ with $\Re s > 1$ as the analytic continuation of

$$E_{\mathfrak{a}}(z, s) = \sum_{g \in F_{\mathfrak{a}} \backslash F} (\Im \sigma_{\mathfrak{a}}^{-1} g z)^s.$$

If F has no cusps (in this case F is said to be co-compact), the last term in the spectral expansion does not appear (it is an empty sum). Typically, the main term in (2.1) comes from the constant eigenfunction $u_0(z) = |F\backslash\mathbb{H}|^{-1/2}$, where $|F\backslash\mathbb{H}|$ is the area of the fundamental domain of F. Note that the eigenfunctions u_j and the eigenpackets $E_{\mathfrak{a}}$ depend strongly on F; consequently, so does (2.1).

In the rest of the section, we focus on the Selberg transform. It is a kind of hyperbolic analogue of the Fourier transform. Firstly, we state two general results.

Lemma 2.1. *We have* $h(i/2) = 4\pi \int_0^{\infty} k(x)\, dx$.

Proof. The result follows from the equalities

$$h(i/2) = \int_{\mathbb{H}} k(u(i,z))\,d\mu(z) = 4\int_0^\infty\int_0^\pi k(u)\,du\,d\varphi = 4\pi\int_0^\infty k(u)\,du,$$

where we have employed hyperbolic polar coordinates (u,φ) (see [12, §1.3]). ∎

Given two functions k_1 and k_2, we define their *hyperbolic convolution*, $k_1 * k_2$, as

$$(k_1 * k_2)(u(z,w)) = \int_{\mathbb{H}} k_1(u(z,v))k_2(u(v,w))\,d\mu(v).$$

Note that the integral depends only on $u(z,w)$ because $z \mapsto gz$, $w \mapsto gw$ with $g \in G$ leaves it invariant.

LEMMA 2.2. *If h_1 and h_2 are the Selberg transforms of k_1 and k_2, then their product h_1h_2 is the Selberg transform of $k_1 * k_2$.*

Proof. A basic result (the Fundamental Lemma 5.1 in [10]) asserts that for any eigenfunction $\phi(z)$ of the Laplace–Beltrami operator, we have

$$\int_{\mathbb{H}} k(u(z,w))\phi(z)\,d\mu(z) = h(t)\phi(w).$$

The proof reduces to a double application of this formula for $\phi(z) = (\Im z)^s$:

$$\begin{aligned}
&\int_{\mathbb{H}} (k_1 * k_2)(u(z,i))\,d\mu(z)\\
&\qquad = \int_{\mathbb{H}} k_2(u(v,i))\Big(\int_{\mathbb{H}} k_1(u(z,v))(\Im z)^{1/2+it}\,d\mu(z)\Big)\,d\mu(v)\\
&\qquad = \int_{\mathbb{H}} k_2(u(v,i))(h_1(t)\cdot(\Im v)^{1/2+it})\,d\mu(v) = h_1(t)h_2(t).
\end{aligned}$$

Of course we implicitly assume that the regularity of k_1 and k_2 ensures the convergence of the integrals. ∎

To get accurate approximate identities from (2.1), we are specially interested in rapidly decreasing Selberg transforms. Due to the involved formula defining this transform, it is not easy to find examples giving explicit results.

LEMMA 2.3. *Let $\mu \in \mathbb{C}$ be a constant with $\Re\mu > 1$. Then the Selberg transform of $k(u) = (u+1)^{-\mu}$ is*

$$h(t) = \frac{4\pi}{\Gamma^2(\mu)}\Gamma(\mu - 1/2 + it)\Gamma(\mu - 1/2 - it).$$

In particular,

$$h(t) = \frac{4\pi^2}{(\mu-1)!^2\cosh(\pi t)}\prod_{n=1}^{\mu-1}((n-1/2)^2 + t^2) \qquad \text{if } \mu \in \mathbb{Z},\ \mu > 1,$$

and

$$h(t) = \frac{(\mu-3/2)!^2 4^{2\mu-1}\pi t}{(2\mu-2)!^2\sinh(\pi t)} \prod_{n=1}^{\mu-3/2}(n^2+t^2) \qquad \textit{if } \mu - 1/2 \in \mathbb{Z},\ \mu > 1.$$

Proof. By the definition of the Selberg transform and the change of variables $x \mapsto (y+1)\sqrt{x}$ we have

$$\begin{aligned} h(t) &= 2\int_0^\infty\int_0^\infty \left(\frac{x^2+(y-1)^2}{4y}+1\right)^{-\mu} y^{-3/2+it}\,dx\,dy \\ &= 4^\mu \int_0^\infty \frac{y^{\mu-3/2+it}}{(1+y)^{2\mu-1}} \int_0^\infty \frac{x^{-1/2}}{(1+x)^\mu}\,dx\,dy \\ &= 4^\mu B(1/2,\mu-1/2)B(\mu-1/2+it,\mu-1/2-it), \end{aligned}$$

where B is the classical Beta function that admits the integral representation

$$B(z_1,z_2) = \int_0^\infty \frac{u^{z_2-1}}{(1+u)^{z_1+z_2}}\,du$$

and satisfies $\Gamma(z_1)\Gamma(z_2) = \Gamma(z_1+z_2)B(z_1,z_2)$. Using this relationship as well as the duplication formula for the Gamma function we obtain the result.

