Rigorous computation of Maass cusp forms

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Abstract

We describe three new algorithms related to the rigorous computation of Maass cusp forms.

Firstly, we describe a novel algorithm to compute and rigorously verify the Laplace eigenvalue and Hecke eigenvalues of Maass cusp forms of squarefree level and trivial character. The main tool we use is an explicit version of the Selberg trace formula.

We then describe a new algorithm to unconditionally compute the class numbers of real quadratic fields. Again, the main tool used here is an explicit trace formula for Maass forms of level 1 and a dataset of rigorously verified Maass forms.

Finally, we describe a method to extend Hejhal's algorithm to rigorously zoom into a Laplace eigenvalue of a Maass form, once we know it exists in a small interval. With this, we derive a test to show whether or not the main matrix appearing in this algorithm for level 1 Maass forms is well-conditioned as the matrix size increases.

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Author's declaration

I declare that the work in this dissertation was carried out in accordance with the requirements of the University's Regulations and Code of Practice for Research Degree Programmes and that it has not been submitted for any other academic award. Except where indicated by specific reference in the text, the work is the candidate's own work. Work done in collaboration with, or with the assistance of, others, is indicated as such. Any views expressed in the dissertation are those of the author.

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Contents

Introduction

The theory of modular forms has been studied for over 200 years. Mathematicians in the early 19th century, such as Gauss and Jacobi, discovered early examples of modular forms through elliptic functions. Later in the 19th century, Klein further developed the theory of elliptic functions and modular forms. This was followed by work by Ramanujan in the early 20th century with work on his τ function, which gave the first construction of what we now call a *cusp form*, and further “modular” identities with certain infinite products.

One of the biggest breakthroughs in the theory of modular forms came from Hecke, who studied the structures of the spaces of modular forms. In his work he introduced certain operators, now known as *Hecke operators*, to these objects to help prove the multiplicity of the Fourier coefficients of modular forms, generalising the work of Mordell on the τ function. Hecke's research helped to describe the framework with which to study modular forms. The theory of modular forms has grown immeasurably since and, as a result, has found connections in many different areas. Most notably in the theory of elliptic curves, culminating in Wiles' remarkable proof of Fermat's last theorem [Wil95]. Modular forms have also been used in sphere packing [Via17, CKM$^+$17] and in the proof of the monstrous moonshine conjecture and its connections to string theory [Bor92].

Up until the mid-20th century, all modular forms that had been constructed or known to exist were holomorphic. This changed, when in 1949 Maass [Maa49] (a student of Hecke) constructed the first examples of non-holomorphic analogues of modular forms. Hecke in 1926 constructed his *Hecke L-function* over imaginary quadratic fields and showed that they were in correspondence with holomorphic modular forms. He then gave Maass the problem of doing the same thing but for real quadratic fields. For this, Maass did not get the classical holomorphic modular forms and instead had to construct non-holomorphic modular forms to show this correspondence, giving examples of the general object we now call *Maass forms*. These connections between various types of modular forms and other objects are now heavily studied under the *Langlands program*.

However, after Maass' work, it was still not known if Maass forms existed in general in the same way as modular forms. For odd Maass forms, their existence and infinitude can be shown directly from the automorphic and Dirichet boundary conditions. For even Maass forms, this was answered by Selberg [Sel56] in the 1950s with his construction of the Selberg trace formula. Not only did Selberg prove their existence, but also proved that there are infinitely many of them. For a more modern proof of their existence and infinitude, see [LV07]. The Selberg trace formula plays a pivotal role in the study of Maass forms and is the main tool used throughout this thesis. More in depth studies on the theory of Maass forms can be found in [Iwa02, Bum97, CS17, Gol06].

When it comes to constructing examples of Maass forms, the only known explicit cases are the ones due to Maass or the ones appearing from certain Galois representations [Lan80, Tun81]. Instead in general, we rely on numerical computations. Associated with each Maass form is its Laplace eigenvalue and its (infinite) list of Hecke eigenvalues. By computing Maass forms, we mean computing numerical approximations to each Maass form's Laplace eigenvalue and Hecke eigenvalues up to some limit. Further, by rigorous computation, we mean that we can also compute rigorously provable error bounds on each of these approximations.

The history on the numerical computations of Maass cusp forms is quite broad, with the first numerical computations occurring in the early 1970s [Car71]. The main development came when Hejhal introduced an algorithm to numerically compute Maass cusp forms in the 1990s [Hej99]. This was later generalised to general congruence and non-congruence subgroups by his student Strömberg in 2006 [Str05]. This algorithm remains state of the art and works very well in practice. Unfortunately however, this algorithm is non-rigorous since it relies on a heuristic argument.

Since then, there has been progress towards numerically verifying numerical computations of Maass cusp forms, most notably from Booker, Strömbergsson and Venkatesh [BSV06], who derived a method to numerically verify Maass cusp forms for $\mathrm{PSL}(2,\mathbb{Z})$. Using this method they verified the first 10 Laplace eigenvalues to 100 decimal places. This method has recently been generalised to general level N and character by Child in 2022 [Chi22] in his thesis.

Computations of Maass cusp forms have also been studied from a physics background, mainly due to their connection to quantum chaos. Roughly, if we consider a free quantum particle with mass m_0 on a surface $\mathcal{M}$, then quantum mechanics tells us that we can describe the system by a wave function ψ. The Schrödinger equation describes the evolution of this quantum system over time and is given by

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m_0}\Delta\psi,$$

where $\hbar$ is Planck's constant and Δ is the Laplace–Beltrami operator on the surface. By separation of variables, we find that the time independent part of ψ, denoted by

ϕ, satisfies the *time independent Schrödinger equation*, given by

$$\Delta\phi = \lambda\phi.$$

Since ψ is a probability measure, we must have that $\langle\phi, \phi\rangle = 1$, where $\langle\cdot, \cdot\rangle$ denotes the L^2 norm on the space. Now if we consider certain surfaces, namely hyperbolic surfaces that correspond to subgroups of the modular group $\mathrm{PSL}(2, \mathbb{Z})$, then we get precisely *Maass forms*. For applications of Maass forms to physics, see [BGGS97] for results related to quantum chaos and [AST12] for cosmology.

The main result of this thesis is a novel way to compute and rigorously verify examples of Maass cusp forms. As noted before, the main tool used throughout this work is an explicit version of the Selberg trace formula, derived by Strömbergsson [Str16]. We note that explicit forms of the Selberg trace formula have been used before by Booker and Strömbergsson [BS07] for computations to numerically verify the Selberg eigenvalue conjecture. However, they were mainly focused on proving the non-existence of Maass forms in an interval, rather than computing individual examples.

Throughout this thesis, the computations described are predominately implemented in interval arithmetic, namely using the ball-arithmetic C-library `Arb` [Joh17]. The main reason for this, is that it allows us to describe our numerical results as rigorous. The main downside to this is the extra work required in deriving explicit error bounds and how to efficiently implement these. Thankfully the `Arb` library makes this process considerably easier and we highly encourage any reader to give it a try.

Summary of the chapters

Chapter 1 gives a background to the study of Maass forms, stating the main preliminary theory needed for this thesis. Those with a background in classical modular forms should find a lot of this theory familiar.

In Chapter 2 we introduce and describe the novel way to compute Maass forms using the Selberg trace formula. The main tool used is an explicit version of the Selberg trace formula with Hecke operators. Briefly, this allows us to compute sums of the form

$$\sum_{j=1}^{\infty} a_j(m)h(r_j)$$

for some test function h, where the r_j are the Laplace eigenvalues describing the

Maass forms, and the $a_j(m)$ are their corresponding Hecke eigenvalues. The main idea is that we construct a quadratic form, with matrix elements relating to Selberg trace formula values. We then construct a Rayleigh quotient to calculate the error for each Laplace eigenvalue. A lot of this chapter is describing how to implement an explicit form of the Selberg trace formula for computations like these.

In Chapter 3 we introduce a novel method to unconditionally compute real quadratic class numbers. Again, the main tool used here is an explicit version of the Selberg trace formula. The reason for this is that in the Selberg trace formula there is a term that sums over real quadratic class numbers (L-function values more specifically). The main idea is to first compute the class numbers conditionally, which will give us a lower bound on this sum, then we use the Selberg trace formula as an upper bound and numerically show that they match up. All these steps are made rigorous and we implement this algorithm and unconditionally compute the class number for all real quadratic fields with discriminant up to $d = 10^{11}$.

Finally, in Chapter 4 we describe a method to implement a version of Hejhal's algorithm rigorously, once we know our Laplace eigenvalue exists in some provable interval. However, we do not currently know beforehand whether or not this algorithm converges. We then describe a test to show whether or not the main matrix appearing in Hejhal's algorithm for level 1 Maass forms is well-conditioned as you increase the matrix size, once we know our Laplace eigenvalue exists in some provable interval.

Chapter 1

Background

Let $\mathbb{H} = \{z = x + iy \in \mathbb{C} \mid y > 0\}$ denote the hyperbolic upper half-plane with hyperbolic metric and area measure

$$ds^2 = \frac{1}{y}(dx^2 + dy^2), \quad d\mu = \frac{1}{y^2}\, dx\, dy,$$

respectively. The *general linear group* $\mathrm{GL}(2, \mathbb{R})$ acts on $\mathbb{H}$ via the the group action

$$\gamma z = \begin{pmatrix} a & b \\ c & d \end{pmatrix} z = \begin{cases} \dfrac{az + b}{cz + d} & \text{if } \det \gamma > 0, \\ \dfrac{a\overline{z} + b}{c\overline{z} + d} & \text{if } \det \gamma < 0, \end{cases}$$

for all $\gamma \in \mathrm{GL}(2, \mathbb{R})$. We note that any scalar multiple of γ does not change this action, hence we can instead just consider the group of all isometries given by $\mathrm{PGL}(2, \mathbb{R}) = \mathrm{GL}(2, \mathbb{R})/\{\pm\mathrm{Id}\}$, which we call the *projective general linear group.*

We shall consider the subgroup of $\mathrm{PGL}(2, \mathbb{R})$ of orientation persevering isometries $\mathrm{PSL}(2, \mathbb{R}) = \mathrm{SL}(2, \mathbb{R})/\{\pm\mathrm{Id}\}$, which we call the *projective special linear group.* This is a subgroup of index 2 and has a coset representative of

$$J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which corresponds to the map $z \mapsto -\overline{z}$. We call this map the *reflection operator* and it will be discussed in Section 1.5. We note that all the matrices in $\mathrm{SL}(2, \mathbb{R})$ have determinant 1.

For us, the only subgroups of $\mathrm{PSL}(2, \mathbb{R})$ we are interested in are the discrete subgroups. The main discrete subgroup, which we will call the *full modular group*, is

$$\mathrm{PSL}(2, \mathbb{Z}) \cong \mathrm{SL}(2, \mathbb{Z})/\{\pm\mathrm{Id}\}.$$

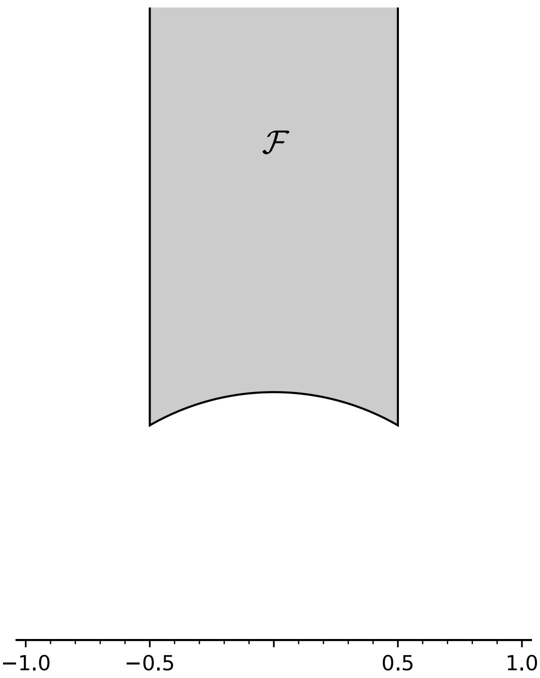


Figure 1.1: Plot of the fundamental domain $\mathcal{F}$ for $\mathrm{PSL}(2,\mathbb{Z})$.

We note that $\mathrm{SL}(2,\mathbb{Z})$ is generated by the two matrices

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

with Möbius transformations $z \mapsto z+1$ and $z \mapsto -\frac{1}{z}$ respectively.

We further define the fundamental domain $\mathcal{F}$ of this action of $\mathrm{PSL}(2,\mathbb{Z})$ by

$$\mathcal{F} = \{z = x+iy \in \mathbb{H} \mid |x| \leq 1/2, |z| \geq 1\}.$$

1.1 Hecke congruence subgroups

We shall now describe certain subgroups of $\mathrm{PSL}(2,\mathbb{Z})$, namely the congruence subgroups. Let N be a positive integer. We define the *principal congruence subgroup* $\Gamma(N) \subset \mathrm{PSL}(2,\mathbb{Z})$ of level N to be

$$\Gamma(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{PSL}(2,\mathbb{Z}) \,\middle|\, \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \mod N \right\}.$$

This is a normal subgroup of $\mathrm{PSL}(2,\mathbb{Z})$ with finite index. Furthermore, we call a subgroup $\Gamma \subset \mathrm{PSL}(2,\mathbb{Z})$ a *congruence subgroup* if $\Gamma(N) \subset \Gamma$, for some N. The main example of a congruence subgroup we shall be using are the *Hecke congruence subgroups* $\Gamma_0(N)$ defined by

$$\Gamma_0(N) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{PSL}(2,\mathbb{Z}) \middle| c \equiv 0 \mod N \right\}.$$

The index of this subgroup is given by

$$[\mathrm{PSL}(2,\mathbb{Z}) : \Gamma_0(N)] = N \prod_{p|N} \left(1 + \frac{1}{p}\right).$$

We note that $\Gamma_0(1) = \mathrm{PSL}(2,\mathbb{Z})$.

1.2 Maass forms

With the hyperbolic metric defined before on $\mathbb{H}$, we have the Laplace–Beltrami operator given by

$$\Delta = -y^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right).$$

We define a *Maass form of level N* and weight 0 to be a non-constant, smooth function $f : \Gamma_0(N)\backslash\mathbb{H} \to \mathbb{C}$ that satisfies the following properties:

1. $f(\gamma z) = f(z)$ for all $z \in \mathbb{H}$ and $\gamma \in \Gamma_0(N)$;
2. f has polynomial growth at the cusps of $\Gamma_0(N)$;
3. $f \in L^2(\Gamma_0(N)\backslash\mathbb{H})$;
4. f is an eigenfunction of the Laplace–Beltrami operator Δ on $\mathbb{H}$.

We shall also write the Laplace eigenvalue as $\lambda = \frac{1}{4} + r^2$ (we shall refer to both λ and r as the Laplace eigenvalue). Furthermore, if f vanishes at the cusps of $\Gamma_0(N)$, then we call f a *Maass cusp form*. For the rest of this thesis, we shall only focus on the case of Maass cusp forms. Additionally, we remark that here, and throughout this thesis, we shall only be considering the case when we have trivial character.

We shall denote $S(\Gamma_0(N))$ to be the space of Maass cusp forms of level N and similarly, denote $S_\lambda(\Gamma_0(N))$ to be the space of Maass cusp forms of level N and Laplace eigenvalue λ.

Furthermore, the space $S_\lambda(\Gamma_0(N))$ is a finite-dimensional Hilbert space with respect to the *Petersson inner product*, defined by

$$\langle f, g\rangle = \int_{\Gamma_0(N)\backslash\mathbb{H}} f\overline{g}\, d\mu,$$

where the integration is taken over the fundamental domain for $\Gamma_0(N)$.

Similar to classical modular forms, we shall also define the (weight 0) *slash operator* for $f \in S_\lambda(\Gamma_0(N))$ by

$$f_{|\gamma}(z) = f(\gamma z)$$

for all $z \in \mathbb{H}$ and $\gamma \in \mathrm{PGL}(2, \mathbb{Z})$.

1.3 Fourier series

Since we have that the matrix $T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \in \Gamma_0(N)$ for all $N \in \mathbb{N}$ with corresponding Möbius transformation $z \mapsto z+1$, we have that our Maass forms admit a Fourier series. Before we can give a description of this series, we must first introduce the *K-Bessel function*.

Definition 1.3.1 (K-Bessel function)**.** Let x be a positive real number and $\nu \in \mathbb{C}$. Then we define the K-Bessel function by

$$K_\nu(x) := \frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh(t)+\nu t}\, dt = \int_0^\infty \cosh(\nu t) e^{-x\cosh(t)}\, dt.$$

We have that $y = K_\nu(x)$ satisfies the differential equation

$$y'' + \frac{y'}{x} - \left(1 + \frac{\nu^2}{x^2}\right) y = 0.$$

For all the work that we will be doing, we shall assume ν is purely imaginary, i.e $\nu = ir$ for some real r. We shall also mainly be considering the *Whittaker function* of the form $W_{ir}(x) = \sqrt{x}K_{ir}(x)$. This function plays a key role in the computation of Maass forms, and will appear many times in this thesis. In Appendix A we shall provide further facts about this function.

We can now state the Fourier series for a Maass cusp form.

Proposition 1.3.1. *Let $f \in S_\lambda(\Gamma_0(N))$ be a Maass cusp form of level N and Laplace eigenvalue $\lambda = \frac{1}{4} + r^2 > 0$. Then, for all $z \in \mathbb{H}$, f admits a Fourier series of the* *form*

$$f(z) = f(x+iy) = \sum_{n\neq 0} \frac{a_n}{\sqrt{|n|}} W_{ir}(2\pi|n|y)e^{2\pi i n x}, \tag{1.1}$$

where the a_n *are its Fourier coefficients.*

1.4 Involutions

In linear algebra, an *involution* on a vector space V is a linear operator $T : V \to V$ such that $T^2 = I$, where I is the identity matrix. For us, we call a linear operator $T : S_\lambda(\Gamma_0(N)) \to S_\lambda(\Gamma_0(N))$ a $\Gamma_0(N)$-*involution* if

$$T^2 f = f,$$

for all $f \in S_\lambda(\Gamma_0(N))$, i.e. T^2 is the identity operator. These involutions will allow us to categorise Maass forms in many different ways.

The two main involutions we shall be using are the:

1. *Fricke involution* - Let $W_N = \begin{pmatrix} 0 & -\frac{1}{\sqrt{N}} \\ \sqrt{N} & 0 \end{pmatrix} \in \mathrm{PSL}(2,\mathbb{R})$. This is a $\Gamma_0(N)$-involution, called the *Fricke involution* when acting through the slash operator. The corresponding Möbius transformation is $z \mapsto \frac{-1}{Nz}$. A Maass cusp form $f \in S_\lambda(\Gamma_0(N))$ will have an eigenvalue of ± 1 with respect to this involution which we call the *Fricke sign*.

2. *Reflection operator* - Let $J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We saw this matrix at the start of this chapter and this is an involution by the map $z \mapsto -\overline{z}$. More details of this operator are given in the next section.

1.5 Reflection operator

From Figure 1.1 we see that the fundamental domain of $\mathrm{PSL}(2,\mathbb{Z})$ has an obvious symmetry, namely reflection in the imaginary axis. This symmetry will allow us to split our Maass forms into two separate groups called *even* and *odd* forms. This categorisation will occur due to certain boundary conditions of the fundamental domain.

Precisely, we shall consider the reflection operator $J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, with corresponding map $z \mapsto -\overline{z}$. Now, we can diagonalise $S_\lambda(\Gamma_0(N))$ with respect to J

and the eigenvalues of this involution will be 1 or -1. We say that f is *even* if $f(z) = f(-\overline{z})$ and *odd* is $f(z) = -f(-\overline{z})$. For an even form, its Fourier coefficients a_n satisfy $a_n = a_{-n}$, and similarly, for a odd form $a_n = -a_{-n}$. From the Fourier series given in Proposition 1.3.1, we can replace the exponentials with a cosine/sine series for even/odd forms respectively.