The well-known formulas

$$|\Gamma(1/2+it)|^2 = \frac{\pi}{\cosh(\pi t)}, \qquad |\Gamma(1+it)|^2 = \frac{\pi t}{\sinh(\pi t)},$$
$$\Gamma(n+1/2) = \frac{(2n-1)!}{2^{n-1}(n-1)!}\sqrt{\pi}$$

give the particular expressions for μ integral and half-integral. ∎

LEMMA 2.4. *The Selberg transform of $k(u) = e^{-\mu u}$, with $\mu > 0$, is $4e^{\mu/2}\sqrt{\pi/\mu}\,K_{it}(\mu/2)$, where $K_\nu(z)$ is the modified Bessel function of the second kind.*

Proof. Manipulating the definition shows that

$$\begin{aligned} h(t) &= \int_0^\infty e^{-\mu(y-1)^2/4y}\Big(\int_{-\infty}^\infty e^{-\mu x^2/4y}\,dx\Big)y^{-3/2+it}\,dy \\ &= (4\pi e^\mu)^{1/2}\mu^{-1/2}\int_0^\infty e^{\frac{\mu}{4}(y+1/y)}y^{-1+it}\,dy \end{aligned}$$

and, by the integral representation (see [9, §8])

$$K_\nu(z) = \frac{1}{2}\int_0^\infty e^{-\frac{z}{2}(t+1/t)}t^{-\nu-1}\,dt,$$

the result follows. ∎

Lemma 2.5. *For $\alpha, \beta > 0$, the Selberg transform of*

$$k(u) = \frac{\sqrt{\alpha\beta}}{4\sqrt{(\alpha+\beta)^2 + 4\alpha\beta u}}\, e^{-\sqrt{(\alpha+\beta)^2+4\alpha\beta u}}$$

is $K_{it}(\alpha)K_{it}(\beta)$.

Proof. For $\mu > 0$, let us define $k_\mu(u) = \sqrt{\mu/(8\pi)}\, e^{-\mu(1+2u)}$. Using the previous lemma, the Selberg transform of this function is $K_{it}(\mu)$. So, according to Lemma 2.2, we just have to prove that $(k_\alpha * k_\beta)(u) = k(u)$. As both sides are $\mathrm{SL}_2(\mathbb{R})$ point-pair invariant, we can restrict ourselves to the points $z = i$ and $w = \lambda i$ for some $\lambda > 0$. Then $u(z,w) = (\lambda-1)^2/4\lambda$, and we have

$$\begin{aligned}(k_\alpha * k_\beta)&(u(w,z))\\ &= \frac{\sqrt{\alpha\beta}}{8\pi e^{\alpha+\beta}} \int_0^\infty \Big(\int_{-\infty}^{\infty} e^{-(\alpha/\lambda+\beta)x^2/2y}\, dx\Big) e^{-(\alpha(y-\lambda)^2/\lambda+\beta(y-1)^2)/2y} y^{-2}\, dy\\ &= \frac{\sqrt{2\pi\alpha\beta}}{8\pi\sqrt{\alpha/\lambda+\beta}} \int_0^\infty e^{-(\alpha/\lambda+\beta)y/2-(\beta+\alpha\lambda)/2y} y^{-3/2}\, dy\\ &= \frac{\sqrt{\alpha\beta}}{4\sqrt{(\alpha/\lambda+\beta)(\beta+\alpha\lambda)}}\, e^{\sqrt{(\alpha/\lambda+\beta)(\beta+\alpha\lambda)}}.\end{aligned}$$

The last integral can be expressed as $K_{1/2}(z)$, which is the elementary function $e^{-z}\sqrt{\pi/2z}$ (see for instance [9, §8]). ∎

Lemma 2.6. *The Selberg transform of $k(u) = u^{-2}((1+2/u)\log(1+u)-2)$, with $k(0)$ defined by continuity as $k(0) = 1/6$, is*

$$h(t) = 2\pi^3\Big(\frac{1/4+t^2}{\cosh(\pi t)}\Big)^2.$$

Note that $k(u)$ is the derivative of $u^{-2}(u-(1+u)\log(1+u))$.

Proof of Lemma 2.6. By Lemmas 2.2 and 2.3, the Selberg transform of $(u+1)^{-2} * (u+1)^{-2}$ is exactly $8\pi h(t)$. Then it is enough to check

$$8\pi k(u(z,w)) = \int_{\mathbb{H}} (u(z,v)+1)^{-2}(u(v,w)+1)^{-2}\, d\mu(v). \tag{2.2}$$

As in the previous proof, we can restrict ourselves to $z = i$ and $w = (2c+1)i$, with $c > -1/2$. With this choice, $u(z,w) = c^2/(2c+1)^2$ and

$$k(u(z,w)) = \frac{(2c+1)^2}{c^4}\Big(\frac{c^2+4c+2}{c^2}\log\frac{(c+1)^2}{2c+1} - 2\Big).$$

On the other hand, the integral in (2.2) is

$$I = 256(2c+1)^2 \int_0^\infty y^2 J(y+1, y+2c+1)\,dy,$$

where

$$J(A,B) = \int_{-\infty}^{\infty} \frac{dx}{(x^2+A^2)^2(x^2+B^2)^2} = \frac{\pi}{2}\,\frac{A^2+3AB+B^2}{A^3B^3(A+B)^3}.$$

The change of variables $y \mapsto y-c-1$ gives

$$I = 16\pi(2c+1)^2 \int_{c+1}^{\infty} \frac{(5y^2-c^2)(y-c-1)^2}{y^3(y^2-c^2)^3}\,dy.$$

Evaluating this rational integral, we obtain the same expression as that for $8\pi k(u(z,w))$, and (2.2) is proved. ■

3. The non-compact case. The most conspicuous examples of Fuchsian groups are the full modular group, $\Gamma = \mathrm{PSL}_2(\mathbb{Z})$, and the congruence modular group $\Gamma_0(N)$. It will be convenient here to consider also $\widetilde{\Gamma}$, defined as the subgroup of Γ such that $a_{11}+a_{22}$ and $a_{12}+a_{21}$ are both even. It is easy to see that actually $\widetilde{\Gamma}$ is a conjugate of $\Gamma_0(2)$, namely

$$\widetilde{\Gamma} = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}^{-1} \Gamma_0(2) \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} / \{\pm \mathrm{Id}\}.$$

A special feature of Γ and $\widetilde{\Gamma}$ is that the automorphic kernels have a rather direct arithmetic interpretation and (2.1) provides a kind of Fourier expansion for these arithmetical quantities.