1.6 Hecke operators

The classical theory of Hecke operators for holomorphic forms translates very easily to the case of Maass forms. Here we shall just give the definition of Hecke operators and some facts.

To begin, let $f \in S_\lambda(\Gamma_0(N))$ and n a non-zero integer coprime to N. We define the nth *Hecke operator* T_n by

$$T_n f(z) = \frac{1}{\sqrt{|n|}} \sum_{\substack{ad=n \\ (a,N)=1 \\ d>0}} \sum_{j=0}^{d-1} \begin{cases} f\left(\dfrac{az+j}{d}\right) & \text{if } n > 0, \\ f\left(\dfrac{a\overline{z}+j}{d}\right) & \text{if } n < 0. \end{cases} \tag{1.2}$$

This maps $S_\lambda(\Gamma_0(N)) \to S_\lambda(\Gamma_0(N))$. Furthermore, these operators commute. Explicitly, for non-zero integers n and m, with $(n, N) = (m, N) = 1$, we have that

$$T_n T_m = \sum_{\substack{d|(m,n) \\ d>0}} T_{\frac{mn}{d^2}}.$$

In addition, the Hecke operators T_n with $(n, N) = 1$ commute with the Laplacian and the reflection operator.

Another important use for Hecke operators, is for their relation to the Fourier coefficients. More precisely, let $f \in S_\lambda(\Gamma_0(N))$ be a eigenfunction of all T_n with $(n, N) = 1$ and let λ_n be the eigenvalue for Hecke operator T_n, that is $T_n f = \lambda_n f$. We call λ_n the *nth Hecke eigenvalue*. Furthermore, let a_m be the Fourier coefficients of f and b_m be the Fourier coefficients of $T_n f$. Then comparing the Fourier expansions of (1.2), we get that

$$b_m = \sum_{\substack{d|(m,n) \\ d>0}} a_{\frac{mn}{d^2}}.$$

Next, comparing the Fourier expansions of either side of $T_n f = \lambda_n f$, we see that

$b_m = \lambda_n a_m$. Combining both of these, we get that

$$a_n = \lambda_n a_1$$

for all $n \neq 0$.

Finally, we note the following important theorem.

Theorem 1.6.1. *There exists an orthogonal basis* $\{f_j\}$ *in* $S_\lambda(\Gamma_0(N))$*, where the* f_j*'s are eigenfunctions to all the Hecke operators* T_n *with* $(n, N) = 1$*.*

1.7 Oldforms and newforms

Atkin–Lehner theory [AL70] for holomorphic forms allows us to distinguish between forms that are new to the level and ones which can be derived from lower levels. This theory directly translates to Maass forms, giving us a normalisation for the Fourier coefficients and relations between these Fourier coefficients and Hecke operators.

Let $K, N \in \mathbb{N}$ and suppose $K \mid N$. Then $\Gamma_0(N) \subseteq \Gamma_0(K)$. Notably, if f is a Maass cusp form of $\Gamma_0(K)$, then $f(kz)$ is a Maass cusp form of $\Gamma_0(N)$ for all $k \mid \frac{N}{K}$. Forms that arise like this for $\Gamma_0(N)$ we call *oldforms.* We define *newforms* to be forms in the orthogonal complement (with respect to the Petersson inner product) of the space spanned by the oldforms. We denote the space of Maass newforms of level N and Laplace eigenvalue λ by $S_\lambda^{\text{new}}(\Gamma_0(N))$. Since oldforms can be derived from lower level newforms, we can just focus our attention on newforms to derive facts about all cusp forms.

As a further refinement, we call a Maass newform $f \in S_\lambda^{\text{new}}(\Gamma_0(N))$ a *normalised newform* if f is an eigenfunction of all Hecke operators T_n with $(n, N) = 1$, and furthermore, its first Fourier coefficient $a_1 = 1$. The motivation for this refinement is given in the following two theorems.

Theorem 1.7.1. *There exists an orthogonal basis of normalised newforms for the space* $S^{\text{new}}(\Gamma_0(N))$*. We call this basis the* Hecke-eigenbasis *of this space.*

Theorem 1.7.2. *Let* $f \in S_\lambda^{\text{new}}(\Gamma_0(N))$ *be a normalised newform with Laplace eigenvalue* λ*, Hecke eigenvalues* λ_n*, Fourier coefficients* a_m*, given by* (1.1) *and parity* $\varepsilon = 1$ *if* f *is even and* $\varepsilon = -1$ *if* f *is odd. Then*

$$\begin{aligned} a_m &= \lambda_m, \text{ and} \\ a_{-m} &= \varepsilon \lambda_m \end{aligned}$$

for all $m \in \mathbb{N}$. Furthmore, we have the following Hecke multiplicativity relations

$$a_m a_n = \sum_{\substack{d|(m,n) \\ d>0}} a_{\frac{mn}{d^2}}, \text{ for } (n, N) = 1, m \in \mathbb{Z},$$

$$a_m a_p = a_{mp}, \text{ for } p \mid N, m \in \mathbb{Z}.$$

Finally, for prime $q \mid N$ but $q^2 \nmid N$, we have that

$$a_q = \frac{w_q}{\sqrt{q}},$$

where $w_q = \pm 1$ is the eigenvalue of the Fricke involution.

For the entirety of this thesis, we shall mainly use normalised Maass newforms.

1.8 L-function

Let f be a normalised Maass newform, with Laplace eigenvalue $\lambda = \frac{1}{4} + r^2$, of level N and trivial character. Moreover, let $a_f(n)$ be the Hecke eigenvalues of f. We define the associated L-function to f by

$$L_f(s) = \sum_{n=1}^{\infty} \frac{a_f(n)}{n^s},$$

where $\mathrm{Re}(s) > 1$. This can be analytically continued to the whole complex plane and satisfies the functional equation

$$\Lambda_f(s) = N^{\frac{s}{2}} \Gamma_{\mathbb{R}}(s + a + ir)\Gamma_{\mathbb{R}}(s + a - ir)L_f(s) = \omega(-1)^a \Lambda_f(1 - s),$$

where

- $\Gamma_{\mathbb{R}}(s) = \pi^{-s/2}\Gamma(s/2)$,
- ω is the eigenvalue of the Fricke involution given by $f(z) = \omega f\left(-\frac{1}{Nz}\right)$,
- $a = 0$ if f is even and $a = 1$ if f is odd.

It is conjectured, analogous to the Riemann zeta function, that L-functions associated to Maass cusp forms on $\Gamma_0(N)$ satisfy a Riemann hypothesis, that is all the zeros of $L_f(s)$ in the strip $\{s \in \mathbb{C} \mid 0 < \mathrm{Re}(s) < 1\}$ lie on the line $s = 1/2 + it, t \in \mathbb{R}$. When computing zeros on the critical line of these L-functions, it is easier to work with the associated real-valued Z-function, defined by

$$Z(t) = \bar{\varepsilon}^{1/2} \frac{\gamma(1/2+it)}{|\gamma(1/2+it)|} L_f(1/2+it), \tag{1.3}$$

where $\gamma(s) = N^{\frac{s}{2}} \Gamma_{\mathbb{R}}(s+a+ir)\Gamma_{\mathbb{R}}(s+a-ir)$ and $\varepsilon = \omega(-1)^a$. Since $|Z(t)| = |L_f(1/2+it)|$, they share the same zeros on the critical line.

1.9 Selberg Trace formula

As stated in the introduction, Selberg [Sel56] introduced the Selberg trace formula to prove the existence of Maass cusp forms in general. The Selberg trace formula can be seen as a generalisation of the Poisson summation formula to non-compact manifolds, where one side is a sum over the spectral eigenvalues, and the other side, is a collection of terms relating to the geometry of the space. More concretely, let $\{f_j\}_{j=1}^{\infty}$ be a sequence of normalised Hecke eigenforms such that it is a basis for $\bigoplus_{\lambda>0} S_\lambda^{\text{new}}(N)$. Let λ_j denote the Laplace eigenvalue of f_j and assume that $\lambda_1 \leq \lambda_2 \leq \dots$. In addition, let $a_j(n)$ be the Hecke eigenvalues for f_j. Then, the Selberg trace formula is an expression for the weighted sum

$$\sum_{j=1}^{\infty} a_j(n) h(r_j),$$

where $n \in \mathbb{Z}\backslash\{0\}$ and h is a suitable test function. We call this side the *spectral side*, and the terms on the right-hand side of the equation the *geometric side*.

There are many different ways to write the geometric side, depending on what one plans to use it for. In this thesis, it is crucial that we have a very explicit form of the geometric side, so that it can be implemented on a computer easily. More details of this are given in Sections 2.2 and 2.3 for level 1 and squarefree level N respectively.

One very important consequence of the Selberg trace formula is an approximation to the density of the eigenvalues, called the *Weyl law*, and is given by

$$\#\{\lambda_j \mid \lambda_j < M\} \sim \frac{\text{vol}(\Gamma_0(N)\backslash\mathbb{H})}{4\pi} M, \tag{1.4}$$

as $M \to \infty$. For $\Gamma_0(N)$, we can write this explicitly using [Ris04] as

$$\#\{\lambda_j \mid \lambda_j < M\} = N \prod_{p|N} \Big(1 + \frac{1}{p}\Big) \frac{M}{12} + O(\sqrt{M} \log \sqrt{M}\,).$$

1.10 Open conjectures

During the 20th century and early 21st century, many open conjectures on holomorphic modular forms have been proven, most notably the Ramanujan conjecture. Most of these results have direct analogues for Maass forms and are still open in this case.

Selberg eigenvalue conjecture

A natural question to ask is how small can the Laplace eigenvalue be for Maass forms? If we let $f \in S_\lambda(\Gamma_0(N))$ be a Maass cusp form with Laplace eigenvalue λ, then the *Selberg eigenvalue conjecture* states that $\lambda \geq \frac{1}{4}$. We call a Maass form *exceptional* if $\lambda \in (0, \frac{1}{4}]$. This was known for the full modular group by Selberg and W. Roelcke independently in the 1950s, and can be proved using elementary methods (see [Hej83, Chap. 11, Prop. 2.1]). For all levels $N \leq 880$, this conjecture has been numerically verified by Booker, Min and Strömbergsson [BLS20]. Theoretically, the best bound we currently have is $\lambda \geq 975/4096 = 0.238037109375$ due to Kim and Sarnak [Kim03].

Ramanujan–Petersson conjecture

Let $f \in S_\lambda^{\text{new}}(\Gamma_0(N))$ be a normalised newform with Laplace eigenvalue λ and Hecke eigenvalues λ_n. Then, the *Ramanujan–Petersson conjecture* states that $|\lambda_p| \leq 2$ for all prime $p \nmid N$. We remark that the Ramanujan–Petersson conjecture for holomorphic modular forms was proven by Deligne [Del74]. For Maass forms however, this is still open with the best bound being $|\lambda_p| \leq p^{7/64} + p^{-7/64}$ due to Kim and Sarnak [Kim03]. From the Hecke relations it follows that for $n \in \mathbb{N}$,

$$|\lambda_n| \leq b(n) := \prod_{p^k \| n} \frac{\sinh((k+1)\theta \log p)}{\sinh(\theta \log p)}, \tag{1.5}$$

where $\theta = 7/64$ and $p^k \| n$ means that $p^k \mid n$ but $p^{k+1} \nmid n$.

Sato–Tate conjecture

The Sato–Tate conjecture is a statistical conjecture about the asymptotic distribution of Hecke eigenvalues λ_p of Hecke operators T_p for primes p. It states that the λ_p should be asymptotically distributed with respect to the Sato–Tate measure given by

$$\mu_\infty = \frac{1}{\pi}\sqrt{1 - \frac{x^2}{4}}\, dx,$$

as $p \to \infty$. This is also sometimes referred to as the *horizontal Sato–Tate conjecture*. A related result, sometimes referred to as *vertical Sato–Tate*, proven by Sarnak in [Sar87], states that instead if we fix a prime $p \nmid N$ and let the level tend to infinity or the Laplace eigenvalue tend to infinity, then the points λ_p of these forms are asymptotically distributed by the measure

$$\mu_p = f_p\, \mu_\infty,$$

where

$$f_p(x) = \frac{p+1}{(p^{1/2} + p^{-1/2})^2 - x^2},$$

for $x \in [-2, 2]$.

Chapter 2

Trace formula algorithm for Maass forms

In this chapter, we introduce a novel method to compute and rigorously verify the Laplace and Hecke eigenvalues of Maass cusp forms of squarefree level and trivial character. The main tool used is an explicit version of the Selberg trace formula due to Strömbergsson [Str16].

The outline of this chapter is as follows. In Section 2.1 we present the novel algorithm. In Sections 2.2 and 2.3 we state the explicit forms of the Selberg trace formula that we use for level 1 and squarefree level N respectively, and explain computational aspects on how to compute it. In Section 2.4 we choose and optimise the test function for the trace formula such that it maximises the precision of the computation. Finally, in Section 2.5 we state the computational results and show some numerical evidence towards the Ramanujan–Petersson conjecture, Sato–Tate conjecture and the Riemann hypothesis for L-functions of Maass cusp forms.

This chapter is heavily based on work by the author which first appeared in [SH22].

2.1 Trace Formula Algorithm

In this section, we derive the algorithm to compute and rigorously verify the Laplace and Hecke eigenvalues of Maass cusp forms of squarefree level N. The central tool used here is the Selberg trace formula with Hecke operators. The main idea here is to use linear algebra to remove the contribution of all the forms up to some limit and isolate just one form. We then use our approximation to this form to see how well it removes the remaining contribution.

2.1.1 Setup

Consider the space of Maass newforms of level N, Laplace eigenvalue λ and trivial character, denoted by $S_\lambda^{\mathrm{new}}(\Gamma_0(N))$. Let $\{f_j\}_{j=1}^\infty$ be a sequence of normalised Hecke eigenforms such that it is a basis for $\bigoplus_{\lambda>0} S_\lambda^{\mathrm{new}}(\Gamma_0(N))$. Let λ_j denote the Laplace eigenvalue of f_j and assume that $\lambda_1 \leq \lambda_2 \leq \ldots$. In addition, let $a_j(n)$ be the Hecke eigenvalues for f_j.

The Selberg trace formula allows us to compute

$$t(n,H) := \sum_{j=1}^{\infty} a_j(n) H(\lambda_j),$$

for any non-zero $n \in \mathbb{Z}$ with $(n,N) = 1$ and any sufficiently nice test function H. Using the Hecke relations, we compute that

$$\left(\sum_{m=1}^{M} c(m) a_j(m)\right)^2 = \sum_{m_1=1}^{M} \sum_{m_2=1}^{M} c(m_1) c(m_2) \sum_{d|(m_1,m_2)} a_j\left(\frac{m_1 m_2}{d^2}\right),$$

for any sequence $\{c(m)\}_{m=1}^{M}$ of real numbers, satisfying $c(m) = 0$ whenever $(m,N) > 1$. Thus, defining

$$Q(c,H) := \sum_{j=1}^{\infty} \left(\sum_{m=1}^{M} c(m) a_j(m)\right)^2 H(\lambda_j),$$

we have

$$Q(c,H) = \sum_{m_1=1}^{M} \sum_{m_2=1}^{M} c(m_1) c(m_2) \sum_{d|(m_1,m_2)} t\left(\frac{m_1 m_2}{d^2}, H\right). \tag{2.1}$$

2.1.2 Computing the forms

Let H be a non-negative test function and let $\widetilde{H}(\lambda) = \lambda H(\lambda)$. Let Q and $\widetilde{Q}$ denote the respective matrices of the quadratic forms $Q(c,H)$ and $Q(c,\widetilde{H})$. We can get approximations of the Laplace eigenvalues by considering the generalised symmetric eigenvalue equation

$$\widetilde{Q}x = \lambda Q x. \tag{2.2}$$

The eigenvalues of this problem correspond directly with the Laplace eigenvalues in the trace formula. To see this, we see that solving (2.2) is equivalent to solving the equation

$$\det(\widetilde{Q} - \lambda Q) = 0.$$

Plugging in the matrix elements of $\widetilde{Q}$ and Q, we see that the above becomes

$$\det\left(\left(\sum_{d|(m_1,m_2)} t\left(\frac{m_1m_2}{d^2},\widetilde{H}\right) - \lambda t\left(\frac{m_1m_2}{d^2},H\right)\right)_{1\le m_1,m_2\le M}\right)$$
$$= \det\left(\left(\sum_{d|(m_1,m_2)}\sum_{j=1}^{\infty} a_j\left(\frac{m_1m_2}{d^2}\right)H(\lambda_j)(\lambda_j-\lambda)\right)_{1\le m_1,m_2\le M}\right) = 0.$$

Here, we see that solutions λ of (2.2) correspond exactly to the Laplace eigenvalues of the Maass cusp forms. Now, these will only be non-rigorous approximations since the tail of the spectrum will have an influence.

We solve this by first diagonalising $Q = PDP^T$, where P is an orthogonal matrix and D is diagonal with positive entries. Then the solutions to (2.2) will just be the eigenvalues of $D^{-1/2}P^T\widetilde{Q}PD^{-1/2}$. For each eigenvalue $\widetilde{\lambda}_i$, we set c_i to be the corresponding eigenvector. We will use the components of c_i to form the sequence $c(m)$ for each eigenvalue. The reason for this, is that the c_i will pick out the ith Maass form. More explicitly, plugging in c_i into the following Rayeigh quotient gives

$$\frac{c_i^T\widetilde{Q}c_i}{c_i^TQc_i} = \widetilde{\lambda}_i.$$

2.1.3 Verifying the forms

Firstly, for the verification we shall prove that there exists a Laplace eigenvalue near $\widetilde{\lambda}_i$. For this, we define the Rayleigh quotient

$$\varepsilon_i := \sqrt{\frac{Q(c_i,\widetilde{H}_i)}{Q(c_i,H)}}, \tag{2.3}$$

where $\widetilde{H}_i(\lambda) = H(\lambda)(\lambda-\widetilde{\lambda}_i)^2$, for the same c_i computed above. Then ε_i^2 is a weighted average of $(\lambda-\widetilde{\lambda}_i)^2$ and hence there exists a cuspidal eigenvalue $\lambda \in [\widetilde{\lambda}_i-\varepsilon_i, \widetilde{\lambda}_i+\varepsilon_i]$. Another way to see this, is that the c_i is just picking out the ith Maass form and we are seeing how well our approximation removes the contribution of this form in the trace formula.

Next we prove completeness of the eigenvalues, i.e. prove that we have not missed any. We choose a test function $H^*(\lambda)$ that is positive and monotonically decreasing for $\lambda > 0$. Then $H^*(\lambda) \ge H^*(\widetilde{\lambda}_i+\varepsilon_i)$ for all $\lambda \in [\widetilde{\lambda}_i-\varepsilon_i, \widetilde{\lambda}_i+\varepsilon_i]$. Hence any eigenvalue λ that is not contained in $\bigcup_i[\widetilde{\lambda}_i - \varepsilon_i, \widetilde{\lambda}_i + \varepsilon_i]$ must satisfy

$$H^*(\lambda) \leq t(1, H^*) + \sum_i H^*(\widetilde{\lambda}_i + \varepsilon_i).$$

Here the second sum ranges over all i such that $[\widetilde{\lambda}_i - \varepsilon_i, \widetilde{\lambda}_i + \varepsilon_i]$ does not overlap the corresponding interval for any smaller value of i. Since H^* is monotonic, this determines numbers $\delta_i > 0$ such that $|\lambda_i - \widetilde{\lambda}_i| \leq \varepsilon_i$ and $|\lambda_j - \widetilde{\lambda}_i| \geq \delta_i$ for $j \in \mathbb{N}\backslash\{i\}$. Note that this approach only works well if the λ_i turn out to be distinct and well separated. It is conjectured that the Laplacian spectrum is simple for squarefree level and trivial character, with Poissonian spacing statistics. There exists some theoretical and numerical evidence for this, namely from [LS94] and [Ste94] respectively. For this algorithm, we will see from the data that this will be the case.

Finally, we consider the Hecke eigenvalues. For $j \geq 1$ and any sequence $\{c(m)\}_{m=1}^{M}$, define

$$L_j(c) = \sum_{m=1}^{M} c(m)a_j(m).$$

Let $H, \widetilde{H}_i$ be as above. Then

$$\begin{aligned}\left(\sum_{j\neq i} L_j(c_i)a_j(n)H(\lambda_j)\right)^2 &\leq \sum_{j\neq i} L_j(c_i)^2 H(\lambda_j) \sum_{j=1}^{\infty}(a_j(n))^2 H(\lambda_j)\\ &\leq \delta_i^{-2} Q(c_i, \widetilde{H}_i)Q(e_n, H) = \varepsilon_i^2\delta_i^{-2}Q(c_i, H)Q(e_n, H),\end{aligned}$$

where $e_n(m) = 1$ if $m = n$ and 0 otherwise. Thus, defining

$$\eta_{i,n} = \frac{\varepsilon_i}{\delta_i}\sqrt{Q(c_i, H)Q(e_n, H)} \quad \text{and} \quad W_i = L_i(c_i)H(\lambda_i), \tag{2.4}$$

we have

$$A_i(n) := a_i(n)W_i = \sum_{m=1}^{M} c_i(m) \sum_{d|(m,n)} t\left(\frac{mn}{d^2}, H\right) + \beta_{i,n}\eta_{i,n},$$

where $\beta_{i,n}$ is some real constant that depends on i and n and satisfies $|\beta_{i,n}| \leq 1$. We can use this to compute $a_i(n)$, with $(n, N) = 1$, by using the fact that $a_i(1) = 1$ to compute W_i to a proven accuracy.

In practice, we will choose one test function H that is both positive and monotonically decreasing and use this throughout.

2.1.4 Computing a_n for $(n, N) > 1$ for squarefree level N

Let f be a primitive Maass newform of squarefree level N, Laplace eigenvalue $\lambda = 1/4 + r^2$ and trivial character, with Fourier coefficients a_n. By Atkin–Lehner theory, see Section 1.7, for each prime $p \mid N$ we have $a_p = \pm 1/\sqrt{p}$. Moreover, defining $w = \mu(N)\sqrt{N}\prod_{p|N} a_p = \prod_{p|N} \operatorname{sign}(-a_p)$, we have $f(z) = wf(-1/Nz)$. Hence, we just need to find the signs of the a_p for $p \mid N$, and then use the Hecke relations to find all a_n for $(n, N) > 1$.

Suppose first that f is even, so its Fourier expansion is of the form

$$f(z) = \sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}} W_{ir}(2\pi n y)\cos(2\pi n x),$$

where $W_{ir}(y) := \sqrt{y}K_{ir}(y)$ and $K_{ir}(y)$ is the K-Bessel function. Substituting $z = iy$ into the relation $f(z) = wf(-1/Nz)$, we have

$$\sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}} \left(W_{ir}(2\pi n y) - wW_{ir}\left(\frac{2\pi n}{Ny}\right)\right) = 0. \tag{2.5}$$

If $w = -1$ then taking $y = 1/\sqrt{N}$ in (2.5) yields

$$\sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}} W_{ir}\left(\frac{2\pi n}{\sqrt{N}}\right) = 0.$$

If $w = 1$ then taking $y = \sqrt{2/N}$ in (2.5) yields

$$\sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}} \left(W_{ir}\left(\frac{2\pi n\sqrt{2}}{\sqrt{N}}\right) - W_{ir}\left(\frac{\pi n\sqrt{2}}{\sqrt{N}}\right)\right) = 0.$$

Now suppose f is odd, so its Fourier expansion takes the form

$$f(z) = \sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}} W_{ir}(2\pi n y)\sin(2\pi n x).$$

In this case plugging in $z = iy$ would only give the trivial relation $0 = 0$, so instead we first differentiate with respect to x. For this we consider

$$\frac{\partial}{\partial x}(f(z) - wf(-1/Nz))|_{z=iy} = 0.$$

After some computation this yields

$$\sum_{n=1}^{\infty} a_n\sqrt{n}\left(W_{ir}(2\pi n y) + \frac{w}{Ny^2}W_{ir}\left(\frac{2\pi n}{Ny}\right)\right) = 0. \tag{2.6}$$

If $w = 1$ then taking $y = 1/\sqrt{N}$ in (2.6) yields

$$\sum_{n=1}^{\infty} a_n\sqrt{n}W_{ir}\left(\frac{2\pi n}{\sqrt{N}}\right) = 0.$$

If $w = -1$ then taking $y = \sqrt{2/N}$ in (2.6) yields

$$\sum_{n=1}^{\infty} a_n\sqrt{n}\left(W_{ir}\left(\frac{2\pi n\sqrt{2}}{\sqrt{N}}\right) - \frac{1}{2}W_{ir}\left(\frac{\pi n\sqrt{2}}{\sqrt{N}}\right)\right) = 0.$$

In summary, if we define

$$W(y) = \begin{cases} W_{ir}(y) & \text{if } f \text{ is even and } w = -1, \\ W_{ir}(y\sqrt{2}) - W_{ir}(y/\sqrt{2}) & \text{if } f \text{ is even and } w = 1, \\ \dfrac{y\sqrt{N}}{2\pi}W_{ir}(y) & \text{if } f \text{ is odd and } w = 1, \\ \dfrac{y\sqrt{N}}{2\pi}\left(W_{ir}(y\sqrt{2}) - \dfrac{1}{2}W_{ir}(y/\sqrt{2})\right) & \text{if } f \text{ is odd and } w = -1, \end{cases}$$

then

$$\sum_{n=1}^{\infty} \frac{a_n}{\sqrt{n}}W\left(\frac{2\pi n}{\sqrt{N}}\right) = 0.$$

Now computationally we will only have accurate approximations of a_n for $n \leq M$, so we must truncate the above sums at M and estimate the error incurred. Using the current best estimate towards to Ramanujan–Petersson conjecture from Kim–Sarnak [Kim03], see (1.5), we get the following.

Lemma 2.1.1. *Let f be a Maass cusp form of level N with Hecke eigenvalues a_m. Then for all non-zero $m \in \mathbb{Z}$ we have*

$$\left|\frac{a_m}{\sqrt{m}}\right| \leq \eta := 1.758.$$

Proof. Using (1.5), we have $\left|\frac{a_m}{\sqrt{m}}\right| \leq \frac{b(m)}{\sqrt{m}}$, and this is maximised at $m = 12$. $\square$

Additionally we also have, from Appendix A, that

$$|W_{ir}(y)| \leq \sqrt{\frac{\pi}{2}} e^{-y} \text{ for } y > 0.$$

With both of these results we can easily find bounds for the tails of the sums and obtain

$$\left| \sum_{n=M+1}^{\infty} \frac{a_n}{\sqrt{n}} W\left(\frac{2\pi n}{\sqrt{N}}\right) \right| \leq \begin{cases} \eta \sqrt{\frac{\pi}{2}} \frac{\exp\left(-\frac{2\pi M}{\sqrt{N}}\right)}{\exp\left(\frac{2\pi}{\sqrt{N}}\right) - 1} & f \text{ even, } w = -1, \\ 2\eta \sqrt{\frac{\pi}{2}} \frac{\exp\left(-\frac{\pi M \sqrt{2}}{\sqrt{N}}\right)}{\exp\left(\frac{\pi\sqrt{2}}{\sqrt{N}}\right) - 1} & f \text{ even, } w = 1, \\ \eta \sqrt{\frac{\pi}{2}} \frac{\left((M+1)\exp\left(\frac{2\pi}{\sqrt{N}}\right) - M\right)}{\exp\left(\frac{2\pi M}{\sqrt{N}}\right)\left(\exp\left(\frac{2\pi}{\sqrt{N}}\right) - 1\right)^2} & f \text{ odd, } w = 1, \\ \frac{3\eta}{2} \sqrt{\frac{\pi}{2}} \frac{\left((M+1)\exp\left(\frac{\pi\sqrt{2}}{\sqrt{N}}\right) - M\right)}{\exp\left(\frac{\pi M\sqrt{2}}{\sqrt{N}}\right)\left(\exp\left(\frac{\pi\sqrt{2}}{\sqrt{N}}\right) - 1\right)^2} & f \text{ odd, } w = -1. \end{cases}$$

To obtain these bounds, we used the fact that

$$\sum_{n=M}^{\infty} n e^{-nx} = \frac{e^{(1-M)x}\left((1-M) + Me^{x}\right)}{(e^{x}-1)^2},$$

which can be seen by differentiating both sides of the geometric series

$$\sum_{n=M}^{\infty} e^{-nx} = \frac{e^{-Mx}}{1-e^{-x}}.$$

To find the signs of the a_p for $p \mid N$ we just test every combination of ± 1 for the signs of the a_p, then use this to compute w and the corresponding sum from the above cases. Heuristically, we expect only one of these sums to be within the error derived. When there is only one sum within the errors, we can say that the result is rigorous. We then take the signs of the a_p for $p \mid N$ and w from that sum. In practice we see this works well, provided the Laplace eigenvalue and Hecke eigenvalues are computed to a high enough precision.

2.2 The Selberg Trace Formula for level 1

In the algorithm given in Section 2.1, an essential tool we need is an explicit version of the Selberg trace formula with Hecke operators. Currently, this has only been derived for squarefree level by Strömbergsson in [Str16]. To make this more suitable for computation, we rewrite it in the following form, following the steps of Proposition 2.1 in [BL17].

Theorem 2.2.1 (The Selberg trace formula for Maass newforms for level 1)**.** *Fix $\delta > 0$, let $h(t)$ be a even analytic function on the strip $\{t \in \mathbb{C} : \mathrm{Im}(t) \leq \frac{1}{2} + \delta\}$ such that $h(r) \in \mathbb{R}$ for $r \in \mathbb{R}$ and $h(r) = O((1 + |r|^2)^{-1-\delta})$. Define g as the Fourier transform of h given by*

$$g(u) = \frac{1}{2\pi} \int_{-\infty}^{\infty} h(r) e^{-iru} \, dr.$$

Let $\{f_j\}$ be a sequence of normalised Hecke eigenforms of level 1, with Laplacian eigenvalues $\lambda_j = \frac{1}{4} + r_j^2$ and respective Hecke eigenvalues $a_j(n)$.

Then, we have

$$
\begin{aligned}
&\frac{\sigma_1(|n|)}{\sqrt{|n|}} h\left(\frac{i}{2}\right) + \sum_{j>0} h(r_j) a_j(n) \\
&= \sum_{\substack{t\in\mathbb{Z} \\ \sqrt{D}=\sqrt{t^2-4n}\notin\mathbb{Q}}} L(1,\psi_D)\cdot \begin{cases} g\left(\log\left(\frac{(|t|+\sqrt{D})^2}{4|n|}\right)\right) & \textit{if } D>0, \\ \frac{\sqrt{|D/4n|}}{2\pi}\int_{-\infty}^{\infty} \frac{g(u)\cosh(u/2)}{\sinh^2(u/2)+|D/4n|}\,du & \textit{if } D<0 \end{cases} \\
&+ \sum_{\substack{ad=n \\ a>0 \\ a\neq d}} \left(\log\pi + \log|a-d| - \frac{\log(X(|a-d|))}{|a-d|}\right)\cdot g\left(\log\left|\frac{a}{d}\right|\right) \\
&+ \frac{1}{2}\sum_{\substack{ad=n \\ a>0 \\ a\neq d}} \int_{|\log|\frac{a}{d}||}^{\infty} g(u)\cdot \frac{e^{u/2}+\varepsilon e^{-u/2}}{e^{u/2}-\varepsilon e^{-u/2}+\left|\sqrt{|a/d|}-\varepsilon\sqrt{|d/a|}\right|}\,du \\
&+ \sum_{\substack{ad=n \\ a>0}} \left[g\left(\log\left|\frac{a}{d}\right|\right)\log(4e^\gamma) + \int_0^\infty \frac{g(u+\log|\frac{a}{d}|)-g(\log|\frac{a}{d}|)}{2\sinh(u/2)}\,du - \frac{1}{4}h(0)\right] \\
&+ 2\sum_{m=2}^{\infty}\sum_{\substack{ad=n \\ a>0}} \frac{\Lambda(m)}{m} g\left(\log\left|\frac{a}{d}\right| - 2\log m\right), \\
&+ \begin{cases} -\frac{1}{12\sqrt{n}}\int_{-\infty}^{\infty}\frac{g'(u)}{\sinh\left(\frac{u}{2}\right)}\,du + \left(\log\left(\frac{\pi\sqrt{n}}{2}\right)+\gamma\right) g(0) & \\ -\int_0^\infty \log\left(2\sinh\left(\frac{u}{2}\right)\right) g'(u)\,du & \text{if } \sqrt{n}\in\mathbb{Z}, \\ 0 & \text{otherwise,} \end{cases}
\end{aligned}
$$

where

$$
L(1,\psi_D) = \frac{L(1,\psi_d)}{l}\prod_{p|l}\left[1+(p-\psi_d(p))\frac{(l,p^\infty)-1}{p-1}\right],
$$

with $D = dl^2$*,* $l > 0$*,* d *a fundamental discriminant and* $\psi_d(p) = \left(\frac{d}{p}\right)$*. Here* (l, p^∞) *denotes the largest power of* p *that divides* l*. Additionally* $\sigma_1(n) = \sum_{d|n} d$ *is the divisor function,* $\Lambda(m)$ *is the von Mangoldt function,* $\varepsilon = \mathrm{sign}(n)$ *and* $X(m) = \prod_{k \bmod m}\gcd(k,m)$*.*

Remark 2.2.1. We refer to the terms in the sum with $D > 0$ as the hyperbolic terms and the terms $D < 0$ as the elliptic terms.

2.2.1 Computational remarks

The main numerical bottleneck of computing the trace formula is from the contribution of the hyperbolic terms, which involves computing the class number and regulator of $\mathbb{Q}(\sqrt{D})$. For numerical stability, it is best to consider a test function g that is compactly supported. This allows one to compute the terms on the geometric side to arbitrary precision with a fixed finite list of class numbers. Precisely we would need class numbers $h_{\mathbb{Q}(\sqrt{D})}$ for $D = t^2 - 4n < (2n\cosh(X/2))^2$.

We can also get a bonus increase in the precision of the algorithm by splitting the spectrum between even and odd forms separately. For this, we recall that for even forms, the Hecke eigenvalues satisfy $a(n) = a(-n)$, and odd forms they satisfy $a(n) = -a(-n)$. Hence, the traces given by $\frac{1}{2}(t(n,h) + t(-n,h))$ and $\frac{1}{2}(t(n,h) - t(-n,h))$ will pick out the even and odd forms respectively. This effectively allows us to consider double the amount of forms for a fixed parity.

Computing the integrals appearing in the elliptic terms to arbitrary precision can also be challenging given the large number of them appearing for values of D and n. We can remedy this by noting that $|D/4n| \in (0,1]$ for $D = t^2 - 4n < 0$, and considering the integrals as functions $f : (0,1] \to \mathbb{R}$ defined by

$$f(x) = \int_0^\infty \frac{g(u)\cosh(u/2)}{\sinh^2(u/2) + x}\, du.$$

This function is analytic with respect to the variable x, hence we can approximate this integral with a Taylor series, where the only integrals we need to compute are given in the Taylor coefficients. Explicitly, for x near x_0, we can approximate $f(x)$ by

$$f(x) = \sum_{k=0}^{K} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + R_K(x),$$

where $R_K(x)$ is the error term given by

$$R_K(x) = \frac{f^{(K+1)}(\xi)}{(K+1)!}(x - x_0)^{K+1},$$

for some ξ in the closed interval between x and x_0. To find the Taylor coefficients, we use Leibniz's integral rule to get

$$\frac{d^k}{dx^k} f(x) = k!(-1)^k \int_0^\infty \frac{g(u)\cosh(u/2)}{(\sinh^2(u/2) + x)^{k+1}}\, du.$$

To bound the error term, let $\xi \in [x_0, x]$ and $M_g = \max_{y\in[0,\infty)} |g(y)|$. Then

$$\begin{aligned} |f^{(K+1)}(\xi)| &= (K+1)! \left| \int_0^\infty \frac{g(u)\cosh(u/2)}{(\sinh^2(u/2)+\xi)^{K+2}}\, du \right| \\ &\leq M_g (K+1)! \int_0^\infty \frac{\cosh(u/2)}{(\sinh^2(u/2)+\xi)^{K+2}}\, du. \end{aligned}$$

Here we have that

$$\int_0^\infty \frac{\cosh(u/2)}{(\sinh^2(u/2)+\xi)^{K+2}}\, du = \pi \xi^{-3/2-K} \prod_{k=1}^{K+1} \left(\frac{2k-1}{2k} \right).$$

Hence we can bound the error term in the Taylor series by

$$|R_K(x)| \leq \frac{\pi M_g}{\sqrt{x_0}} \left| 1 - \frac{x}{x_0} \right|^{K+1} \prod_{k=1}^{K+1} \left(\frac{2k-1}{2k} \right).$$

To compute all the elliptic integrals, we shall need to choose the sample points for our Taylor series, such that it minimises the number of Taylor coefficients that are needed to be computed. Since there is a singularity at $x = 0$, it is best for us to choose our sampling points geometrically, that is $x_j = c^{-j}$ for some $c > 1$. Suppose, we take K terms of a Taylor expansion around the point x_j, we can see that error is of size about $|1 - x/x_0|^K$. For our sample points, we have

$$\left| 1 - \frac{x}{x_0} \right| \leq \left(\frac{c-1}{c+1} \right),$$

hence the worst our error could be is $\left(\frac{c-1}{c+1}\right)^K$. Note, that given x we can choose $j = \lceil \log_c(\frac{2}{(c+1)x}) \rceil$. Thus to choose the number of sampling points needed, we just consider the smallest value of x that we could feasibly have.

We see that the number of sample points is about $\log_c n$, where n is the largest Hecke operator we shall need to consider. So in total we have to compute about $K \log_c n$ integrals, and we want to minimise this with respect to the constraint that $\left(\frac{c-1}{c+1}\right)^K < \varepsilon$ for some fixed error tolerance ε. This surprisingly has the exact solution with $c = 1 + \sqrt{2}$ and $K = \log_c(1/\varepsilon)$.

In addition to this, the other integrals in the trace formula also need be taken with some care when implementing in interval arithmetic, mainly due to their removable singularities. The main integrals where this is a problem are the following from the sum over the divisors of n,

$$\int_0^\infty \frac{g(u + \log|\frac{a}{d}|) - g(\log|\frac{a}{d}|)}{2\sinh(u/2)}\, du.$$

Near $u = 0$, we essentially get $0/0$, which interval arithmetic can struggle to manage. To circumvent this, we can factor out a u from the numerator, and rewrite the denominator in terms of the $\operatorname{sinc}(x) = \sin(x)/x$ function. This does rely on there being a "nice" expression for the numerator divided by u. We do not give details here how one would go about doing this, however if one were to look at the test function in Section 2.4, we see that it is essentially a sum of polynomials in u, so it should not be too difficult to derive such an expression. The method we used to implement numerical integration in interval arithmetic is given in Appendix B.

2.3 The Selberg Trace Formula for squarefree level $N > 1$

Similar to the level 1 case, we use the trace formula derived by Strömbergsson in [Str16], and rewrite it in the following form, following Proposition 2.2 in [BL17].

Theorem 2.3.1 (The Selberg trace formula for Maass newforms for squarefree level and trivial character)**.** *Fix $\delta > 0$, let $h(t)$ be a even analytic function on the strip $\{t \in \mathbb{C} : \operatorname{Im}(t) \le \frac{1}{2} + \delta\}$ such that $h(r) \in \mathbb{R}$ for $r \in \mathbb{R}$ and $h(r) = O((1 + |r|^2)^{-1-\delta})$. Define g as the Fourier transform of h given by*

$$g(u) = \frac{1}{2\pi} \int_{-\infty}^{\infty} h(r) e^{-iru}\, dr.$$

Let $\{f_j\}$ be a sequence of normalised Hecke eigenforms of squarefree level N, with Laplacian eigenvalues $\lambda_j = \frac{1}{4} + r_j^2$ and respective Hecke eigenvalues $a_j(n)$.