PROPOSITION 3.1. *We have the spectral expansions*

(a) $$\sum_{n=0}^{\infty} r(n)r(n+1)k(n) = 8\int_0^\infty k(x)\,dx + 2\sum_{j=1}^{\infty} h(\widetilde{t}_j)|u_j(i)|^2 + \frac{4}{\pi}\int_{-\infty}^{\infty} h(t)\left|\frac{f(t)}{1+2^{1/2+it}}\right|^2 dt,$$

(b) $$\sum_{n=0}^{\infty} (3+(-1)^n) r(n)r(n+4)k(n/4) = 96\int_0^\infty k(x)\,dx + 8\sum_{j=1}^{\infty} h(t_j)|u_j(i)|^2 + \frac{8}{\pi}\int_{-\infty}^{\infty} h(t)|f(t)|^2\,dt,$$

where h is the Selberg transform of k, $f(t) = \zeta(s)L(s,\chi)/\zeta(2s)$ with $s = 1/2+it$, and $1/4+\widetilde{t}_j^2$ and $1/4+t_j^2$ are the non-trivial eigenvalues for $\widetilde{\Gamma}\backslash\mathbb{H}$ and $\Gamma\backslash\mathbb{H}$, respectively.

For the proof we need two summation formulas (cf. [12, §12]) and an explicit description of the Eisenstein series for Γ and $\widetilde{\Gamma}$.

LEMMA 3.2. *We have the identities*

(a) $2\sum_{\gamma\in\widetilde{\Gamma}} k(u(\gamma i,i)) = \sum_{n=0}^{\infty} r(n)r(n+1)k(n)$,

(b) $8\sum_{\gamma\in\Gamma} k(u(\gamma i,i)) = \sum_{n=0}^{\infty}(3+(-1)^n)r(n)r(n+4)k(n/4)$.

LEMMA 3.3. *Let E be the Eisenstein series of Γ and $E_{\mathfrak{a}}$, $E_{\mathfrak{b}}$ the ones corresponding to the cusps $\mathfrak{a}=\infty$ and $\mathfrak{b}=1$ of $\widetilde{\Gamma}$. Then*

$$E(i,s) = (2^s+1)E_{\mathfrak{a}}(i,s) = (2^s+1)E_{\mathfrak{b}}(i,s) = \frac{2\zeta(s)L(s,\chi)}{\zeta(2s)}, \tag{3.1}$$

where χ is the non-principal character modulo 4.

Proof of Lemma 3.2. Let $\gamma=(a_{ij})\in G$. Then

$$\begin{cases} 4u(\gamma i,i) = (a_{11}-a_{22})^2+(a_{12}+a_{21})^2, \\ 4u(\gamma i,i)+4 = (a_{11}+a_{22})^2+(a_{12}-a_{21})^2. \end{cases} \tag{3.2}$$

If $\gamma\in\widetilde{\Gamma}$ these quantities are multiples of 4, say $4n$ and $4n+4$, and recalling that $r(n)=r(4n)$ we derive (a).

For $\gamma\in\Gamma$, if $n=4u(\gamma i,i)$ satisfies $n\equiv 1 \pmod 4$ then the squares in each equation of (3.2) have different parity, and a choice of the parity of the squares in the first equation forces a fixed ordering in the second, contributing $\frac{1}{2}r(n)r(n+4)$ to the total number of solutions. If $n\equiv 0,2 \pmod 4$ then they have the same parity and we obtain $r(n)r(n+4)$ solutions. Hence

$$2\sum_{\gamma\in\Gamma} k(u(\gamma i,i)) = \frac{1}{2}\sum_{n\equiv 1\,(4)}^{\infty} r(n)r(n+4)k(n/4) + \sum_{n\not\equiv 1\,(4)}^{\infty} r(n)r(n+4)k(n/4).$$

Noting that $r(n)=0$ for $n\equiv 3 \pmod 4$, we get (b). ∎

Proof of Lemma 3.3. Taking $z=i$ in the definition of the Eisenstein series yields

$$E(i,s) = \sum_{\gamma\in\Gamma_\infty\backslash\Gamma} \frac{(\Im i)^s}{|j_{\sigma_\infty^{-1}\gamma}(i)|^{2s}} = \frac{1}{2}\sum_{\substack{c,d=-\infty\\(c,d)=1}}^{\infty} \frac{1}{(c^2+d^2)^s} = \frac{1}{2\zeta(2s)}\sum_{n=1}^{\infty}\frac{r(n)}{n^s},$$

where $r(n)$, the number of representations of n as sum of two squares, satisfies $\frac{1}{4}r(n) = 1*\chi(n)$, and this gives the equality between the extremes of (3.1) that is classical. In the case of the group $\widetilde{\Gamma}$, the scaling matrices are

$$\sigma_{\mathfrak{a}} = \begin{pmatrix}\sqrt{2} & 0\\ 0 & 1/\sqrt{2}\end{pmatrix}, \qquad \sigma_{\mathfrak{b}} = \begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix};$$

they give rise to the same conjugate groups:

$$\sigma_{\mathfrak{a}}^{-1}\widetilde{\Gamma}\sigma_{\mathfrak{a}} = \left\{\begin{pmatrix} * & * \\ 2n & m \end{pmatrix} \in \Gamma\right\} = \sigma_{\mathfrak{b}}^{-1}\widetilde{\Gamma}\sigma_{\mathfrak{b}}.$$

Therefore

$$\begin{aligned} E_{\mathfrak{a}}(i,s) &= \sum_{g\in\widetilde{\Gamma}_{\mathfrak{a}}\backslash\widetilde{\Gamma}} (\Im\sigma_{\mathfrak{a}}^{-1}gi)^s = \sum_{\gamma\in\Gamma_\infty\backslash\sigma_{\mathfrak{a}}^{-1}\widetilde{\Gamma}\sigma_{\mathfrak{a}}} (\Im\gamma\sigma_{\mathfrak{a}}^{-1}i)^s \\ &= \frac{1}{2^{s+1}} \sum_{\substack{m,n\in\mathbb{Z} \\ (m,n)=1,\, 2\nmid m-n}} \frac{1}{(m^2+n^2)^s}, \end{aligned}$$

and the same result is obtained for the corresponding series associated to the cusp $\mathfrak{b}$ of $\widetilde{\Gamma}$ using similar arguments. Further

$$\begin{aligned} &2(2^s+1)E_{\mathfrak{a}}(i,s) \\ &= \sum_{\substack{m,n=-\infty \\ (m,n)=1,\, 2\nmid m-n}}^{\infty} \frac{1}{(m^2+n^2)^s} + \sum_{\substack{m,n=-\infty \\ (m,n)=1,\, 2\mid m-n}}^{\infty} \frac{1}{(m^2+n^2)^s} = 2E(i,s), \end{aligned}$$

and we obtain the expected result. ∎

Proof of Proposition 3.1. Substitute the previous lemmas into the spectral expansion of automorphic kernels (2.1). The contribution of the trivial eigenvalue is evaluated using Lemma 2.1, and taking into account that $|\Gamma\backslash\mathbb{H}| = \pi/3$ and $|\widetilde{\Gamma}\backslash\mathbb{H}| = \pi$. ∎

Taking $k(u) = (u+1)^{-m}$ in Proposition 3.1, with m an integer greater than 1, we obtain approximations of π whose accuracy depends on spectral quantities. Consider

$$s_m = \sum_{n=0}^{\infty}(3+(-1)^n)\frac{r(n)r(n+4)}{2(n+4)^m} \quad\text{and}\quad \widetilde{s}_m = \sum_{n=0}^{\infty}\frac{r(n)r(n+1)}{(n+1)^m}.$$

Consider also the integrals

$$\gamma_m = \int_{-\infty}^{\infty} g_m(t)|f(t)|^2\,dt \quad\text{and}\quad \widetilde{\gamma}_m = \int_{-\infty}^{\infty} g_m(t)\left|\frac{f(t)}{1+2^{1/2+it}}\right|^2 dt,$$

where

$$g_m(t) = \operatorname{sech}(\pi t)\prod_{j=1}^{m-1}((j-1/2)^2+t^2),$$

and $f(t)$ is as in Proposition 3.1. We define

$$e_m = (m-1)!^2\,\frac{2^{2m-4}(m-1)s_m - 3}{(m-1)\gamma_m} - \pi, \qquad \widetilde{e}_m = (m-1)!^2\,\frac{(m-1)\widetilde{s}_m - 8}{16(m-1)\widetilde{\gamma}_m} - \pi.$$

We show that these errors when approximating π can be theoretically estimated thanks to a recurrence formula involving a certain eigenvalue (and implicitly the symmetries of the Maass forms).

THEOREM 3.4. *For any integer $m > 1$,*

$$0 < e_m < \frac{\gamma_{m+1}}{((m-1/2)^2 + t_3^2)\gamma_m} e_{m+1},$$

where $\lambda_3 = 1/4 + t_3^2$, with $t_3 = 13.77975\ldots$, is the third non-trivial eigenvalue in $\Gamma\backslash\mathbb{H}$.

Proof. Using Proposition 3.1(a), with $k_m(u) = 4^{-m}(u+1)^{-m}$, and recalling Lemmas 2.3 and 2.1, we have

$$s_m = \frac{48}{4^m(m-1)} + 4\sum_{j=1}^{\infty} h_m(t_j)|u_j(i)|^2 + \frac{4\pi}{4^{m-1}(m-1)!^2}\int_{-\infty}^{\infty} g_m(t)|f(t)|^2\,dt,$$

where we have used the fact that the area of the fundamental domain of Γ is $\pi/3$. We have got an expression for the error term

$$e_m = \frac{4^{m-2}(m-1)s_m - 3}{(m-1)\gamma_m}(m-1)!^2 - \pi = \frac{\pi^2}{\gamma_m}\sum_{j=1}^{\infty} g_m(t_j)|u_j(i)|^2, \tag{3.3}$$

which is positive because $u_j(i) \neq 0$ infinitely often (in fact it is known that the set of these values is unbounded [12, §13.2]). Hence, using $g_{m+1}(t) = ((m-1/2)^2 + t^2)g_m(t)$, we see that

$$\frac{e_m}{e_{m+1}} = \frac{\gamma_{m+1}\sum_{j=1}^{\infty} g_m(t_j)|u_j(i)|^2}{\gamma_m \sum_{j=1}^{\infty} g_{m+1}(t_j)|u_j(i)|^2} \le \frac{\gamma_{m+1}/\gamma_m}{(m-1/2)^2 + t_3^2},$$

where we have taken into account that u_1 and u_2 are odd eigenfunctions so that $u_j(i) = 0$, while $\lambda_3 = 1/4 + t_3^2$ with $t_3 = 13.77975\ldots$ corresponds to an even eigenfunction [4]. ∎

THEOREM 3.5. *For any integer $m > 1$,*

$$0 < \widetilde{e}_m < \frac{\widetilde{\gamma}_{m+1}}{((m-1/2)^2 + \widetilde{t}_1^2)\widetilde{\gamma}_m} \widetilde{e}_{m+1},$$

where $\widetilde{\lambda}_1 = 1/4 + \widetilde{t}_1^2$, with $\widetilde{t}_1 = 8.92287\ldots$, is the smallest non-trivial eigenvalue in $\widetilde{\Gamma}\backslash\mathbb{H}$.

Proof. The proof is similar to that of Theorem 3.4, but in this case $k_m(u) = (u+1)^{-m}$ and the area of the fundamental domain of $\widetilde{\Gamma}$ is π. This gives

$$\widetilde{s}_m = \frac{8}{m-1} + 2\sum_{j=1}^{\infty} h_m(\widetilde{t}_j)|u_j(i)|^2 + \frac{16\pi}{(m-1)!^2}\int_{-\infty}^{\infty} g_m(t)\left|\frac{f(t)}{1+2^{1/2+it}}\right|^2 dt$$

and we obtain

$$\widetilde{e}_m = \frac{\pi^2}{2\widetilde{\gamma}_m}\sum_{j=1}^{\infty} g_m(\widetilde{t}_j)|u_j(i)|^2 > 0, \qquad \frac{\widetilde{e}_m}{\widetilde{e}_{m+1}} \le \frac{\widetilde{\gamma}_{m+1}/\widetilde{\gamma}_m}{(m-1/2)^2+\widetilde{t}_1^2}$$

proceeding as in the previous case. ∎

Numerical analysis and examples in the non-compact case. If we think of $u_j(z)$ as essentially bounded [12, §13] in terms of the eigenvalue, then at first glance one can expect e_m to be comparable to $g_m(t_1)/\gamma_m$, but numerical calculations show a better approximation and a substantial difference between e_m and $\widetilde{e}_m$. For instance, the values for $m = 3, 4$, truncated to four decimal digits, are

$$e_3 = 2.0086\cdot 10^{-12}, \quad \widetilde{e}_3 = 7.2745\cdot 10^{-7},$$
$$e_4 = 4.9016\cdot 10^{-11}, \quad \widetilde{e}_4 = 6.7890\cdot 10^{-6}.$$