Then, for $(N, n) = 1$ *we have*

$$\frac{\mu(N)\sigma_1(|n|)}{\sqrt{|n|}} h\left(\frac{i}{2}\right) + \sum_{j>0} h(r_j)a_j(n)$$
$$= \sum_{\substack{t\in\mathbb{Z} \\ \sqrt{D}=\sqrt{t^2-4n}\notin\mathbb{Q}}} c_N(D) \cdot \begin{cases} g\left(\log\left(\frac{(|t|+\sqrt{D})^2}{4|n|}\right)\right) & \text{if } D > 0, \\ \frac{\sqrt{|D/4n|}}{2\pi} \int_{-\infty}^{\infty} \frac{g(u)\cosh(u/2)}{\sinh^2(u/2) + |D/4n|} du & \text{if } D < 0 \end{cases}$$
$$+ \Lambda(N) \sum_{\substack{ad=n \\ a>0 \\ a\neq d}} \frac{g\left(\log\left|\frac{a}{d}\right|\right)}{(N^\infty, |a-d|)} - 2\Lambda(N) \sum_{\substack{ad=n \\ a>0}} \sum_{r=0}^{\infty} N^{-r} g\left(\log\left|\frac{a}{d}\right| - 2r\log(N)\right)$$
$$+ \begin{cases} -\frac{\prod_{p|N}(p-1)}{12\sqrt{n}} \int_{-\infty}^{\infty} \frac{g'(u)}{\sinh\left(\frac{u}{2}\right)} du & \text{if } \sqrt{n} \in \mathbb{Z}, \\ 0 & \text{otherwise,} \end{cases}$$

where

$$\begin{aligned} c_N(D) &= L(1, \psi_D) \prod_{p|N} (\psi_d(p) - 1) \\ &= \frac{L(1, \psi_d)}{l} \prod_{p|N} (\psi_d(p) - 1) \prod_{p|l} \left[1 + (p - \psi_d(p)) \frac{(l, p^\infty) - 1}{p - 1}\right], \end{aligned}$$

with $D = dl^2$, $l > 0$, d *a fundamental discriminant and* $\psi_d(p) = \left(\frac{d}{p}\right)$. *Here* (l, p^∞) *denotes the largest power of* p *that divides* l. *Additionally* $\sigma_1(n) = \sum_{d|n} d$ *is the divisor function,* $\mu(n)$ *is the Möbius function and* $\Lambda(m)$ *is the von Mangoldt function.*

Remark 2.3.1. We refer to the terms in the sum with $D > 0$ as the hyperbolic terms and the terms $D < 0$ as the elliptic terms. The terms that are multiplied by the von Mangoldt function $\Lambda(N)$ we call the parabolic terms, and the term when $\sqrt{n} \in \mathbb{Z}$ we call the identity term.

The computational remarks from Section 2.2.1 about computing the hyperbolic and elliptic terms are also relevant here.

2.4 Choice of test function

As stated in the previous sections, we will want a test function that is even, positive and monotonically decreasing. Moreover, to aid in computations, we will also want

g, the Fourier transform of h, to be compactly supported. This will make all the integrals and sums on the geometric side have finite bounds which will help when implementing the algorithm.

2.4.1 Candidate test function

A good initial function to consider is powers of the $\operatorname{sinc}(x) = \sin(x)/x$ function. For even powers, this is a positive even function with a compactly supported Fourier transform. However, this function is not monotonically decreasing. To remedy this we consider the test function

$$h_1(t) = \frac{\pi^2}{\pi^2+4}\left[\operatorname{sinc}^2\left(\frac{t}{2}\right) + \frac{1}{2}\operatorname{sinc}^2\left(\frac{t-\pi}{2}\right) + \frac{1}{2}\operatorname{sinc}^2\left(\frac{t+\pi}{2}\right)\right],$$

and let $h_d(t) = h_1(t)^d$ for $d \in \mathbb{N}$. We can see that this is decreasing and positive by noting that $\sin^2(t/2) + 1/2(\sin^2(t/2+\pi/2) + \sin^2(t/2-\pi/2)) = 1$, that is, the waves constructively amplify the signal everywhere. Then $h_d(t)$ is a positive, even and monotonically decreasing function on $\mathbb{R}_{>0}$, satisfying $h_d(0) = 1$ and

$$h_d(t) \sim \left(\frac{4\pi^2}{\pi^2+4}\right)^d t^{-2d},$$

as $|t| \to \infty$. Moreover, its Fourier transform

$$g_d(x) = \frac{1}{\pi}\int_0^\infty h_d(t)\cos(tx)\,dt, \tag{2.7}$$

is compactly supported on $[-d, d]$. For a fixed d we can express g_d in the form

$$g_d(x) = \sum_{m\in\{-1,0,1\}} A_m(x)e^{\pi i m x},$$

where

$$A_m(x) = A_{m,j}\left(x - j - \frac{1}{2}\right) \qquad \text{for } x \in [j, j+1), j \in \{-d, \ldots, d-1\},$$

for some $A_{m,j} \in \mathbb{C}[x]$ satisfying $A_{m,-1-j}(x) = A_{-m,j}(-x) = \overline{A_{m,j}(-x)}$. Note that all the $A_{m,j}$ are determined by those with $m \in \{0,1\}$ and $j \in \{0, \ldots, d-1\}$.

Specifically, for $d = 1$, we have

$$A_{0,0}(x) = \frac{\pi^2}{\pi^2+4}\left(\frac{1}{2} - x\right) \qquad \text{and} \qquad A_{1,0}(x) = \frac{1}{2}A_{0,0}(x).$$

For $d > 1$, we compute the functions using convolutions. More explicitly, suppose we are given functions

$$A(x) = \sum_{m\in\{-1,0,1\}} A_m(x)e^{\pi imx} \quad \text{and} \quad B(x) = \sum_{m\in\{-1,0,1\}} B_m(x)e^{\pi imx},$$

and we wish to compute their convolution $C = A * B$, which is again a function of the same form. For a set S, we define the indicator function $\mathbf{1}_S(x) = 1$ if $x \in S$ and 0 if $x \notin S$. It suffices to consider the constituent functions

$$A_{m,j}\left(x - j - \frac{1}{2}\right) e^{\pi imx}\mathbf{1}_{[j,j+1)}(x) \quad \text{and} \quad B_{n,k}\left(x - k - \frac{1}{2}\right) e^{\pi inx}\mathbf{1}_{[k,k+1)}(x),$$

with convolution

$$\int_{\mathbb{R}} A_{m,j}\left(y - j - \frac{1}{2}\right) e^{\pi imy}\mathbf{1}_{[j,j+1)}(y)B_{n,k}\left(x - y - k - \frac{1}{2}\right) e^{\pi in(x-y)}\mathbf{1}_{[k,k+1)}(x-y)\,dy.$$

Consider $x \in [j+k+\delta, j+k+\delta+1)$ for some $\delta \in \{0,1\}$, and let $t = x - \big(j + k + \delta + \frac{1}{2}\big)$. We make the change of variable $y \mapsto y + j + \frac{1}{2}$ to get

$$\begin{aligned}
&\int_{\mathbb{R}} A_{m,j}(y)e^{\pi im\left(y+j+\frac{1}{2}\right)}\mathbf{1}_{\left[-\frac{1}{2},\frac{1}{2}\right)}(y)B_{n,k}\left(t + \delta - \frac{1}{2} - y\right) e^{\pi in\left(x-y-j-\frac{1}{2}\right)}\mathbf{1}_{(t+\delta-1,t+\delta]}(y)\,dy \\
&= e^{\pi i(m-n)\left(j+\frac{1}{2}\right)+\pi inx}(-1)^\delta \int_{\delta-\frac{1}{2}}^{t} A_{m,j}(y)B_{n,k}\left(t + \delta - \frac{1}{2} - y\right) e^{\pi i(m-n)y}\,dy. \qquad (2.8)
\end{aligned}$$

When $m \neq n$ we apply repeated integration by parts to see that (2.8) becomes

$$\begin{aligned}
&e^{\pi i(m-n)\left(j+\frac{1}{2}\right)+\pi inx}(-1)^\delta \sum_{r=0}^{\deg A_{m,j}} \sum_{s=0}^{\deg B_{n,k}} \frac{(-1)^s\binom{r+s}{s}}{(-\pi i(m-n))^{r+s+1}} \\
&\cdot \left(A_{m,j}^{(r)}\left(\delta - \frac{1}{2}\right) B_{n,k}^{(s)}(t)e^{\pi i(m-n)\left(\delta-\frac{1}{2}\right)} - A_{m,j}^{(r)}(t)B_{n,k}^{(s)}\left(\delta - \frac{1}{2}\right) e^{\pi i(m-n)t}\right) \\
&= (-1)^{(m-n+1)\delta} \sum_{r=0}^{\deg A_{m,j}} \sum_{s=0}^{\deg B_{n,k}} \frac{(-1)^s\binom{r+s}{s}}{(-\pi i(m-n))^{r+s+1}} \\
&\cdot \left(A_{m,j}^{(r)}\left(\delta - \frac{1}{2}\right) B_{n,k}^{(s)}(t)(-1)^{(m-n)j}e^{\pi inx} - A_{m,j}^{(r)}(t)B_{n,k}^{(s)}\left(\delta - \frac{1}{2}\right)(-1)^{(m-n)k}e^{\pi imx}\right).
\end{aligned}$$

Note that this will contribute to both the $C_{m,j+k+\delta}$ and $C_{n,j+k+\delta}$ terms.

When $m = n$, we define polynomials $P_{\delta,l} \in \mathbb{C}[y]$ such that $P_{\delta,0} = A_{m,j}(y)$ and

$$P_{\delta,l} = \int_{\delta-\frac{1}{2}}^{y} P_{\delta,l-1}(u)\,du,$$

for $l \geq 1$. Then applying integration by parts, (2.8) becomes

$$(-1)^\delta \sum_{l=1}^{\deg B_{n,k}+1} B_{n,k}^{(l-1)} \left(\delta - \frac{1}{2}\right) P_{\delta,l}(t) e^{\pi imx}.$$

Dilations

As will be explained later, we will optimise some of the values that comes from defining the test function such as the support and power d. Part of this is to consider the test function $h(t) = h_d(at)$ for some $a \in \mathbb{R}$. Thus, by (2.7), we have that its Fourier transform is of the form

$$g(u) = \frac{1}{a} g_d\left(\frac{u}{a}\right).$$

If g_d is supported on $[-d, d]$, then g is supported on $[-ad, ad]$. Thus, we get the more general form of g being

$$g(x) = \sum_{m \in \{-1,0,1\}} B_m(x) e^{\pi imx/a},$$

where $B_m(x) = A_m\left(\frac{x}{a}\right)$.

Derivatives

In the verification of Maass forms in Section 2.1, we needed to consider test functions of the form $\tilde{h}(\lambda) = \lambda^n h(\lambda)$ for some $n \in \mathbb{N}$. In the world of Fourier analysis, this just amounts to the derivative of the Fourier transform. More explicitly, by (2.7), we have for $n > 0$

$$\frac{d^n g_d(x)}{dx^n} = \begin{cases} \dfrac{(-1)^{(n+1)/2}}{\pi} \displaystyle\int_0^\infty t^n h_d(t) \sin(tx)\, dt & \text{if } n \text{ is odd,} \\ \dfrac{(-1)^{n/2}}{\pi} \displaystyle\int_0^\infty t^n h_d(t) \cos(tx)\, dt & \text{if } n \text{ is even.} \end{cases}$$

Since we will still want the Fourier transform of $\lambda^n h(\lambda)$ to be even, we will only be considering even n. Explicitly to compute the derivative of (2.7), we have

$$\frac{dg_d(x)}{dx} = \sum_{m \in \{-1,0,1\}} \left(A'_m(x) + \pi im A_m(x)\right) e^{\pi imx},$$

which is again in the form

$$\sum_{m\in\{-1,0,1\}} C_m(x)e^{\pi imx}$$

for polynomials $C_m(x) = A'_m(x) + \pi imA_m(x)$. To compute higher degree derivatives we then use $\frac{d^n g}{dx^n} = \frac{d^{n-1}}{dx^{n-1}}\frac{dg}{dx}$. We note that we shall also be taking derivatives of a dilated test function. In this case, we apply the same idea as above, noting that we are replacing x with x/a.

2.4.2 Optimising the test function

We wish to optimise the decay of the test function for certain given constants such that we maximise the precision with which we compute the trace formula. Suppose we aim for a final precision of B bits. Due to the square roots in (2.3) and (2.4), we must consider terms larger than 2^{-2B} to be significant, and use a working precision of at least $2B$ bits. Let $X \in \mathbb{R}_{>0}, d \in \mathbb{N}$ and consider the test function

$$h(r) = h_d\left(\frac{Xr}{d}\right). \tag{2.9}$$

From this we see that g, the Fourier transform of h, is compactly supported on $[-X, X]$. We take the edge of the precision window to be the point $R_{\max}$ at which

$$h(R_{\max}) = h_1(XR_{\max}/d)^d = 2^{-2B}. \tag{2.10}$$

Fix a level N. Let M be the number of level N newforms with trivial character, fixed parity and Laplace eigenvalue $\lambda \leq \frac{1}{4} + R_{\max}^2$ and let $D_{\max}$ be the largest size of discriminant appearing in the hyperbolic sum. The value M will control the size of the matrices appearing in the linear algebra and $D_{\max}$ will control how many hyperbolic terms will appear. We want the ability to choose these values since these are the main sections of the algorithm that are constrained by external factors. For example, we will only have a list of class numbers up to a certain limit that that could feasibly be computed. The idea of this section is to first fix N, M and $D_{\max}$, then find $R_{\max}, X$ and d such that it maximises the precision B.

So fix N, M and $D_{\max}$. To find $R_{\max}$, we have from [Ris04] that

$$M = \frac{R_{\max}^2}{24}N + O(\sqrt{\lambda}\log\lambda),$$

which we can rearrange to compute $R_{\max}$ by

$$R_{\max} \approx \sqrt{\frac{24M}{N}}.$$

To find X, we use the fact that g is compactly supported on $[-X, X]$ and hence, we have that

$$D_{\max} = \left(2M \cosh\left(\frac{X}{2}\right)\right)^2,$$

which we can rearrange to compute X by

$$X = 2\cosh^{-1}\left(\frac{\sqrt{D_{\max}}}{2M}\right).$$

Once we have values for $R_{\max}$ and X, we can find d by first rearranging (2.10) to obtain

$$-\log_2\left(h_1\left(\frac{XR_{\max}}{d}\right)\right)d = 2B.$$

We can now find a d which maximises the left side of this equation, which in turn will maximise our final precision B. Note that since $d \in \mathbb{N}$, we can find the maximum by sampling the left side of the equation over integer values of d and choosing the largest value.

Thus, once we have computed these values, the test function we use for the computation is given by (2.9). In practice, when choosing the level N, we pick N to be the largest level we are computing with and use this test function for all smaller levels as well.

2.5 Computational results

2.5.1 Computing the forms

We implemented this algorithm in the C programming language, predominately using the ball-arithmetic library `Arb` [Joh17] throughout our computations to manage round-off errors. For the main computation, following the notation from Section 2.4.2, we chose the numbers $D_{\max} = 10^9, M = 2000$ and the maximum level we consider is $N = 105$. Using `SageMath` [The20], we find $X \approx 5.51341, R_{\max} \approx 21.38089, d = 13$ and $2B \approx 63$. We we used `Pari` [The22] to compute the real class numbers and regulators required, and verified the calculations with the algorithm from Chapter 3.

With these numbers, we computed a total of 33214 Laplace eigenvalues of Maass cusp forms, each with all Hecke eigenvalues a_n with $n \leq 2000$ and $(n, N) = 1$, for squarefree levels $2 \leq N \leq 105$. The range of the ε_i's computed is between 10^{-15} and 10^{-2}. Of these forms 17243 are even and 15971 are odd.

Of these Laplace eigenvalues, we proved completeness for 16207 of them and hence, their Hecke eigenvalues have rigorous error bounds. We could only compute completeness for all prime levels $2 \leq N \leq 67$ and all composite squarefree levels $6 \leq N \leq 105$ due to the precision of the computed trace formula values in the linear algebra. Each of these complete Laplace eigenvalues will correspond to a provably unique Maass cusp form. Of these forms 8419 are even and 7788 are odd.

We observed that the closest distance between two Maass forms in the completed range was approximately 3×10^{-6} from the level 23 Laplace eigenvalues of $10.85166055\ldots$ and $10.8516021\ldots$. The closest distance between two even forms was approximately 1.4×10^{-5} from the level 53 Laplace eigenvalues of $5.876312\ldots$ and $5.876299\ldots$. The closest distance between two odd forms was approximately 3×10^{-6} from the level 55 Laplace eigenvalues of $8.350572\ldots$ and $8.350569\ldots$.

The entire computation took just under two weeks of time on 64 cores of 2.5GHz AMD Opteron processors. As predicted, the computation was dominated by computing the hyperbolic terms. We now provide some statistical evidence towards various conjectures described in Section 1.10.

2.5.2 Ramanujan–Petersson conjecture

We recall, the Ramanujan–Petersson conjecture states that for prime p, the pth Fourier coefficient a_p for a Maass cusp form on $\Gamma_0(N)$ should satisfy $|a_p| \leq 2$. For the data we computed, we verified this was true for all Hecke eigenvalues with $p \leq 2000$ for 13271 of our Maass forms that we proved completeness for.

2.5.3 Sato–Tate conjecture

The Sato–Tate conjecture states that the a_p should be asymptotically distributed with respect to the Sato–Tate measure given by

$$\mu_\infty = \frac{1}{\pi}\sqrt{1 - \frac{x^2}{4}}\, dx,$$

as $p \to \infty$. A related result, proven by Sarnak in [Sar87], states that instead if we fix a prime $p \nmid N$ and let the level tend to infinity or the Laplace eigenvalue tend

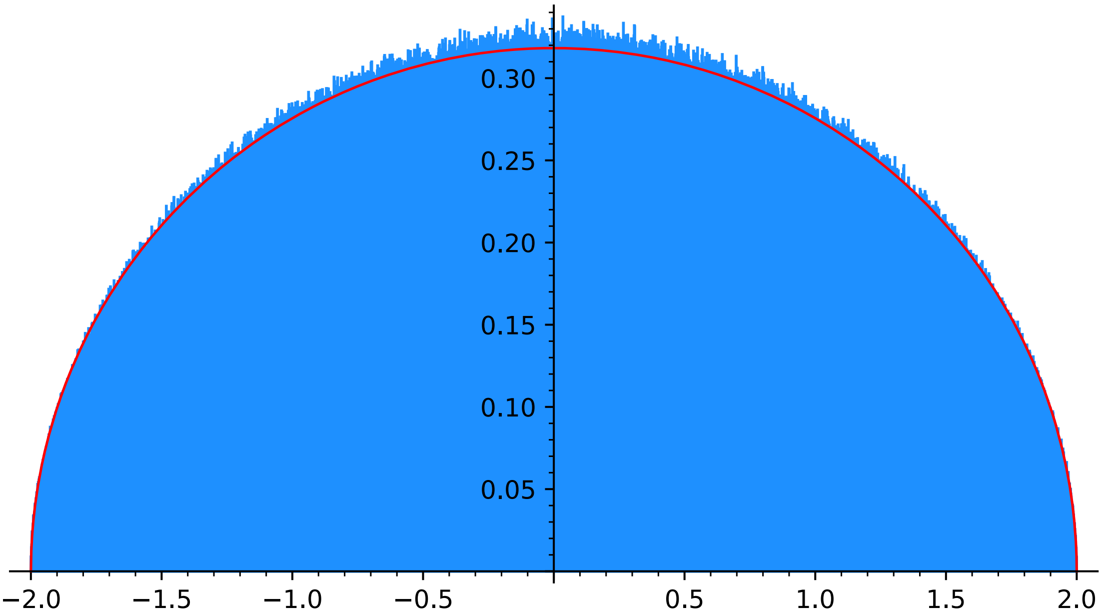


Figure 2.1: Comparison of our data to the predicted Sato–Tate measure. The data is all a_p from our 33214 Maass forms with $2 \leq p \leq 2000$ and p not dividing the respective levels of these forms. The histogram has 10003411 data points in 3162 bins.

to infinity, then the points a_p of these forms are asymptotically distributed by the measure

$$\mu_p = f_p \, \mu_\infty,$$

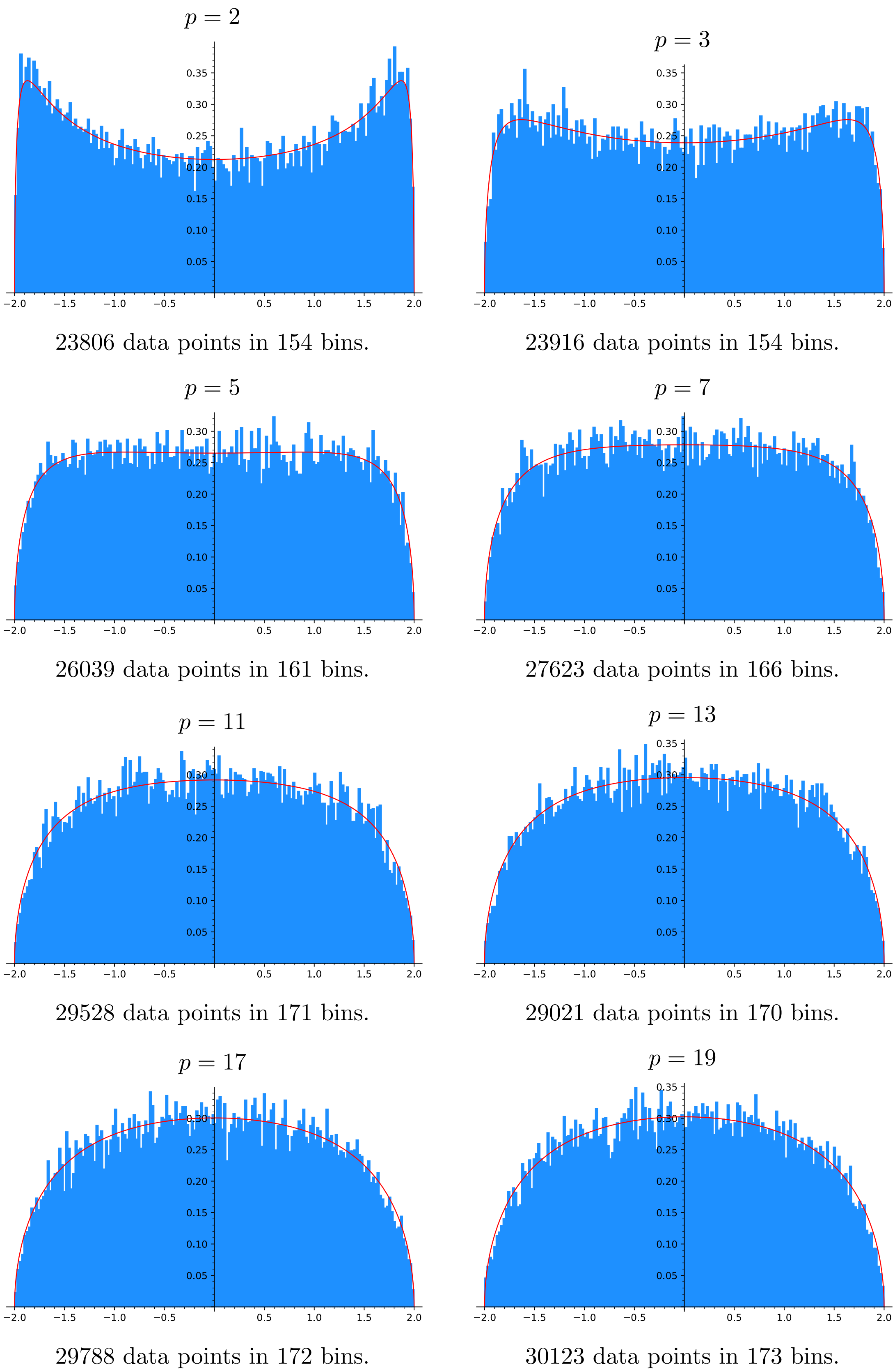
where

$$f_p(x) = \frac{p+1}{(p^{1/2} + p^{-1/2})^2 - x^2},$$

for $x \in [-2, 2]$. As an example, for $p = 2$, the points should be distributed asymptotically with respect to

$$\mu_2 = \frac{3\sqrt{4 - x^2}}{9 - 2x^2} \frac{dx}{\pi}. \tag{2.11}$$

We used the Maass form data to create Figures 2.1 and 2.2, which illustrates a strong connection to the predicted result of the Sato–Tate conjecture and the result proven by Sarnak.



23806 data points in 154 bins.

23916 data points in 154 bins.

26039 data points in 161 bins.

27623 data points in 166 bins.

29528 data points in 171 bins.

29021 data points in 170 bins.

29788 data points in 172 bins.

30123 data points in 173 bins.

Figure 2.2: Comparison of our data to Sarnak's theorem [Sar87] for a_p with prime $2 \leq p \leq 19$.

2.5.4 L-function and the Riemann hypothesis

Let f be a Maass cusp form, with Laplace eigenvalue $\lambda = \frac{1}{4} + r^2$, of level N and trivial character. Moreover, let $a_f(n)$ be the Hecke eigenvalues of f. We define the associated L-function to f by

$$L_f(s) = \sum_{n=1}^{\infty} \frac{a_f(n)}{n^s},$$

where $\mathrm{Re}(s) > 1$.

It is conjectured, analogous to the Riemann zeta function, that L-functions associated to Maass cusp forms on $\Gamma_0(N)$ satisfy a Riemann hypothesis, that is all the zeros of $L_f(s)$ in the strip $\{s \in \mathbb{C} \mid 0 < \mathrm{Re}(s) < 1\}$ lie on the line $s = 1/2 + it$, $t \in \mathbb{R}$. For computations, it is easier to work with the associated real-valued Z-function, defined by (1.3), since they share the same zeros on the critical line. An example of a Z-function is shown in Figure 2.3.

For the Maass forms we computed we used Rubenstein's library `lcalc` [Rub] to compute the L-function and calculate the zeros in the strip. We did this for all complete forms with $\varepsilon_i \leq 10^{-10}$ and found no zeros off the line, up to height $t = 100$. To do this we computed the $a_f(n)$ with $(n, N) > 1$ up to $n \leq 2000$ using the method in Section 2.1.4. The method employed in `lcalc` to find zeros on the critical line is heuristic, however computing zeros on the critical line could be made rigorous with more work using the method in [BT18].

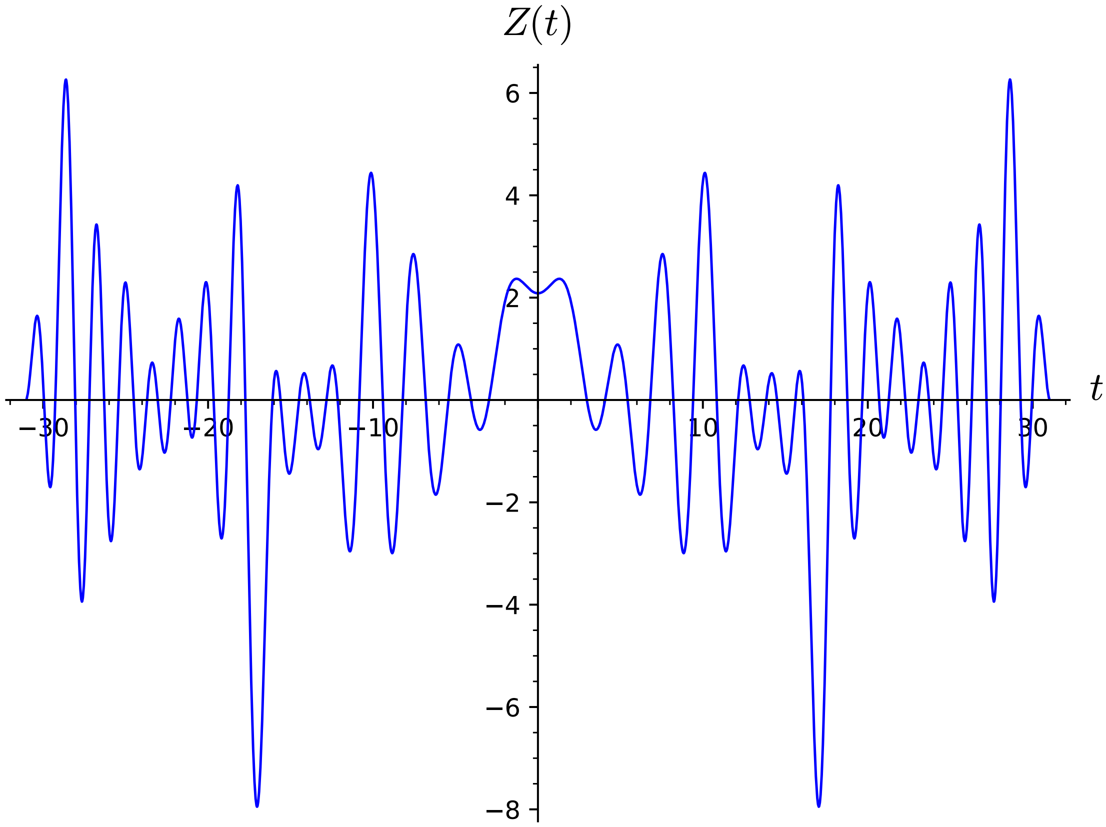


Figure 2.3: Plot of the Z-function on the critical line associated to the first level 105 Maass cusp form with Laplace eigenvalue $r = 0.4366582\ldots$.

Chapter 3

Unconditional computation of real quadratic class numbers

Class groups are fundamental objects in number theory and have been studied in various forms for several centuries. Over the years several authors, including Gauss, have produced tables of the various invariants of the class group of quadratic fields, most notably the class number. With his computations, Gauss stated his famous conjecture that there are infinitely many real quadratic fields with class number one. A further use of computations of class groups is in the statement of the Cohen–Lenstra heuristics [CL84], which were inspired by numerical data.

When using this numerical data to aid in giving evidence towards conjectures, it would be ideal that these objects were computed unconditionally. Unfortunately, the current fastest algorithms for computing class numbers rely on the generalised Riemann hypothesis (GRH).

The current best algorithm for computing class numbers, due to Hafner and McCurley [HM89], computes real quadratic class numbers in an expected subexponential runtime of $O(\exp((\log d)^{1/2+\varepsilon}))$, where d is the discriminant of the quadratic number field $\mathbb{Q}(\sqrt{d})$. Unfortunately, this algorithm relies on GRH and also the runtime analysis is heuristic. Later, Buchmann [BV07] generalised their work to all number fields and gave a deterministic algorithm for quadratic fields, still reliant on GRH, that runs in time $O(d^{1/4+\varepsilon})$. Booker [Boo06] used Buchmann's algorithm to derive a verification algorithm that unconditionally terminates and, under GRH, runs in $O(d^{1/4+\varepsilon})$. An alternative algorithm given by Lenstra [Len82], based on Shanks' method of "baby step-giant step", has runtime of $O(d^{1/5+\varepsilon})$. This is also completely dependent on GRH to provably give correct answers in this runtime.

For imaginary quadratic fields, Jacobson, Ramachandran and Williams [JRW06] resolved the issue of conditional computation by deriving a batch verification algorithm to verify the entire table of class groups. The main tool used was an explicit version of the Eichler–Selberg trace formula for holomorphic modular forms. In this chapter, we follow the same approach for real quadratic fields, however we use an explicit version of the Selberg trace formula for Maass forms as the basis for a novel algorithm to verify a list of class numbers.

The main difference between using Maass forms and holomorphic modular forms is that the trace formula for holomorphic forms isolates a fixed weight, resulting in a finite-dimensional space. In fact, the approach in [JRW06] used a space of dimension 0, so no modular form computations were needed in order to compute traces. By contrast, the trace formula for Maass forms necessarily involves infinitely many forms. In practice this means that we need to truncate certain infinite sums and estimate the error, and we require explicit, rigorous numerical computations of Maass forms.

This chapter is heavily based on work by Ce Bian, Andrew R. Booker, Austin Docherty, Michael J. Jacobson and the author [BBD$^+$23], soon to appear. Additional details on how to compute the class groups and further analysis regarding testing various conjectures can also be found in the paper.

3.1 Verification algorithm

Let $\{f_j\}_{j=1}^{\infty}$ be a Hecke-eigenbasis for Maass forms of the full modular group $\mathrm{PSL}(2,\mathbb{Z})$, with Laplace eigenvalues $\lambda_j = \frac{1}{4} + r_j^2$ and Hecke eigenvalues $a_j(n)$. The r_j may be taken to be positive real numbers, and we may assume that the f_j are ordered such that $r_1 \le r_2 \le r_3 \le \ldots$. Additionally, the f_j have a Fourier expansion of the form

$$f_j(x+iy) = \sum_{n=1}^{\infty} \frac{a_j(n)}{\sqrt{n}} \widetilde{W}_{ir_j}(2\pi ny) \cos^{(\omega_j)}(2\pi nx),$$

where $\widetilde{W}_{ir}(x) = e^{\frac{\pi}{2}r} W_{ir}(x) = \sqrt{x} e^{\frac{\pi}{2}r} K_{ir}(x)$ and $K_{ir}(x)$ is the K-Bessel function. In addition, we define $\cos^{(\omega)} = \cos$ if $\omega = 0$ and $\cos^{(\omega)} = \sin$ if $\omega = 1$. We remark that the normalising factor $e^{\frac{\pi}{2}r}$ is non-standard; it is designed to compensate for the exponential decay of the K-Bessel function as $r \to \infty$ and is convenient for numerical purposes.

3.1.1 The Selberg trace formula

The Selberg trace formula is an expression for the weighted sum

$$\sum_{j=1}^{\infty} a_j(n) h(r_j),$$

where $n \in \mathbb{Z}\backslash\{0\}$ and h is a suitable test function (see Proposition 3.1.1 for more details). For us the key interest in this formula is that it involves the values $L(1,\chi)$

for quadratic Dirichlet characters χ, which are in turn related to quadratic class groups via Dirichlet's class number formula.

To state the formula precisely, we recall some notation from Section 1.1 in [BL17]. Let $\mathcal{D}$ denote the set of discriminants, that is

$$\mathcal{D} = \{D \in \mathbb{Z} : D \equiv 0 \text{ or } 1 \pmod 4\}.$$

Any non-zero $D \in \mathcal{D}$ can be uniquely expressed in the form $d\ell^2$, where d is a fundamental discriminant and $\ell > 0$. We define

$$\psi_D(n) = \left(\frac{d}{n/\gcd(n,\ell)}\right),$$

where $(-)$ denotes the Kronecker symbol. We see that ψ_D is periodic modulo D, and if D is a fundamental discriminant, then ψ_D is the usual quadratic character modulo D. We set

$$L(s,\psi_D) = \sum_{n=1}^{\infty} \frac{\psi_D(n)}{n^s} \quad \text{for } \operatorname{Re}(s) > 1.$$

When we set $D = d\ell^2$, we can rewrite this as

$$L(s,\psi_D) = L(s,\psi_d) \prod_{p|\ell} \left[1 + (1-\psi_d(p)) \sum_{j=1}^{\operatorname{ord}_p(\ell)} p^{-js}\right].$$

Here we see that $L(s,\psi_D)$ has analytic continuation to $\mathbb{C}$, apart from a simple pole at $s = 1$ when D is square. When D is not a square, we have

$$L(1,\psi_D) = \frac{L(1,\psi_d)}{\ell} \prod_{p|\ell} \left[1 + (1-\psi_d(p)) \frac{(\ell,p^\infty)-1}{p-1}\right].$$

Here (l, p^∞) denotes the largest power of p that divides l. We can now state the Selberg trace formula for the modular group using results from [BL17].

Proposition 3.1.1 (The Selberg trace formula for the modular group)**.** *Let n be a non-zero integer and $f \in C^3(\mathbb{R})$ be even of compact support. Define*

$$h(r) = 2|n|^{-ir} \int_0^\infty f\left(v - \frac{n}{v}\right) v^{2ir} \frac{dv}{v} \quad \textit{for } r \in \mathbb{R},$$

and for $a \in \mathbb{N}$ with $a \mid n$ define

$$
\begin{aligned}
\Phi(a) &= 2\sum_{m=1}^{\infty} \frac{\Lambda(m)}{m} f\Big(am - \frac{n}{am}\Big) + 2a\int_a^{\infty} \frac{f(v-\frac{n}{v}) - f(a-\frac{n}{a})}{v^2-a^2}\,dv \\
&\quad + \big(\gamma + \log(4\pi)\big) f\Big(a - \frac{n}{a}\Big) - \frac{1}{2}\int_0^{\infty} f\Big(v - \frac{n}{v}\Big)\,\frac{dv}{v} \\
&\quad - a^{-1}\int_{\mathbb{R}} f\Big(\sqrt{y^2 - \min(4n,0)}\Big)\,dy \\
&+ \begin{cases} \displaystyle\sum_{\substack{m\in\mathbb{N} \\ m|(a-\frac{n}{a})}} \Lambda(m)\big(1-m^{-1}\big) f\Big(a-\frac{n}{a}\Big) + \int_{|a-\frac{n}{a}|}^{\infty} \frac{f(y)}{y + |a-\frac{n}{a}|}\,dy & \text{if } a \neq \dfrac{n}{a}, \\ \displaystyle(\gamma - \log 2) f(0) + \frac{1}{2}\int_0^{\infty} \frac{f(y)+f(y^{-1})-f(0)}{y}\,dy & \\ \displaystyle+ \frac{1}{3}\int_0^{\infty} \frac{f(0)-f(y)}{y^2}\,dy & \text{if } a = \dfrac{n}{a}, \end{cases}
\end{aligned}
$$

where γ is the Euler–Mascheroni constant and $\Lambda(m)$ is the von Mangoldt function.

Then,

$$
\sum_{j=1}^{\infty} a_j(n)h(r_j) = \sum_{\substack{a\in\mathbb{N} \\ a|n}} \Phi(a) + \sum_{\substack{t\in\mathbb{Z} \\ \sqrt{D}=\sqrt{t^2-4n}\notin\mathbb{Q}}} L(1,\psi_D)\cdot \begin{cases} f\big(\sqrt{D}\big) & \text{if } D>0, \\ \dfrac{\sqrt{|D|}}{\pi}\displaystyle\int_{\mathbb{R}} \frac{f(y)}{y^2+|D|}\,dy & \text{if } D<0. \end{cases}
$$

Proof. Suppose first that f is smooth. In [BL17, Proposition 2.1][1] we find the following trace formula:

$$
\sum_{j=0}^{\infty} a_j(n)h(r_j) = \sum_{\substack{a\in\mathbb{N} \\ a|n}} F(a) + \sum_{\substack{t\in\mathbb{Z} \\ \sqrt{D}=\sqrt{t^2-4n}\notin\mathbb{Z}}} W(D), \tag{3.1}
$$

[1] There is a minor error in [BL17, Proposition 2.1]; the definition of $W(0)$ should be divided by 2.

where

$$W(D) = \begin{cases} L(1,\psi_D) f\big(\sqrt{D}\big) & \text{if } 0 < \sqrt{D} \notin \mathbb{Z}, \\ L(1,\psi_D) \dfrac{\sqrt{|D|}}{\pi} \displaystyle\int_{\mathbb{R}} \frac{f(y)}{y^2+|D|}\, dy & \text{if } D < 0, \\ \displaystyle\sum_{m|\sqrt{D}} \Lambda(m)(1-m^{-1}) f(\sqrt{D}) + \int_{\sqrt{D}}^{\infty} \frac{f(y)\, dy}{y+\sqrt{D}} & \text{if } 0 < \sqrt{D} \in \mathbb{Z}, \\ \dfrac{1}{2}(\gamma - \log 2) f(0) + \dfrac{1}{6}\displaystyle\int_0^\infty \frac{f(0)-f(y)}{y^2}\, dy & \\ +\dfrac{1}{4}\displaystyle\int_0^\infty \frac{f(y)+f(y^{-1})-f(0)}{y}\, dy & \text{if } D = 0, \end{cases}$$

and

$$\begin{aligned} F(a) = {} & 2\sum_{m=1}^{\infty} \frac{\Lambda(m)}{m} f\left(am - \frac{n}{am}\right) + 2a \int_a^\infty \frac{f\left(v - \frac{n}{v}\right) - f\left(a - \frac{n}{a}\right)}{v^2 - a^2}\, dv \\ & + \big(\gamma + \log(4\pi)\big) f\left(a - \frac{n}{a}\right) - \frac{1}{4} h(0). \end{aligned}$$

To begin, we note that

$$h(0) = 2\int_0^\infty f\left(v - \frac{n}{v}\right) \frac{dv}{v}.$$

Thus, we see that $\Phi(a)$ and $F(a)$ only differ by the final line of $\Phi(a)$ and the term $-a^{-1}\int_{\mathbb{R}} f\left(\sqrt{y^2 - \min(4n,0)}\right) dy$. The latter term comes from the $j = 0$ term on the left-hand side of (3.1), which corresponds to the constant eigenfunction with $r = \frac{i}{2}$ and Hecke eigenvalues $\sigma_{-1}(|n|)\sqrt{|n|}$. Averaging the integral formulas for $h(i/2) = h(-i/2)$ and making the substitution $v \mapsto \frac{y+\sqrt{y^2+4|n|}}{2}$, we have

$$\begin{aligned} \sigma_{-1}(|n|)\sqrt{|n|}\, h\left(\frac{i}{2}\right) &= \sum_{\substack{a\in\mathbb{N} \\ a|n}} a^{-1} \int_0^\infty f\left(v - \frac{n}{v}\right) \left(1 + |n| v^{-2}\right) dv \\ &= \sum_{\substack{a\in\mathbb{N} \\ a|n}} a^{-1} \int_{\mathbb{R}} f\left(\sqrt{y^2 - \min(4n,0)}\right) dy, \end{aligned}$$

as required.