The explanation is that, as mentioned in the proof of Theorem 3.4, the first and the second non-trivial eigenvalues correspond in Γ to odd eigenfunctions so that $u_1(i) = u_2(i) = 0$, while $\lambda_3 = 1/4 + t_3^2$ with $t_3 = 13.77975\ldots$ comes from an even eigenfunction [4]. On the other hand, for $\widetilde{\Gamma}\backslash\mathbb{H}$ the first non-trivial eigenvalue $\widetilde{\lambda}_1$ corresponds to an even eigenfunction (see [8]). The large size of the quotient $\cosh(\pi t_3)/\cosh(\pi\widetilde{t}_1) = 4.23\cdot 10^6$ explains why the approximations of π are about 6 orders of magnitude worse.

Note also that g_m is increasing in m. Then we expect s_2 to give the best example to approximate π because for $m = 2$ we have the quickest decay of the spectral expansion. In principle the half-integral case $s_{3/2}$ would be even better, but actually it gives an approximate formula not involving π. In both cases, the convergence of the series is very slow and a direct computation is unfeasible to control the error term. With the previous analysis, a result in this direction can be deduced.

PROPOSITION 3.6. *Let e_m and s_m be as above. Then*

$$0 < e_2 < 3.62\cdot 10^{-14}, \qquad 0 < s_{3/2} - 12 - 8\int_{-\infty}^{\infty}\frac{t|f(t)|^2}{\sinh(\pi t)}\,dt < 1.55\cdot 10^{-15}.$$

Proof. The integrals γ_2 and γ_3 are quickly convergent and with numerical calculations we have $\gamma_2 = 0.23223\ldots$ and $\gamma_3 = 0.80239\ldots$. More extensive calculations give the value of e_3 mentioned before, and substituting these data in Theorem 3.4 with $m = 2$, we get the first part of the result.

For the second, note that Proposition 3.1(b) with $k(u) = (u+1)^{-3/2}$ reads

$$16 s_{3/2} = 192 + 128\pi\sum_{j=1}^{\infty}\frac{t_j}{\sinh(\pi t_j)}|u_j(i)|^2 + 128\int_{-\infty}^{\infty}\frac{t|f(t)|^2}{\sinh(\pi t)}\,dt.$$

The function $g(t) = t^{-1}(1/4+t^2)(9/4+t^2)\tanh(\pi t)$ is increasing for $t > t_3 = 13.77975$ and $u_1(i) = u_2(i) = 0$. Hence

$$0 < s_{3/2} - 12 - 8\int_{-\infty}^{\infty} \frac{t|f(t)|^2}{\sinh(\pi t)}\,dt < \frac{8\pi}{g(t_3)}\sum_{j=3}^{\infty}\frac{(1/4+t_j^2)(9/4+t_j^2)}{\cosh(\pi t_j)}|u_j(i)|^2.$$

The last sum equals $\gamma_3 e_3/\pi^2$ by (3.3). Substituting the numerical values of the quantities involved, we get the result. ∎

Theorems 3.4 and 3.5 also extend to the non-converging case $m = 1$ upon redefining $e_1 = s_1/4\gamma_1$ and $\widetilde{e}_1 = \widetilde{s}_1/16\widetilde{\gamma}_1$ where

$$s_1 = \sum_{n=0}^{\infty}\frac{(3+(-1)^n)r(n)r(n+4)-24}{2(n+4)}, \qquad \widetilde{s}_1 = \sum_{n=0}^{\infty}\frac{r(n)r(n+1)-8}{n+1},$$

which can be proved to converge.

We can use the same ideas with other kernels, for example,

$$\sum_{n=0}^{\infty} r(n)r(n+1)\,\frac{e^{1-\sqrt{n+1}}}{\sqrt{n+1}}.$$

The Selberg transform of $k(u) = e^{1-\sqrt{u+1}}/\sqrt{u+1}$ is $h(t) = 8eK_{it}^2(1/2)$ by Lemma 2.5 with $\alpha = \beta = 1/2$. Now, denoting the previous sum by S, we get

$$S = 64e\int_0^{\infty} k(x)\,dx + 16e\sum_{j=1}^{\infty} h(\widetilde{t}_j)|u_j(i)|^2 + \frac{32e}{\pi}\int_{-\infty}^{\infty} K_{it}^2(1/2)\left|\frac{f(t)}{1+2^{1/2+it}}\right|^2 dt.$$

Let I be the last integral. With some chiliads of terms in S and approximating I, one obtains

$$\frac{S-16}{32I} = 0.8652559794526\ldots,$$

which differs from e/π by less than $2.04\cdot 10^{-11}$.

It is also possible to prove approximate formulas associated to general congruence modular groups, but they have a less direct arithmetical interpretation.

Since the pioneering works of H. Maass and A. Selberg, there are many examples showing the influence of the eigenvalues associated to $\mathrm{PSL}_2(\mathbb{Z})$ or to congruence modular groups on some arithmetic quantities. A neat example [12, Th. 12.3], motivating some of our results, is the error term in the asymptotic formula

$$\sum_{n\le x} r(n)r(n+1) \sim 8x.$$

The novelty in this paper is to consider convergent series that approximate known constants in an extended setting that also covers co-compact examples.

4. The compact case. Let H be the indefinite quaternion algebra $\left(\frac{A,B}{\mathbb{Q}}\right)$ such that A and B are squarefree and $A > 0$. Then there is an embedding of H into $M_2(\mathbb{R})$, given by

$$\Phi(\lambda_1 + \lambda_2 i + \lambda_3 j + \lambda_4 k) = \begin{pmatrix} \lambda_1 + \lambda_2\sqrt{A} & \lambda_3 + \lambda_4\sqrt{A} \\ B(\lambda_3 - \lambda_4\sqrt{A}) & \lambda_1 - \lambda_2\sqrt{A} \end{pmatrix}.$$

By Th. 5.2.13 of [13], given an order $\mathcal{O} \subset H$, the image under Φ of the elements of norm one in $\mathcal{O}$ is a Fuchsian group of the first kind. Moreover, it is co-compact if H is a division algebra.