As for the final line of $\Phi(a)$, we define the map

$$\left\{t \in \mathbb{Z} : \sqrt{t^2 - 4n} \in \mathbb{Z}\right\} \to \{a \in \mathbb{N} : a \mid n\},$$
$$t \mapsto a = \left|\frac{t + \sqrt{t^2 - 4n}}{2}\right|.$$

Then for $t \in \mathbb{Z}$ with $\sqrt{t^2 - 4n} \in \mathbb{Z}$, we have that a is a positive divisor of n with $t^2 - 4n = (a - n/a)^2$. Furthermore, this map is a bijection unless n is a square, in which case the value $a = \sqrt{n}$ is assumed twice (from $t = \pm 2\sqrt{n}$). Hence the corresponding terms on the right-hand side of (3.1) contribute as the final line of $F(a)$. Note that the contribution from $a = n/a$ is doubled.

Finally, we remove the assumption from [BL17, Proposition 2.1] that the test function is smooth. Under our hypotheses on f, we can apply integration by parts three times to the definition of h to see that $h(r) \ll |r|^{-3}$. By the Weyl estimate $\#\{j : r_j \leq r\} \ll r^2$, it follows that the left-hand side of (3.1) is absolutely convergent. The conclusion now follows by a straightforward approximation argument. □

We call the terms where $D > 0$ and $\sqrt{D} \notin \mathbb{Q}$ *hyperbolic* and the terms where $D < 0$ *elliptic*.

3.1.2 Specialising the test function

In order to apply the trace formula as a certification tool, it is necessary to choose a test function f that allows us to work out explicit expressions for the terms occurring in Proposition 3.1.1. For this we consider the test function

$$f(y) = \max\left(0, 1 - \frac{y^2}{X}\right)^k, \tag{3.2}$$

where $k \geq 4$ is an integer and X is a positive real number. We see this is an even, C^3 function that is supported on $[-\sqrt{X}, \sqrt{X}]$, so it satisfies our criteria in Proposition 3.1.1. The next proposition makes each term in the trace formula explicit for this test function.

Proposition 3.1.2. *Let n, D be non-zero integers, a, X be positive real numbers and $k \geq 4$ be an integer. Assume that $D \geq -4n$ and $X > \max(D, (a - n/a)^2)$, and set*

$$b = \frac{\sqrt{X} + \sqrt{X + 4n}}{2a}, \quad A = \frac{n + ab\sqrt{X}}{|n|}, \quad x = \sqrt{X/|D|}.$$

Then, with f and h as defined in (3.2) and Proposition 3.1.1, we have *(i)* $h(r) = 2 \cdot k! \left(\frac{A|n|}{X}\right)^k \sum_{j=0}^{k} (-1)^j \binom{k}{j} \operatorname{Re}\left(\frac{A^{ir-2j}}{\prod_{l=-j}^{k-j}(l+ir)}\right)$ *for* $r \in \mathbb{R} \setminus \{0\}$*;*

(ii) $h(0) = 2\int_0^\infty f\left(v - \frac{n}{v}\right)\frac{dv}{v} = 2\left(\frac{A|n|}{X}\right)^k \sum_{j=0}^{k} \binom{k}{j}^2 A^{-2j}\left(\log A + \sum_{l=1}^{j}\frac{1}{l} - \sum_{l=1}^{k-j}\frac{1}{l}\right)$*;*

(iii) $\int_{\mathbb{R}} f\left(\sqrt{y^2 - \min(4n,0)}\right) dy = 2\sqrt{X}\left(1 + \frac{\min(4n,0)}{X}\right)^{k+\frac{1}{2}} \prod_{j=1}^{k}\frac{2j}{2j+1}$*;*

(iv) $\int_{\sqrt{|D|}}^\infty \frac{f(y)\,dy}{y + \sqrt{|D|}} = (1-x^{-2})^k \log\left(\frac{x+1}{2}\right) - \sum_{j=0}^{k}\binom{k}{j}(-x^2)^{-j}\sum_{l=1}^{2j}(-1)^{l-1}\frac{x^l - 1}{l}$*;*

(v) $\sqrt{|D|}\int_{\mathbb{R}} \frac{f(y)\,dy}{y^2 + |D|} = 2(1+x^{-2})^k \arctan x - 2\sum_{j=0}^{k}\binom{k}{j}x^{-2j}\sum_{l=1}^{j}\frac{(-1)^{l-1}}{2l-1}x^{2l-1}$*;*

(vi) $$2a\int_a^\infty \frac{f(v-\frac{n}{v}) - f(a-\frac{n}{a})}{v^2 - a^2}\,dv = f\left(a - \frac{n}{a}\right)\log\left(\frac{b-1}{b+1}\right)$$
$$+ 2\sum_{m=-k}^{k}\left(-\frac{a^2}{n}\right)^m \sum_{j=|m|}^{k}\binom{k}{j}\binom{2j}{j+|m|}\left(\frac{n}{X}\right)^j \sum_{l=1}^{|m|}\frac{b^{(2l-1)\operatorname{sgn} m} - 1}{2l-1};$$

(vii) $\int_0^\infty \frac{f(0) - f(y)}{y^2}\,dy = \frac{2k+1}{\sqrt{X}}\prod_{j=1}^{k}\frac{2j}{2j+1}$*;*

(viii) $\int_0^\infty \frac{f(y) + f(y^{-1}) - f(0)}{y}\,dy = \log X - \sum_{j=1}^{k}\frac{1}{j}$.

Proof. Using the definition of h and making the change of variables $v \mapsto \sqrt{|n|u}$, we have

$$\begin{aligned} h(r) &= 2|n|^{-ir}\int_0^\infty \max\left(0, 1 - \frac{v^2 - 2n + (n/v)^2}{X}\right)^k v^{2ir}\,\frac{dv}{v} \\ &= \int_0^\infty \max\left(0, 1 + \frac{2n}{X} - \frac{|n|}{X}\left(u + u^{-1}\right)\right)^k u^{ir}\,\frac{du}{u} \\ &= \left(\frac{|n|T}{X}\right)^k \int_0^\infty \max\left(0, 1 - \frac{u+u^{-1}}{T}\right)^k u^{ir}\,\frac{du}{u}, \end{aligned}$$

where $T = \frac{X+2n}{|n|} \geq 2$.

Now let $F : [2, \infty) \to \mathbb{C}$ be a k-times differentiable function of compact support and let $s \in \mathbb{C}$. Applying integration by parts inductively, we derive

$$\int_0^\infty F(u+u^{-1})u^s \frac{du}{u} = \int_0^\infty F^{(k)}(u+u^{-1}) \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(s+2j-k)u^{s+2j-k}}{\prod_{l=0}^{k}(s+j-l)} \frac{du}{u}.$$

We can apply this to our specific test function $F(t) = \max\left(0, 1-\frac{t}{T}\right)^k$, noting that

$$F^{(k)}(t) = \begin{cases} \dfrac{(-1)^k k!}{T^k} & \text{if } t < T, \\ 0 & \text{if } t > T. \end{cases}$$

Thus, using the above formula we obtain

$$\begin{aligned} \int_0^\infty \max\left(0, 1-\frac{u+u^{-1}}{T}\right)^k u^{ir}\frac{du}{u} &= \frac{(-1)^k k!}{T^k} \int_{\frac{1}{A}}^{A} \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(ir+2j-k)u^{ir+2j-k}}{\prod_{l=0}^{k}(ir+j-l)} \frac{du}{u} \\ &= \frac{(-1)^k k!}{T^k} \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{A^{ir+2j-k} - A^{-ir-2j+k}}{\prod_{l=0}^{k}(ir+j-l)}, \end{aligned}$$

where $A = \frac{T+\sqrt{T^2-4}}{2} = \frac{X+2n+\sqrt{X^2+4nX}}{2|n|}$, so that $A + A^{-1} = T$. Replacing (j, l) by $(k-j, k-l)$ in the above sum, we see that it becomes

$$\frac{2k!}{T^k} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} \operatorname{Re}\left(\frac{A^{ir+2j-k}}{\prod_{l=0}^{k}(ir+j-l)}\right).$$

Now multiplying by $\left(\frac{|n|T}{X}\right)^k$ and replacing (j, l) by $(k-j, k-j-l)$ in the above sum yields (i).

To evaluate $h(0)$, we write

$$h(r) = \frac{A^{ir}H(r) - A^{-ir}H(-r)}{2ir},$$

where

$$H(r) = 2 \cdot k! \left(\frac{A|n|}{X}\right)^k \sum_{j=0}^{k} (-1)^j \binom{k}{j} A^{-2j} \prod_{\substack{-j \le l \le k-j \\ l \ne 0}} (l+ir)^{-1}.$$

By l'Hôpital's rule, we have

$$h(0) = (\log A)H(0) - iH'(0).$$

Hence, a straightforward evaluation of $H(0)$ and $H'(0)$ gives (ii).

Next, making the substitution $y \mapsto u\sqrt{X + \min(4n, 0)}$, we obtain

$$\begin{aligned}\int_{\mathbb{R}} f\Big(\sqrt{y^2 - \min(4n,0)}\Big)\, dy &= \int_{\mathbb{R}} \max\left(0, 1 - \frac{y^2 - \min(4n,0)}{X}\right)^k dy \\ &= \sqrt{X}\left(1 + \frac{\min(4n,0)}{X}\right)^{k+\frac{1}{2}} \int_{-1}^{1} \big(1-u^2\big)^k\, du,\end{aligned}$$

which yields (iii).

For the next term, making the substitution $y \mapsto u\sqrt{X}$, we have

$$\int_{\sqrt{|D|}}^{\sqrt{X}} \frac{f(y)\, dy}{y + \sqrt{|D|}} = \int_{x^{-1}}^{1} \frac{(1-u^2)^k}{u + x^{-1}}\, du.$$

Writing $(1-u^2)^k = (1-x^{-2})^k + (1-u^2)^k - (1-x^{-2})^k$ and applying the binomial theorem to the last two terms, we get

$$\int_{x^{-1}}^{1} \frac{(1-u^2)^k}{u+x^{-1}}\, du = \int_{x^{-1}}^{1} \frac{(1-x^{-2})^k}{u+x^{-1}}\, du + \sum_{j=0}^{k} \binom{k}{j} (-1)^j \int_{x^{-1}}^{1} \frac{u^{2j} - x^{-2j}}{u+x^{-1}}\, du.$$

Expanding the right-most integrand into a geometric series, we obtain

$$\frac{u^{2j} - x^{-2j}}{u + x^{-1}} = -x^{1-2j} \sum_{l=1}^{2j} (-xu)^{l-1}.$$

Integrating each term of this sum over $[x^{-1}, 1]$ yields (iv).

Similarly,

$$\begin{aligned}\sqrt{|D|}\int_{\mathbb{R}} \frac{f(y)\, dy}{y^2 + |D|} &= x^{-1} \int_{-1}^{1} \frac{(1-u^2)^k}{u^2 + x^{-2}}\, du \\ &= x^{-1}\int_{-1}^{1} \frac{(1+x^{-2})^k}{u^2+x^{-2}}\, du + x^{-1} \sum_{j=0}^{k} \binom{k}{j} \int_{-1}^{1} \frac{(-u^2)^j - (x^{-2})^j}{u^2 + x^{-2}}\, du \\ &= 2\big(1 + x^{-2}\big)^k \arctan x - 2\sum_{j=0}^{k} \binom{k}{j} x^{-2j} \sum_{l=1}^{j} \frac{(-1)^{l-1}}{2l-1} x^{2l-1}.\end{aligned}$$

For (vi), we begin by noting that $(v - n/v)^2 \leq X$ for $a \leq v \leq ab$, hence

$f(n-n/v) = (1-(v-n/v)^2/X)^k$ in this region. Applying the binomial theorem twice, we find that

$$\frac{f(v-\frac{n}{v})-f(a-\frac{n}{a})}{v^2-a^2} = \sum_{j=0}^{k} \binom{k}{j} \left(\frac{n}{X}\right)^j \sum_{m=-j}^{j} \binom{2j}{j+|m|} (-n)^{-m} \frac{v^{2m}-a^{2m}}{v^2-a^2}.$$

Now, expanding the right-most fraction into a geometric series, we find that

$$a\int_a^{ab} \frac{v^{2m}-a^{2m}}{v^2-a^2}\,dv = a^{2m}\sum_{l=1}^{|m|} \frac{b^{(2l-1)\operatorname{sgn} m}-1}{2l-1}.$$

Plugging this into the above equation and rearranging the sum over the values of m to go between $m=-k$ to k yields the first part of (vi). The second part arises from the contribution of the integral over $v > ab$, where $f(v-n/v) = 0$. That is,

$$2a\int_{ab}^{\infty} \frac{f\left(v-\frac{n}{v}\right)-f\left(a-\frac{n}{a}\right)}{v^2-a^2}\,dv = -f\left(a-\frac{n}{a}\right)\int_b^{\infty}\frac{2\,du}{u^2-1} = -f\left(a-\frac{n}{a}\right)\log\frac{b+1}{b-1}.$$

Turning to (vii), we use integration by parts and the substitution $y \mapsto u\sqrt{X}$ to obtain

$$\int_{\mathbb{R}} \frac{f(0)-f(y)}{y^2}\,dy = -\int_{\mathbb{R}}\frac{f'(y)}{y}\,dy = \frac{2k}{\sqrt{X}}\int_{-1}^{1}\left(1-u^2\right)^{k-1}du = \frac{4k+2}{\sqrt{X}}\prod_{j=1}^{k}\frac{2j}{2j+1}.$$

Finally, for (viii), we have

$$\begin{aligned}\int_0^{\infty}\frac{f(y)+f(y^{-1})-f(0)}{y}\,dy &= 2\int_0^1 \frac{f(y)+f(y^{-1})-f(0)}{y}\,dy \\ &= 2\int_0^1\frac{f(y)-f(0)}{y}\,dy + 2\int_1^{\infty}\frac{f(y)}{y}\,dy \\ &= 2\int_0^{\sqrt{X}}\frac{f(y)-f(0)}{y}\,dy + 2f(0)\int_1^{\sqrt{X}}\frac{1}{y}\,dy.\end{aligned}$$

Now using the substitution $y \mapsto u\sqrt{X}$ and noting that $f(0)=1$, this becomes

$$\log X - 2\int_0^1 \frac{1-(1-u^2)^k}{u}\,du = \log X - \int_0^1 \frac{1-v^k}{1-v}\,dv = \log X - \sum_{j=1}^{k}\frac{1}{j}.$$

$\square$

3.1.3 Idea of the algorithm

As noted before, we see the class number for real quadratic fields appearing in the hyperbolic terms in the Selberg trace formula in Proposition 3.1.1. The main idea of our algorithm is to compute the spectral side of the trace formula with known Maass form data, bound its tail and see if the two sides of the trace formula match with our class group data. For this section we shall assume that we are using the test function f defined by (3.2).

To begin, suppose we have rigorously computed values for r_j and $a_j(n)$ for $j \leq J$ and $|n| \leq M$, so that we may compute the spectral side of the trace formula to high accuracy. There will be some error arising from the terms with $j > J$, for which we have no data. More details on how to explicitly estimate the tail of the spectral sum will be given in Section 3.1.3, but suppose for now that we can bound by the tail by some positive real number E_n. By the explicit form of the trace formula we derived in Proposition 3.1.1, we have

$$\begin{aligned}\sum_{\substack{t\in\mathbb{Z}\\ D=t^2-4n<0}} L(1,\psi_D)\frac{\sqrt{|D|}}{\pi}\int_{\mathbb{R}}\frac{f(y)\,dy}{y^2+|D|} + \sum_{\substack{t\in\mathbb{Z}\\ \sqrt{D}=\sqrt{t^2-4n}\notin\mathbb{Q}\\ 0<D\leq X}} L(1,\psi_D)\left(1-\frac{D}{X}\right)^k \\ = \sum_{j=1}^{\infty} a_j(n)h(r_j) - \sum_{\substack{a\in\mathbb{N}\\ a\mid n}}\Phi(a) \\ \leq \sum_{j=1}^{J} a_j(n)h(r_j) + E_n - \sum_{\substack{a\in\mathbb{N}\\ a\mid n}}\Phi(a).\end{aligned} \tag{3.3}$$

Now, suppose we have a list of class numbers computed using our conditional algorithm. *A priori* we do not know that the class numbers are correct, but we know that each computed value is a factor of the true value (being the order of some subgroup of the class group). Hence our data can be used to compute a rigorous lower bound for the left-hand side of (3.3), since the terms are non-negative. (In order to compute $L(1,\psi_D)$ for $D > 0$, we also need the corresponding regulators. Although the fastest algorithms for that also rely on GRH, they can be independently verified using the method of [dHJW07]. Hence we may assume that the regulators are known unconditionally.)

Moreover, any incorrect value must be off by at least a factor of 2. Hence, in order to certify a given class number, we just need to show that it is not at least twice as large as we think it is. To this end, we double the corresponding term in the hyperbolic sum and then compute the full hyperbolic sum. If the sum exceeds the right-hand side of (3.3) then we get a contradiction, and hence our purported value of the class number must have been correct. Heuristically we expect the truncation error to be much smaller than our rigorous estimate E_n, so we expect to be able to certify all d for which $L(1, \psi_d)(1 - d/X)^k$ exceeds E_n. Note that considering all $n \in \mathbb{Z} \setminus \{0\}$ with $|n| \leq \frac{1}{2}\sqrt{X-1}$ suffices to cover all non-square discriminants $d \leq X$.

In our case, we have the first 2184 Laplace eigenvalues with $r \in (0, 177.75]$ computed by Andreas Strömbergsson using Hejhal's algorithm [Hej99] and certified using the program from [BSV06]. The proof of their completeness is given in Corollary 1.2 in [BP19]. In Section 3.2 we use a rigorous version of Hejhal's "Phase 2" algorithm to compute all of the needed Hecke eigenvalues, $a_j(n)$. The next few sections discuss how to explicitly bound the tail of the spectral sum, and estimate the efficiency of the algorithm with our given data.

Bounding the tail of the spectral sum

In order to apply the above algorithm we require an explicit bound on the tail of the spectral sum. To begin, using Proposition 3.1.2 (i), we have that

$$|h(r)| \leq \frac{2 \cdot k!}{|r|^{k+1}},$$

which becomes sharp in the limit as $X \to \infty$. Using this estimate, we can bound the tail of the spectral sum without needing specific estimates of the terms of the trace formula. Namely, we need to find an explicit bound for the sum

$$\sum_{j: r_j > R} r_j^{-k-1},$$

for some positive real R.

The main idea here is to use the fact that the eigenvalue counting function $N(t) = \#\{j : r_j \leq t\}$, is majorised by its Weyl asymptotic. More precisely, let

$$M(t) = \frac{t^2}{12} - \frac{2t}{\pi} \log \frac{t}{e\sqrt{\frac{\pi}{2}}} - \frac{131}{144} \quad \text{and} \quad S(t) = N(t) - M(t).$$

Then, from [Hej83, Ch. 10, Thm. 2.29] we have

$$S(t) = O\left(\frac{t}{\log t}\right) \quad \text{for } t > 1.$$

In order to apply this numerically, we require an explicit constant for the big-O. Currently this has not been worked out, however we can remedy this by using an integrated version derived in [BP19, Theorem 1.1]. Explicitly, define

$$S_1(t) = \frac{1}{t}\int_0^t S(u)\,du \quad \text{and} \quad E(t) = \left(1 + \frac{6.59125}{\log t}\right)\left(\frac{\pi}{12\log t}\right)^2.$$

Then,

$$S_1(t) \le E(t) \quad \text{for all } t > 1. \tag{3.4}$$

Consider

$$\sum_{j:r_j>R} r_j^{-k-1} = \int_R^\infty t^{-k-1}\,dN(t) = \int_R^\infty t^{-k-1}M'(t)\,dt + \int_R^\infty t^{-k-1}\,dS(t).$$

Applying integration by parts to the last integral twice, the above becomes

$$\sum_{j:r_j>R} r_j^{-k-1} = \int_R^\infty t^{-k-1}M'(t)\,dt - \frac{S(R) + (k+1)S_1(R)}{R^{k+1}} + (k+1)(k+2)\int_R^\infty t^{-k-2}S_1(t)\,dt.$$

Using the bound (3.4) and our explicit form of $M(t)$, we obtain

$$\sum_{j:r_j>R} r_j^{-k-1} \le \frac{1}{6(k-1)R^{k-1}} - \frac{2\log(R\sqrt{2/\pi}) + 2/k}{\pi k R^k} - \frac{S(R) + (k+1)S_1(R)}{R^{k+1}} + \frac{(k+2)E(R)}{R^{k+1}}.$$

For given values of R and k, we can easily check that the non-principal terms contribute a negative amount. Thus, using our data with $R \le 177$ and $k \le 15$, we find that

$$\sum_{j:r_j>R} r_j^{-k-1} \le \frac{R^{1-k}}{6(k-1)}.$$

Using this and the bound on the Hecke eigenvalues (1.5) due to Kim and Sarnak, we can bound the tail by

$$\left|\sum_{j:r_j>R} a_j(n)h(r_j)\right| \le b(n)\sum_{j:r_j>R}|h(r_j)| \le 2b(n)k!\sum_{j:r_j>R} r_j^{-k-1} \le \frac{b(n)k!}{3(k-1)}R^{1-k}. \tag{3.5}$$

3.1.4 Efficiency

We can use our explicit bound of the spectral tail (3.5) to get an idea of how efficient this algorithm will be. We will be able to certify a given d provided that the corresponding hyperbolic term on the right-hand side of (3.3) exceeds the amount that we overestimate the tail by. More explicitly, we should get

$$L(1,\psi_d)\left(1-\frac{d}{X}\right)^k > \frac{b(n)k!}{3(k-1)}R^{1-k} - \sum_{j:r_j>R} a_j(n)h(r_j).$$

We do not know the sum over j in advance, but we expect it to be much smaller than our estimate (3.5). Thus, we should succeed in certifying d as long as

$$\frac{d}{X} \lessapprox 1-\frac{1}{R}\left(\frac{b(n)k!R}{3(k-1)L(1,\psi_d)}\right)^{1/k}.$$

For instance, if $X = 10^{11}$ then the worst case value of $b(n)$ is $164.397\ldots$, attained at $n = 151200$. If we assume that $L(1,\chi_d)$ has roughly the same minimum value as among the negative discriminants up to 10^{11} (viz., 0.17448, as computed in [JRW06]), then the optimal k is 11, for which the above is about 94%. However, already with $k = 6$ we get 92%, and that may allow us to get by with significantly lower floating point precision. (Note that the total sum over d has size roughly $\sqrt{X}$, but we are trying to detect variations of size $L(1,\chi_d)(1-d/X)^k$, which can be less than 10^{-7} even with $k = 6$. Hence it is also essential that we work with interval arithmetic in order to control for cancellation; we made use of the `Arb` library [Joh17] for this purpose.) This analysis is also highly pessimistic in assuming that the worst case for $b(n)$ occurs simultaneously with the worst case for $L(1,\chi_d)$.

3.2 Rigorous computation of the Hecke eigenvalues

In order to compute the truncated sum on the spectral side of the trace formula, we require a large list of Hecke eigenvalues for each of the Laplace eigenvalues. As noted before, we have approximations of the Laplace eigenvalues of the first 2184 Maass forms of level 1, as well as a rigorously verified list of the first several Hecke eigenvalues for each form. All this data has been computed and verified to better than 300 bits of precision, which allows us to compute a given Maass form $f(z)$ for any z in the fundamental domain to approximately this accuracy. In turn, we can compute many more Hecke eigenvalues using the "Phase 2" part of Hejhal's algorithm [Hej99]. In this section we explain how to carry out the Phase 2 algorithm rigorously. (See [Str05, Sec. 1.3.3] for more details on this Phase 2 algorithm).

Let f be a Maass cusp form on $\mathrm{PSL}(2,\mathbb{Z})$ with Laplace eigenvalue $\lambda = \frac{1}{4} + r^2$ and Hecke eigenvalues a_m. Let $\omega = 0$ if f is even and $\omega = 1$ if f is odd. Its Fourier expansion is of the form

$$f(x+iy) = \sum_{m=1}^{\infty} \frac{a_m}{\sqrt{m}} \widetilde{W}_{ir}(2\pi m y) \cos^{(\omega)}(2\pi m x)$$

where $\widetilde{W}_{ir}(x) = e^{\frac{\pi r}{2}} W_{ir}(x) = \sqrt{x} e^{\frac{\pi}{2} r} K_{ir}(x)$ and $K_{ir}(x)$ is the K-Bessel function. In addition, $\cos^{(\omega)} = \cos$ if $\omega = 0$ and $\cos^{(\omega)} = \sin$ if $\omega = 1$.

Fix $N \in \mathbb{N}, Y > 0$ and define the $2N$ points

$$z_j = x_j + iY = \frac{j - \frac{1}{2}}{2N} + iY,$$

where $1 - N \leq j \leq N$. Now if we consider the discrete Fourier transform of f, for some integer k, on these points we get

$$\begin{aligned}\sum_{j=1}^{N} f(z_j) \cos^{(\omega)}(2\pi k x_j) &= \sum_{j=1}^{N} \sum_{m=1}^{\infty} \frac{a_m}{\sqrt{m}} \widetilde{W}_{ir}(2\pi m Y) \cos^{(\omega)}(2\pi m x_j) \cos^{(\omega)}(2\pi k x_j) \\ &= \sum_{m=1}^{\infty} \frac{a_m}{\sqrt{m}} \widetilde{W}_{ir}(2\pi m Y) \sum_{j=1}^{N} \cos^{(\omega)}(2\pi m x_j) \cos^{(\omega)}(2\pi k x_j).\end{aligned}$$

Here we can use the trigonometric identity $\cos^{(\omega)}(x)\cos^{(\omega)}(y) = \frac{1}{2}\cos(x-y) +$

$(-1)^\omega \cos(x+y)$, to obtain

$$\sum_{j=1}^{N} f(z_j)\cos^{(\omega)}(2\pi k x_j)$$
$$= \frac{1}{2}\sum_{m=1}^{\infty}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi mY)\left[\sum_{j=1}^{N}\cos(2\pi(m-k)x_j)+(-1)^\omega\sum_{j=1}^{N}\cos(2\pi(m+k)x_j)\right]. \tag{3.6}$$

Our goal is to extract the k-th term of the series on the right-hand side and then get an expression for the rest of the sum which we will bound later. We have

$$\begin{aligned}\sum_{j=1}^{N}\cos(2\pi(m\pm k)x_j) &= \frac{1}{2}\sum_{j=1}^{N}\left(e^{2\pi(m\pm k)x_j}+e^{-2\pi(m\pm k)x_j}\right)\\ &= \frac{1}{2}e^{-\frac{m\pm k}{2N}\pi i}\sum_{j=1}^{N}e^{2\pi i\frac{(m\pm k)j}{2N}}+\frac{1}{2}e^{\frac{m\pm k}{2N}\pi i}\sum_{j=1}^{N}e^{-2\pi i\frac{(m\pm k)j}{2N}}.\end{aligned}$$

Now if $2N \mid (m\pm k)$, then $\sum_{j=1}^{N} e^{\pm 2\pi i\frac{(m\pm k)j}{2N}} = N$. Otherwise, using the fact that this sum is a geometric series, we get 0. Thus we can simplify the above sum to

$$\sum_{j=1}^{N}\cos(2\pi(m\pm k)x_j) = \begin{cases}(-1)^{\frac{(m\pm k)}{2N}}N & \text{if } 2N\mid(m\pm k),\\ 0 & \text{otherwise.}\end{cases} \tag{3.7}$$

Hence combining the results of (3.6) and (3.7), we have

$$\begin{aligned}\frac{2}{N}\sum_{j=1}^{N}f(z_j)\cos^{(\omega)}(2\pi kx_j) &= \sum_{\substack{m\geq 1\\ m\equiv k(2N)}}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi mY)(-1)^{\frac{(m-k)}{2N}}\\ &\quad+(-1)^\omega\sum_{\substack{m\geq 1\\ m\equiv -k(2N)}}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi mY)(-1)^{\frac{(m+k)}{2N}}\\ &= \frac{a_k}{\sqrt{k}}\widetilde{W}_{ir}(2\pi kY)+\mathcal{E}_0,\end{aligned}$$

where

$$\mathcal{E}_0 = \sum_{j=1}^{\infty}(-1)^j\left[\frac{a_{2jN+k}}{\sqrt{2jN+k}}\widetilde{W}_{ir}(2\pi(2jN+k)Y)+(-1)^\omega\frac{a_{2jN-k}}{\sqrt{2jN-k}}\widetilde{W}_{ir}(2\pi(2jN-k)Y)\right]. \tag{3.8}$$

In order for the above truncation to be valid we require $k\leq N$. Let z_j^* be the pullback of z_j into the fundamental domain defined by $\left\{z=x+iy\in\mathbb{H}\mid |z|\geq 1 \text{ and } |x|\leq\frac{1}{2}\right\}$.

Then by the modularity of f, we have $f(z_j) = f(z_j^*)$. Thus

$$\begin{aligned}
\frac{a_k}{\sqrt{k}}\widetilde{W}_{ir}(2\pi kY) &= \frac{2}{N}\sum_{j=1}^{N} f(z_j^*)\cos^{(\omega)}(2\pi kx_j) - \mathcal{E}_0 \\
&= \frac{2}{N}\sum_{j=1}^{N}\sum_{m=1}^{\infty}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi my_j^*)\cos^{(\omega)}(2\pi mx_j^*)\cos^{(\omega)}(2\pi kx_j) - \mathcal{E}_0 \\
&= \frac{2}{N}\sum_{j=1}^{N}\left(\sum_{m=1}^{L_j}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi my_j^*)\cos^{(\omega)}(2\pi mx_j^*) + \mathcal{E}_j\right)\cos^{(\omega)}(2\pi kx_j) - \mathcal{E}_0,
\end{aligned}$$

where $L_j \in \mathbb{N}$ depending on j and

$$\mathcal{E}_j = \sum_{m=L_j+1}^{\infty}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi my_j^*)\cos^{(\omega)}(2\pi mx_j^*). \tag{3.9}$$

Here we can consider the total error given by

$$\mathcal{E} = \frac{2}{N}\sum_{j=1}^{N}\mathcal{E}_j\cos^{(\omega)}(2\pi kx_j) - \mathcal{E}_0. \tag{3.10}$$

Hence our main computation formula becomes

$$\frac{a_k}{\sqrt{k}}\widetilde{W}_{ir}(2\pi kY) = \frac{2}{N}\sum_{j=1}^{N}\sum_{m=1}^{L_j}\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(2\pi my_j^*)\cos^{(\omega)}(2\pi mx_j^*)\cos^{(\omega)}(2\pi kx_j) + \mathcal{E}.$$

Computationally, we can see this is just a discrete cosine/sine transformation with respect to the Hecke eigenvalues. Thus, once we have values of Y and N, discussed in Subsection 3.2.2, we can apply a standard computational library on Fast Fourier Transforms to compute these sums.

Our goal now is to bound the total error $\mathcal{E}$ explicitly so that it can aid us in our computations.

3.2.1 Bounding the error

To begin, we have

$$|\mathcal{E}| \le \left|\frac{2}{N}\sum_{j=1}^{N}\mathcal{E}_j\cos^{(\omega)}(2\pi kx_j)\right| + |\mathcal{E}_0| \le 2\max_{1\le j\le N}\{|\mathcal{E}_j|\} + |\mathcal{E}_0|.$$

We now want to bound the individual parts appearing in the above bound. For this we require the following two lemmas. The first is bound on the Fourier coefficients from Kim–Sarnak [Kim03], which we already saw in Section 2.1.4.

Lemma 3.2.1. *Let f be a Maass cusp form of level 1 with Hecke eigenvalues a_m. Then for all non-zero $m \in \mathbb{Z}$ we have*

$$\left|\frac{a_m}{\sqrt{m}}\right| \leq \eta := 1.758.$$

The second lemma we require is a bound on the K-Bessel function due to Booker, Strömbergsson and Then [BT18, Prop. 1].

Lemma 3.2.2. *For all $y > r > 0$ we have*

$$|\widetilde{W}_{ir}(y)| = e^{\frac{\pi}{2}r}\sqrt{y}|K_{ir}(y)| \leq \sqrt{\frac{\pi}{2}}\frac{\sqrt{y}}{\sqrt[4]{y^2-r^2}}e^{-ru(y/r)},$$

where $u(t) = \sqrt{t^2-1} - \arctan(\sqrt{t^2-1})$ for $t \geq 1$.

We can now directly apply the above lemmas to bound the sums appearing in $\mathcal{E}$.

Proposition 3.2.3. *Let b_m be an increasing arithmetic sequence for $1 \leq m \leq \infty$ with $b_1 > r$ and arithmetic difference d. Then*

$$\sum_{m=1}^{\infty}\left|\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(b_m)\right| < \mathcal{B}_{r,b_1,d} := \eta\sqrt{\frac{\pi}{2}}\frac{\sqrt{b_1}}{\sqrt[4]{b_1^2-r^2}}e^{-ru(b_1/r)}\left(1 + \frac{b_1}{d\sqrt{b_1^2-r^2}}\right).$$

Proof. We begin by noting that the function $\frac{\sqrt{y}}{\sqrt[4]{y^2-r^2}}$ is decreasing for $y > r$. Hence by applying both of the above lemmas we get

$$\sum_{m=1}^{\infty}\left|\frac{a_m}{\sqrt{m}}\widetilde{W}_{ir}(b_m)\right| < \eta\sqrt{\frac{\pi}{2}}\frac{\sqrt{b_1}}{\sqrt[4]{b_1^2-r^2}}\sum_{m=1}^{\infty}e^{-ru(b_m/r)}.$$

The goal here is to majorise the exponential sum by a geometric series. For this, we note that the function $e^{-ru(y/r)}$ is decreasing for $y > r$ and $u'(t) = \sqrt{1-t^{-2}}$ is increasing for $t > 1$. Hence for all $t_2 > t_1 > 1$, we have

$$u(t_2) \geq u(t_1) + (t_2 - t_1)u'(t) = u(t_1) + (t_2 - t_1)\sqrt{1 - t_1^{-2}}.$$

Thus, for all $m \geq 1$ we obtain

$$ru(b_m/r) \geq ru(b_1/r) + \sqrt{b_1^2 - r^2}\frac{b_m - b_1}{b_1}.$$

We can now bound the exponential sum by

$$\begin{aligned}\sum_{m=1}^{\infty} \exp(-ru(b_m/r)) &\leq \exp(-ru(b_1/r)) \exp(\sqrt{b_1^2 - r^2}) \sum_{m=1}^{\infty} \exp\left(-\frac{\sqrt{b_1^2 - r^2}}{b_1} b_m\right) \\ &\leq \exp(-ru(b_1/r)) \left(1 - \exp\left(-\frac{\sqrt{b_1^2 - r^2}}{b_1} d\right)\right)^{-1}.\end{aligned}$$

To get the final result we use the fact that $(1 - e^{-x})^{-1} < 1 + x^{-1}$ for $x > 0$. □

Using Proposition 3.2.3 we can compute bounds for the errors $\mathcal{E}_0$ and $\mathcal{E}_j$.

Proposition 3.2.4. *Let $L, M \in \mathbb{N}$ with $0 < k \leq M < N$, $2\pi Y(2N - M) > r$, and $\sqrt{3}\pi(L + 1) > r$. Then we have*

$$\begin{aligned}|\mathcal{E}_0| &\leq 2\mathcal{B}_{r,2\pi Y(2N-M),4\pi YN}, \\ |\mathcal{E}_j| &\leq \mathcal{B}_{r,\sqrt{3}\pi(L+1),\sqrt{3}\pi}\end{aligned}$$

for all $1 \leq j \leq N$.

Proof. From Lemma 3.2.2, we see that $|W_{ir}(y)|$ is decreasing for $y > r$. Now using the definition of $\mathcal{E}_0$ from (3.8), we have

$$\begin{aligned}|\mathcal{E}_0| &\leq \left| \sum_{j=1}^{\infty} \frac{a_{2jN+k}}{\sqrt{2jN+k}} W_{ir}(2\pi(2jN+k)Y) + (-1)^{\omega} \sum_{j=1}^{\infty} \frac{a_{2jN-k}}{\sqrt{2jN-k}} W_{ir}(2\pi(2jN-k)Y) \right| \\ &\leq \sum_{j=1}^{\infty} \left| \frac{a_{2jN+1}}{\sqrt{2jN+1}} W_{ir}(2\pi(2jN+1)Y) \right| + \sum_{j=1}^{\infty} \left| \frac{a_{2jN-M}}{\sqrt{2jN-M}} W_{ir}(2\pi(2jN-M)Y) \right|.\end{aligned}$$

Thus applying Proposition 3.2.3 we obtain the result.

For $\mathcal{E}_j$, we note that since all the z_j^* are in the fundamental domain, we have $y_j^* > \sqrt{3}/2$ for all j. Hence from the definition of $\mathcal{E}_j$ from (3.9) we get

$$|\mathcal{E}_j| \leq \sum_{m=L+1}^{\infty} \left| \frac{a_m}{\sqrt{m}} W_{ir}(2\pi m y_j^*) \right| < \mathcal{B}_{r,2\pi(L+1)y_j^*,2\pi y_j^*} \leq \mathcal{B}_{r,\sqrt{3}\pi(L+1),\sqrt{3}\pi},$$

by Proposition 3.2.3. □

In practice we choose L to be the number of initial Fourier coefficients that we know. We ensure this is sufficiently large that the error is dominated by our estimate for $|\mathcal{E}_0|$, i.e. that $\mathcal{B}_{r,\sqrt{3}\pi(L+1),\sqrt{3}\pi} \leq \mathcal{B}_{r,2\pi Y(2N-M),4\pi YN}$. Hence we can bound the overall truncation error by

$$|\mathcal{E}| \leq 4\mathcal{B}_{r,2\pi Y(2N-M),4\pi YN}.$$

3.2.2 Choosing Y and N

For our code, we let M be the largest indexed Fourier coefficient we wish to compute. We will only need to consider the Fourier coefficients a_p for $p \leq M$ prime since the others can be computed using the Hecke relations from this data. To help control the error we have to carefully choose the parameters Y and N. To begin we note that the $\widetilde{W}_{ir}(y)$ decays exponentially for $y > r$ from the K-Bessel function.