The spectrum of these groups coincides, under certain conditions, with the point spectrum of $\Gamma_0(N)$ with N depending on the discriminant and on the levels of the order [3], [11]. On the other hand, the Selberg trace formula proves that the eigenvalues for $\Gamma_0(N)$ cluster at the conjectural bottom of the spectrum $1/4$ when N grows [12, (11.18)]. Therefore, to get approximate formulas as before, it is advantageous to consider small discriminants and levels.

Following [1] (see specially Proposition 1.60), we consider the orders

$$\mathbb{Z}\Big[1, i, j, \frac{1}{2}(1+i+j+k)\Big] \subset \left(\frac{p,-1}{\mathbb{Q}}\right),$$
$$\mathbb{Z}\Big[1, i, \frac{1}{2}(1+j), \frac{1}{2}(i+k)\Big] \subset \left(\frac{2,q}{\mathbb{Q}}\right),$$

with $p \equiv 3 \pmod 4$ and $q \equiv 5 \pmod 8$ prime numbers, that correspond to the Shimura curves $X(2p, 1)$ and $X(2q, 1)$ in the notation of [1].

A calculation proves that the corresponding co-compact groups under the embedding Φ are, respectively,

$$G_p = \left\{ \frac{1}{2}\begin{pmatrix} a + b\sqrt{p} & c + d\sqrt{p} \\ -c + d\sqrt{p} & a - b\sqrt{p} \end{pmatrix} \in \mathrm{SL}_2(\mathbb{R}) : \\ a, b, c, d \in \mathbb{Z} \text{ with the same parity} \right\} / \{\pm \mathrm{Id}\}$$

and

$$G_{2,q} = \left\{ \frac{1}{2}\begin{pmatrix} a + b\sqrt{2} & c + d\sqrt{2} \\ q(c - d\sqrt{2}) & a - b\sqrt{2} \end{pmatrix} \in \mathrm{SL}_2(\mathbb{R}) : \\ a, b, c, d \in \mathbb{Z};\ a \equiv c,\ b \equiv d \pmod 2 \right\} / \{\pm \mathrm{Id}\}.$$

The spectral expansions resemble that of Γ but are neater because the integrals associated to the continuous spectrum do not appear.

Proposition 4.1. *For $p \equiv 3 \pmod 4$ and $q \equiv 5 \pmod 8$ prime numbers, the following spectral expansions hold:*

$$\sum_{n=0}^{\infty} r(n)r(pn+2)k(pn/2) = \frac{24}{p-1}\int_0^{\infty} k(x)\,dx + 2\sum_{j=1}^{\infty} h(t_j)|u_j(i)|^2,$$

$$\sum_{n=0}^{\infty} r_{2,q}(n)r_{1,2q}(n+4)k(n/4) = \frac{24}{q-1}\int_0^{\infty} k(x)\,dx + 2\sum_{j=1}^{\infty} h(t_j)|u_j(i/\sqrt{q})|^2,$$

where h is the Selberg transform of k, and $r_{s,t}(n)$ denotes the number of pairs $(a,b)\in\mathbb{Z}^2$ such that $n = sa^2+tb^2$.

For the proof we again need an arithmetic expression for automorphic kernels.

Lemma 4.2. *For p and q as above, we have*

$$2\sum_{\gamma\in G_p} k(u(\gamma i, i)) = \sum_{n=0}^{\infty} r(n)r(pn+2)k(pn/2),$$

$$2\sum_{\gamma\in G_{2,q}} k\big(u(\gamma(i/\sqrt{q}), i/\sqrt{q})\big) = \sum_{n=0}^{\infty} r_{2,q}(n)r_{1,2q}(n+4)k(n/4).$$

Proof. Note first that for $\gamma\in G_p$, $4u(\gamma i, i) = p(b^2+d^2)$. In addition, $\gamma\in \mathrm{SL}_2(\mathbb{R})$ implies $p(b^2+d^2)+4 = a^2+c^2$. Since a,b,c,d have the same parity, $2\,|\,b^2+d^2$. Moreover, this condition determines G_p up to the identification $\pm\gamma$. Hence

$$2\sum_{\gamma\in G_p} k(u(\gamma i, i)) = \sum_{n=0}^{\infty} r(2n)r(2pn+4)k(pn/2),$$

and, noting that $r(n) = r(2n)$, the proof of the first equality is concluded.

For the second, given n, note that the numbers of solutions $(a,b,c,d)\in\mathbb{Z}^4$ of

$$\begin{cases} n = 2b^2+qc^2,\\ n+4 = a^2+2qd^2\end{cases}$$

is $r_{2,q}(n)r_{1,2q}(n+4)$. It is clear that a and c have the same parity, and this implies that so do b and d. Then (a,b,c,d) gives rise to an element $\gamma\in G_{2,q}$ with $4u(\gamma(i/\sqrt{q}), i/\sqrt{q}) = 2b^2+qc^2$. Conversely, $\gamma\in G_{2,q}$ gives two solutions $\pm(a,b,c,d)$ of the previous equations with $n = 4u(\gamma(i/\sqrt{q}), i/\sqrt{q})$. ∎

Proof of Proposition 4.1. Use the previous lemma in the spectral expansion (2.1). Note that, according to [3, (2.1)], the area of the fundamental domain is $|G_p\backslash\mathbb{H}| = (p-1)\pi/3$ in the first case and $|G_{2,q}\backslash\mathbb{H}| = (q-1)\pi/3$ in the second. ∎

Numerical analysis and examples in the compact case. We illustrate Proposition 4.1 with an explicit example (mentioned in the introduction) in which numerical and theoretical arguments are combined to control the precision of the approximation. The underlying group is G_3, which is optimal in the sense that it has the largest spectral gap among the possible choices of p.

PROPOSITION 4.3. *Consider*

$$S = \sum_{n=1}^{\infty} r(n)r(3n+2)\sqrt{n}\, e^{-(\log(n)/4)^2}. \tag{4.1}$$

Then

$$1.29 \cdot 10^{-7} < 1 - \frac{S}{72e^9\sqrt{\pi}} < 3 \cdot 10^{-7}.$$

For the proof we shall employ an explicit upper bound for the hyperbolic circle problem (the spectral analysis gives asymptotic formulas but not explicit error terms [12, §12]).

LEMMA 4.4. *Let ρ be the distance on Poincaré's upper half-plane. Then*

$$\#\{\gamma \in G_3 : \rho(\gamma i, i) < R\} \le 3(2+\sqrt{3})\cosh R.$$

Proof. Let D be the fundamental domain of $G_3\backslash\mathbb{H}$. By Theorem 5.46 of [1], D is the polygon with vertices

$$v_1 = \frac{-\sqrt{3}+i}{2}, \quad v_2 = \frac{-1+i}{1+\sqrt{3}}, \quad v_3 = (2-\sqrt{3})i,$$
$$v_4 = \frac{1+i}{1+\sqrt{3}}, \quad v_5 = \frac{\sqrt{3}+i}{2}, \quad v_6 = i.$$

The distance from v_6 to any other vertex is at most $\cosh^{-1} 2$. Hence, $D \subset B(i, \cosh^{-1} 2)$, where $B(z_0, r) = \{z \in \mathbb{H} : \rho(z, z_0) \le r\}$. Let $\mathcal{A} = \{\gamma \in G_3 : \rho(\gamma i, i) < R\}$. Then

$$\bigcup_{\gamma\in\mathcal{A}} \gamma D \subset B(i, R + \cosh^{-1} 2).$$

By the definition of fundamental domain, the interiors of the sets on the left hand side are disjoint. Hence

$$\#\mathcal{A} \le \frac{|B(i, R+\cosh^{-1} 2)|}{|D|} = 3(2\cosh R + \sqrt{3}\sinh R - 1),$$

where we have used the formula for the area of the hyperbolic circle [12, §1.1] and the fact that $|D| = 2\pi/3$. ∎

Proof of Proposition 4.3. We split the sum as

$$S = \sum_{n<N} + \sum_{n\ge N} = S_1 + S_2 \quad \text{with } N = 2.2 \cdot 10^{12}.$$

An extensive numerical computation shows that

$$2\cdot 10^{-7} < 1 - \frac{S_1}{72e^9\sqrt{\pi}} < 3\cdot 10^{-7}. \tag{4.2}$$

For S_2 we notice that Lemma 4.2 with $\cosh R = 1+3X$ and Lemma 4.4 imply

$$\sum_{n\le X} r(n)r(3n+2) \le 18(2+\sqrt{3})X - 6(1+\sqrt{3}).$$

Subdividing into dyadic intervals yields

$$\begin{aligned} S_2 &\le \sum_{M=2^jN} \sqrt{M}e^{-(\log M)^2/16} \sum_{n\le 2M} r(n)r(3n+2) \\ &\le 36(2+\sqrt{3}) \sum_{M=2^jN} M^{3/2}e^{-(\log M)^2/16}. \end{aligned}$$

We extract the terms corresponding to $j=0,1$, and bound the rest with an integral:

$$\begin{aligned} S_2 &\le 36(2+\sqrt{3})\Big(3.8977\cdot 10^{-4} + 9.1185\cdot 10^{-5} + \frac{1}{\log 2}\int_{\log 2N}^{\infty} e^{3x/2-x^2/16}\,dx\Big) \\ &\le 6.4619\cdot 10^{-2} + \frac{36(2+\sqrt{3})}{\log 2}\,\frac{8}{\log 2N - 12}\int_{\log 2N}^{\infty} \frac{x-12}{8}\,e^{3x/2-x^2/16}\,dx. \end{aligned}$$

This gives

$$0 < \frac{S_2}{72e^9\sqrt{\pi}} < 7.0479\cdot 10^{-8}.$$

The result follows from these inequalities and (4.2). ∎

Choosing suitable kernels, it is possible to get rather cheaply upper bounds for the first non-trivial eigenvalue in G_p with $u_j(i)\ne 0$. For instance, choosing the kernel

$$k(u) = \frac{0.7676}{(u+1)^{3/2}} - \frac{1.6153}{(u+1)^2} + \frac{0.6550}{(u+1)^{5/2}}$$

in Proposition 4.1, with $p=3$, the left hand side and the integral term cancel; and the Selberg transform, after Lemma 2.3, is positive for $t>3.377$. Hence, the first eigenvalue in G_3 with $u_j(i)\ne 0$ is less than 3.377. The actual value is about 2.592.

5. Applying Hecke operators. In analogy with the classical theory [13] one can introduce the Hecke operators [12, §8.5]

$$T_m f(z) = \frac{1}{\sqrt{m}} \sum_{\gamma\in\Gamma\backslash\Gamma_m} f(\gamma z)$$

acting on (non-holomorphic) functions $f\in L^2(\Gamma\backslash\mathbb{H})$, where Γ_m are the integral matrices having determinant m. Note that they clearly commute with Δ.

These operators are self-adjoint and the eigenfunctions $\{u_j(z)\}_{j=0}^{\infty}$ can be chosen to be also eigenfunctions of T_m with eigenvalues that we denote $\{\lambda_j(m)\}_{j=0}^{\infty}$. In $\Gamma_0(N)$, the theory is identical for $\gcd(N,m)=1$ and there is an Atkin–Lehner theory to cover the rest of the cases.

Hecke operators are also defined in the same way in co-compact groups corresponding to indefinite quaternion algebras over $\mathbb{Q}$ (see [2], [13, §5.3]), where now the summation runs over $\gamma \in R(1)\backslash R(m)$ and $R(k)$ means the image under the embedding in $M_2(\mathbb{R})$ of the elements of norm k of an order R.

When we apply T_m to an automorphic kernel with respect to the full modular group Γ, the sum unfolds as

$$T_m\Big(\sum_{\gamma\in\Gamma} k(\gamma(\cdot),w)\Big)(z) = \frac{1}{\sqrt{m}}\sum_{\gamma\in\Gamma_m} k(\gamma z,w).$$

Then, formally, the application of the Hecke operator corresponds to considering, in the automorphic kernel, integral matrices of determinant m instead of 1.

On the other hand, the action of T_m on (2.1) is

$$\sum_{j=0}^{\infty}\lambda_j(m)h(t_j)u_j(z)\overline{u_j(w)} + \frac{1}{4\pi}\int_{-\infty}^{\infty}\eta_t(m)h(t)E(z,1/2+it)\overline{E(w,1/2+it)}\,dt, \tag{5.1}$$

where $\eta_t(m)$ is the divisor-like function $\sum_{ab=m}(a/b)^{it}$ (see [12]).

Similar formulas apply in the case associated to quaternion algebras when m is coprime to the discriminant of the algebra and to the level of the order (of course the integral corresponding to the continuous spectrum does not appear).

We focus here on the roup Γ and on the order $R=\mathbb{Z}\big[1,i,j,\frac12(1+i+j+k)\big]$ that was employed to define G_p. In this latter case, we write the automorphic kernel in terms of the correlation of $r(n)$ with itself in arithmetic progressions.

Lemma 5.1. *With Γ_m as above, we have*

$$8\sum_{\gamma\in\Gamma_m} k(u(\gamma i,i)) = \sum_{n=0}^{\infty}(3+(-1)^n)r(n)r(n+4m)k\Big(\frac{n}{4m}\Big).$$

And for the order $R=\mathbb{Z}\big[1,i,j,\frac12(1+i+j+k)\big]$,

$$2\sum_{\gamma\in R(m)} k(u(\gamma i,i)) = \sum_{n=0}^{\infty} r(n)r(pn+2m)k\Big(\frac{pn}{2m}\Big),$$

where, as above, $p \equiv 3 \pmod 4$ is prime and $R(m)$ denotes the image of the elements of norm m.

Proof. For $\gamma \in (a_{ij})$ with determinant m,

$$\begin{cases} 4mu(\gamma i, i) = (a_{11} - a_{22})^2 + (a_{12} + a_{21})^2, \\ 4mu(\gamma i, i) + 4m = (a_{11} + a_{22})^2 + (a_{12} - a_{21})^2, \end{cases}$$

Using this, the first formula of the lemma follows by modifying appropriately the proof of Lemma 3.2.

In the same way, the second formula follows as in the proof of Lemma 4.2 by noting that $4u(\gamma i, i) = p(b^2 + d^2)/m$ for $\gamma \in R(m)$ and $p(b^2 + d^2) + 4m = a^2 + c^2$. ∎

We have $|\Gamma \backslash \Gamma_m| = \sigma(m)$, the sum of divisors of m. Analogously, if m and $2p$ are relatively prime (see p. 217 of [13]) then $|R(1)\backslash R(m)| = \sigma(m)$. Therefore if the Selberg transform of k decays quickly we expect (cf. Propositions 3.1 and 4.1)

$$\sum_{n=0}^{\infty} (3 + (-1)^n) r(n) r(n + 4m) k\left(\frac{n}{4m}\right) \approx 96\sigma(m) \int_0^{\infty} k(x)\, dx + \frac{8\sqrt{m}}{\pi} \int_{-\infty}^{\infty} \eta_t(m) h(t) |f(t)|^2\, dt \tag{5.2}$$

and

$$\sum_{n=0}^{\infty} r(n) r(pn + 2m) k\left(\frac{pn}{2m}\right) \approx \frac{24\sigma(m)}{p-1} \int_0^{\infty} k(x)\, dx \qquad \text{for } 2\nmid m,\ p \nmid m. \tag{5.3}$$

For instance, consider

$$S = \sum_{n=0}^{\infty} (3 + (-1)^n) r(n) r(n + 2012) \frac{2012^3}{(n + 2012)^3},$$

$$I = \int_{-\infty}^{\infty} \frac{\cos(t \log 503)}{\cosh(\pi t)} \left(\frac{1}{4} + t^2\right)\left(\frac{9}{4} + t^2\right) |f(t)|^2\, dt.$$

Then by (5.2) and Lemma 2.3 with $m = 503$ and $k(u) = (u+1)^{-3}$, we infer

$$S \approx 24192 + 16\pi\sqrt{503}\, I.$$

The actual numerical values give

$$\frac{S - 24192}{16I} = 70.45857658\ldots,$$

which coincides wih $\pi\sqrt{503}$ in all the displayed digits. In fact the actual error seems to be comparable to 10^{-12}.

Despite the accuracy achieved in this example, the formulas (5.2) and (5.3) are not expected to be uniform in m because of the wild behavior of $\lambda_j(m)$ on the number of divisors of m. See [6] for an analysis of the uniformity in a close context.

It is interesting to note that the multiplicative properties of Hecke eigenvalues can be observed numerically and employed to improve approximations. Consider for instance

$$S_m = \sum_{n=0}^{\infty} r(n)r(7n+2m)g(7n/2m)$$

where g is the function k in Lemma 2.6. According to (5.3), it should approximate $2\sigma(m)$ but the approximation is poor because of the existence of small eigenvalues at the bottom of the spectrum. In fact we have

$$S_1 - 2 = 0.047039, \qquad S_3 - 8 = -0.109461, \qquad S_9 - 26 = 0.119267.$$

The spectral expansion (5.1) and Lemma 5.1 suggest that

$$S_m \approx 2\sigma(m) + 2\sqrt{m}\,\lambda_1(m)h(t_1)|u_1(i)|^2$$

with h as in Lemma 2.6 is a better approximation. On the other hand, the multiplicative properties of Hecke eigenvalues [12, §8.5] ensure $(\lambda_j(3))^2 = 1 + \lambda_j(9)$ that translates into $(8 - S_3)^2 \approx 3(2 - S_1)^2 + (26 - S_9)(2 - S_1)$. Hence, we expect the improved approximation

$$S_3 + \sqrt{3(2 - S_1)^2 + (26 - S_9)(2 - S_1)} \approx 8.$$

In fact the left hand side is 8.001211, improving the previous approximation $S_3 \approx 8$ by two orders of magnitude.

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