We start by choosing $Y = r/M$. Then we compute $\widetilde{W}_{ir}(2\pi pY)$ for all primes $p \leq M$. The aim of this is to see if we are near any of the zeros of the K-Bessel function in its oscillatory region, which would cause our error bound to blow up. If we are too close to a zero, we can change Y slightly so that we move away from this zero. However, we have to make sure we do not make any other values of $\widetilde{W}_{ir}(2\pi pY)$ close to a different zero. This is essentially a min-max problem of minimising the value of Y whilst maximising the distance of the values of $\widetilde{W}_{ir}(2\pi pY)$ away from zero.

Once we have a value for Y, we can work on finding N. To do this we first fix a precision of B bits, and then we bound our error $|\mathcal{E}|$ to be roughly 2^{-B}, that is

$$|\mathcal{E}| \leq 4\mathcal{B}_{r,2\pi Y(2N-M),4\pi YN} = 2^{-B}.$$

Note, in practice we will want to choose B larger than our desired error due to rounding errors and the fact we will be dividing by $\widetilde{W}_{ir}$. Now, we know all the constants r, Y, M and B, hence we can rearrange the above to become

$$Q(N) := \frac{1}{\eta}\sqrt{\frac{2}{\pi}}\mathcal{B}_{r,2\pi Y(2N-M),4\pi YN} = \frac{1}{\eta}\sqrt{\frac{2}{\pi}}2^{-B-2}.$$

Hence to find N, we just need to find the root of

$$Q(N) - \frac{1}{\eta}\sqrt{\frac{2}{\pi}}2^{-B-2}.$$

We can find this numerically by just applying a bisection algorithm to this function.

3.3 Computation

3.3.1 Theoretical complexity

The computation of the Maass forms is possible in polynomial time, [Str05, §1.3.4]. Since we can take k arbitrarily large in the analysis in Section 3.1.4, the eigenvalue cutoff R can grow slowly as a function of X, and the time to compute the spectral side is therefore dominated by the computation of the Hecke eigenvalues, which is $O(X^{\frac{1}{2}+\varepsilon})$ for each form (see Section 3.2).

Thus, the slowest part of the computation of the right-hand side of (3.3) is the sum over m appearing in Φ, which has roughly $\frac{\sqrt{X}}{a\log X}$ non-zero terms. Summing over $a \mid n$ and $|n| \leq \sqrt{X}$ gives $O(\frac{X}{\log X})$ terms in total. However, this is still swamped by the roughly X terms appearing on the left-hand side of (3.3) in the hyperbolic sum. This motivates our choice of our test function, which makes the hyperbolic terms simple to compute. This gives overall complexity of $O(X^{1+\varepsilon})$ for the verification.

As described in the introduction, the complexity to conditionally compute the class group for a fixed discriminant d is $O(d^{1/4+\varepsilon})$ using Buchmann's algorithm [BS05]. Further to this, we also require the computation of the regulator, which can be computed and unconditionally verified in $O(d^{1/6+\varepsilon})$ [dHJW07]. Hence, the computation of the class group and regulator up to discriminant X will be done in time $O(X^{\frac{5}{4}+\varepsilon})$ overall. Asymptotically one could turn to an index calculus based algorithm with heuristic complex $O(X^{1+\varepsilon})$. Unfortunately, the correctness of the index calculus approach depends on GRH in several ways, and there is currently no known method of verifying its output in subexponential time. This analysis shows that the verification part should be faster than the time it takes to compute the class numbers and regulators in the first place.

3.3.2 Implementation

We implemented this verification algorithm on data computed with a modification of the generic group structure algorithm of Buchmann and Schmidt [BS05] for producing the table of class groups, which allowed us to extend significantly the table of known class groups to include all fields of discriminant up to 10^{11}. Most importantly, thanks to the new verification algorithm, our results are unconditionally correct for $d \leq 10^{11}$, requiring no assumptions of Riemann hypotheses.

Using the ideas and reasoning in Section 3.3.1 we ran our verification with $k = 6$. We made two runs on a machine with 64 cores (2.5 GHz AMD Opteron processors), with the following results:

X	certified up to	running time
1.1×10^{10}	10 378 129 942	5 hours
1.1×10^{11}	103 455 923 536	57 hours

In both runs, the efficiency was better than 94%, and about 1.3% of the computation time was spent on the right-hand side of (3.3).

Chapter 4

Rigorous implementation of Hejhal's algorithm

In the 1990s, Hejhal [Hej99] introduced an algorithm to compute the Laplace and Hecke eigenvalues of Maass cusp forms. This algorithm was generalised to general congruence and non-congruence subgroups by Strömberg in 2006 [Str05]. This algorithm works very well in practice, however it relies on a heuristic argument and thus is not rigorous.

In this chapter we describe a method to rigorously implement Hejhal's algorithm, once you already know the Laplace eigenvalue of the Maass forms exists in some interval. Essentially, the main idea here is to apply Newton's method on the Hejhal system matrix where the derivatives are taken with respect to the Laplace eigenvalue r.

The main result of this chapter is a test to prove whether or not the matrix appearing from Hejhal's algorithm for level 1 Maass forms is well behaved as the matrix size increases. This will form part of joint work with David Lowry-Duda on actually implementing this algorithm to improve the precision of Maass forms in general.

4.1 Hejhal's algorithm for level 1

Let $\mathbb{H} = \{z = x + iy \mid y > 0\}$ denote the upper half plane and let $\mathcal{F} = \{z = x + iy \mid |x| \leq 1/2, |z| \geq 1\}$ denote the fundamental domain for $\mathrm{PSL}(2,\mathbb{Z})$ acting on $\mathbb{H}$ by Möbius transformations. To begin, we shall only describe in detail Hejhal's algorithm for even forms, however it is very easy to adapt this for odd forms by swapping all the cosines with sines.

Let f be a even Maass cusp form with Laplace eigenvalue $\lambda = \frac{1}{4} + r^2$ and Hecke eigenvalues a_m. It has a Fourier series, see Section 1.3, given by

$$f(z) = f(x+iy) = \sum_{m=1}^{\infty} \frac{a_m}{\sqrt{m}} W_{ir}(2\pi m y)\cos(2\pi m x).$$

The overall aim of Hejhal's algorithm is to create a linear system to solve for the Fourier coefficients for a fixed value r. We then use an auxiliary equation to help zoom in on the values of r that give suspected genuine Maass forms. For this description of Hejhal's algorithm, we shall ignore any error analysis. To begin, we truncate the above Fourier series for some $M \in \mathbb{N}$, to get

$$f(z) \approx \sum_{m=1}^{M} \frac{a_m}{\sqrt{m}} W_{ir}(2\pi m y) \cos(2\pi m x). \tag{4.1}$$

We can now view the sum in (4.1) as a discrete cosine transform in x. We shall now perform an inverse discrete cosine transform along the following horocycle below $\mathcal{F}$:

$$\left\{ z_m = x_m + iY \,\middle|\, x_m = \frac{1}{2Q}\left(m - \frac{1}{2}\right), 1 - Q \leq m \leq Q \right\},$$

for some $Y < Y_0 = \frac{\sqrt{3}}{2}$ and $Q > M$. Taking the inverse transform for some $0 < n \leq M < Q$, we obtain

$$\begin{aligned} \frac{a_n}{\sqrt{n}} W_{ir}(2\pi n Y) &\approx \frac{1}{Q} \sum_{m=1-Q}^{Q} f(z_m) \cos(2\pi n x_m) \\ &\approx \frac{1}{Q} \sum_{m=1-Q}^{Q} f(z_m^*) \cos(2\pi n x_m), \end{aligned}$$

where $z_m = x_m + iy_m = x_m + iY \in \mathbb{C}$ and $z_m^* = x_m^* + iy_m^*$ is its $\mathcal{F}$-pullback. From this relation we get the following linear system valid for all $0 < n \leq M < Q$,

$$\frac{a_n}{\sqrt{n}} W_{ir}(2\pi n Y) \approx \sum_{0<k\leq M} a_k V_{nk} \tag{4.2}$$

where

$$V_{nk} = \frac{1}{Q} \sum_{m=1-Q}^{Q} W_{ir}(2\pi k y_m^*) \cos(2\pi k x_m^*) \cos(2\pi n x_m). \tag{4.3}$$

Restricting to $1 \leq n \leq M$, we obtain a system of M linear equations for M unknowns $\{a_n\}_{1 \leq n \leq M}$. We can rewrite the linear system to get

$$0 \approx \sum_{0<k\leq M} a_k \widetilde{V}_{nk} \tag{4.4}$$

where $\widetilde{V}_{nk} = V_{nk} - \delta_{nk} W_{iR}(2\pi n Y)$. This system can be solved by normalising the system with $a_1 = 1$ and removing the first column from $\widetilde{V}_{nk}$. Explicitly, let $V(r)$

denote the $(M-1)\times(M-1)$-matrix $\widetilde{V}_{nk}$ after removing the first row and column, C denote the $(M-1)$-vector of Fourier coefficients $(a_n)_{M\geq n\geq 2}$ and $b(r)$ denote the negative of the first column vector separated from $\widetilde{V}_{nk}$ corresponding to $a_1 = 1$. Then we can rewrite our linear system as

$$V(r)C \approx b(r), \tag{4.5}$$

which can be solved. We also separate the first row of (4.4) as an auxiliary equation and write it as

$$c(r) = C \cdot v(r) + w(r) \approx 0, \tag{4.6}$$

where $v(r)$ is the first row of $V(r)$ and $w(r)$ is $\widetilde{V}_{11}$.

Note, this linear system relies on the value of r, which we currently do not know. To find the value of r, we shall first start with some initial guess of r, use this to solve (4.5) to get approximations to the coefficients a_n, and then iterate this procedure to minimise the error in the auxiliary equation (4.6). We repeat this for multiple values of r until we believe we have found all of them up to some limit by comparing to the Weyl law, see (1.4).

Alternatively, one could minimise the error of the multiplicativity of the Fourier coefficients, say the equation $a_2a_3 = a_6$, or solve (4.5) for two different values of Y and minimise the difference of the coefficients, since for a true Maass form, the Hejhal system will be invariant by the choice of Y. For more details on how one would implement Hejhal's algorithm in practice, see [Str05].

This final part of Hejhal's algorithm is non-rigorous since we do not know beforehand whether the Hejhal system is well behaved or if it will continue to converge.

4.2 Implementing Hejhal's algorithm rigorously to improve precision

In this section, we will setup the system of equations (4.5) and (4.6) so that they can be implemented rigorously, once we know our Laplace eigenvalue exists in some interval. To begin, let r be the numerical approximation for the Laplace eigenvalue of a Maass form and $\varepsilon > 0$, such that we know the interval $[r-\varepsilon, r+\varepsilon]$ contains the value of the unique and true (but unknown) Laplace eigenvalue r^* of the purported Maass form. This may seem quite restrictive, since the original Hejhal's algorithm does not give you this. However, we can use the rigorous data from the trace formula algorithm in Chapter 2 or from [BSV06] as a starting point.

Let δ be such that $r^* = r+\delta$. To make Hejhal's algorithm rigorous, we shall need to setup the Hejhal system whilst also keeping track of the various errors occurring. Recall, the equations we shall be working with are

$$\begin{aligned} V(r)C &\approx b(r), \\ c(r) &= C \cdot v(r) + w(r) \approx 0. \end{aligned}$$

We wish to change the $\approx$ with $=$ in the above equations. Let $b^\natural$ denote the vector we get by truncating the Fourier series at M and setting up the system ignoring all the error terms. Define $e = V(r^*)C - b^\natural(r^*)$ and set $b(t) = b^\natural(t) + e$. Thus, $b(t)$ is precisely defined, although we are ignorant of its exact value. Let $C(r)$ denote the vector of Fourier coefficients obtained by the now well-defined Hejhal system at r with $V(r)C = b(r)$, such that $C(r^*) = (a_2, \ldots, a_M)$ gives the exact solution.

In practice, we just work in interval arithmetic and bound the tails of the truncation, however we need this setup to describe the algorithm theoretically. Now, we compute (using interval arithmetic) $C(r)$ for our r and look at the auxiliary equation

$$c(r) = C(r) \cdot v(r) + w(r) = 0,$$

where $v(r)$ and $w(r)$ are defined as before, but for our well-defined Hejhal system. Near r^*, have that

$$c(r^*) = c(r) + c'(r)\delta + \frac{c''(\widetilde{r})\delta^2}{2},$$

for some $\widetilde{r}$ between r and r^*. Rearranging, we get that

$$|\delta| = \frac{|c(r) - c(r^*)|}{|c'(r) + c''(\widetilde{r})\delta/2|}.$$

To use this formula, we first numerically compute (using interval arithmetic) interval approximations to $c(r)$ and $c'(r)$ and rigorously bound $c(r^*)$ and $c''(\widetilde{r})$. Furthermore, since $|\delta| \leq \varepsilon$, if we have that $\varepsilon|c''(\widetilde{r})| < |c'(r)|$, then

$$|\delta| \leq 2\left|\frac{c(r) - c(r^*)}{c'(r)}\right|.$$

Thus, if we run this system and we find the above to be true, then we would have rigorously zoomed in on our Laplace eigenvalue. Unfortunately in this setup, there is no way to know beforehand whether the matrix $V^{-1}(r)$ is well-conditioned or that

$c'(r)$ is not very small, meaning we cannot guarantee this algorithm will work all the time. We will only be able to check this at runtime.

This implementation of improving the precision can be easily generalised to Hejhal's algorithm for higher levels. In the near future, David Lowry-Duda and the author will be implementing this algorithm to improve the precision of the low-precision estimates derived by the trace formula algorithm. In this we shall discuss how to get rigorous bounds for $c(r^*)$ and $c''(\widetilde{r})$.

4.3 Proof of well-conditioned Hejhal system for even forms

For the rest of this chapter, we shall discuss how to test beforehand whether the matrix $V^{-1}(r)$ is well conditioned as we increase the matrix size M. In this section we shall setup Hejhal's algorithm for even Maass forms for $\mathrm{PSL}(2,\mathbb{Z})$ in such a way that we can use it theoretically. This version differs from how you would actually implement this numerically.

Let f be an even Maass form on $\mathrm{PSL}(2,\mathbb{Z})$ with Laplace eigenvalue $\lambda = \frac{1}{4} + r^2$ and Hecke eigenvalues a_m. Let $\mathbb{H} = \{z = x + iy \mid y > 0\}$ denote the hyperbolic upper half plane and let $\overline{\mathcal{F}} = \{z = x + iy \in \mathbb{H} \mid 0 \leq |x| \leq 1/2, |z| \geq 1\}$ be the fundamental domain of $\mathrm{PSL}(2,\mathbb{Z})$ along with the reflection operator $z \mapsto -\overline{z}$.

4.3.1 Explicitly defining Hejhal's Algorithm

Let $Y \in (0, \sqrt{3}/2)$ such that $W_{ir}(2\pi mY) \neq 0$ for any $m \in \mathbb{N}$. We shall assume that the values of Y and r are fixed. Let $N, Q \in \mathbb{Z}$, such that $Q > N > 1$. We set $x_m = \frac{a_m}{\sqrt{m}} W_{ir}(2\pi mY)$. We shall define Hejhal's algorithm for x_m with the parameters (r, Y, N, Q).

To begin, consider the horocycle $z(t) = t + iY$ for $t \in [-1/2, 1/2]$. This can be pulled back into a unique closed path $z^*(t) = x^*(t) + iy^*(t) \in \overline{\mathcal{F}}$. We work in $\overline{\mathcal{F}}$ instead of the full fundamental domain $\mathcal{F} = \{z = x + iy \in \mathbb{H} \mid |x| \leq 1/2, |z| \geq 1\}$ since $z^*(t) \in \overline{\mathcal{F}}$ is continuous and piecewise smooth with respect to t here and f is invariant under the reflection operator since it is even. For $m \in \mathbb{Z}_{>0}$, set

$$f_m(t) = \frac{W_{ir}(2\pi m y^*(t))}{W_{ir}(2\pi mY)} \cos\left(2\pi m x^*(t)\right).$$

Next, define for $n \in \mathbb{Z}_{\geq 0}$,

$$h_Q(n,m) = \begin{cases} \dfrac{2}{Q}\displaystyle\sum_{j=1}^{Q} f_m\left(\frac{j-\frac{1}{2}}{2Q}\right)\cos\left(2\pi n\frac{j-\frac{1}{2}}{2Q}\right) & \text{if } n>0, \\ \dfrac{1}{Q}\displaystyle\sum_{j=1}^{Q} f_m\left(\frac{j-\frac{1}{2}}{2Q}\right) & \text{if } n=0. \end{cases} \tag{4.7}$$

Further defining

$$H_{N,Q} = (\delta_{nm} - h_Q(n,m))_{2\leq n,m\leq N} \quad \text{and} \quad b_{N,Q} = (h_Q(n,1))_{2\leq n\leq N},$$

we can set up the Hejhal system as follows,

$$H_{N,Q}\begin{pmatrix} x_2 \\ \vdots \\ x_N \end{pmatrix} = b_{N,Q}.$$

4.3.2 Proof of well-conditioned Hejhal system

For a square matrix with real entries, let $\|A\|$ denote the Frobenius norm $\sqrt{\mathrm{Tr}(A^T A)}$. We make the convention $\|A^{-1}\| = \infty$ if A is not invertable. We now state the main result of this section.

Theorem 4.3.1. *Let I_{N-1} denote the $(N-1)\times(N-1)$ identity matrix. Then either,*

(i) there exists a constant $N_0 = N_0(r,y)$ such that $\|H_{N,Q}^{-1} - I_{N-1}\| \ll_{r,Y} 1$ for all $Q > N \geq N_0$, or

(ii) $1 + \|H_{N,Q}^{-1} - I_{N-1}\| \gg_{r,Y} N^{3/2}$ for all $Q > N > 1$, with an effectively computable constant.

Since the constant in (ii) is effective, we can detect which case we are in at run time by taking N sufficiently large. Moreover, the set of r for which case (i) holds is open, so if we get close enough to a true eigenvalue r^* at which case (i) holds, then it will continue to hold as we zoom in. We can prove this by using the effective bound to establish a uniform upper bound for $\|H_{N,Q}^{-1} - I_{N-1}\|$ for r in an interval.

Proof. Define

$$h_\infty(n,m) = \lim_{Q\to\infty} h_Q(n,m) = \begin{cases} 4\displaystyle\int_0^{1/2} f_m(t)\cos(2\pi n t)\,dt & \text{if } n>0, \\ 2\displaystyle\int_0^{1/2} f_m(t)\,dt & \text{if } n=0, \end{cases} \tag{4.8}$$

so that

$$f_m(t) = \sum_{n=0}^{\infty} h_\infty(n,m)\cos(2\pi n t).$$

For any t at which $f_m(t)$ is smooth, we have using the bounds from Appendix A that

$$\frac{\partial^k}{\partial t^k} f_m(t) \ll_{r,Y,k} m^k e^{-2\pi m\left(\frac{\sqrt{3}}{2}-Y\right)} \ll_{r,Y,k} e^{-\delta m},$$

for any fixed $\delta \in (0, 2\pi(\frac{\sqrt{3}}{2}-Y))$. Since f_m is continuous, we can apply integration by parts twice in (4.8) to see that

$$h_\infty(n,m) = O_{r,Y}(n^{-2}e^{-\delta m}). \tag{4.9}$$

Thus, for any n with $1 \le n < Q$, we have

$$\begin{aligned} h_Q(n,m) &= \sum_{\substack{k\ge 0 \\ k\equiv n \pmod{2Q}}} (-1)^{\frac{k-n}{2Q}} h_\infty(k,m) + \sum_{\substack{k\ge 0 \\ k\equiv -n \pmod{2Q}}} (-1)^{\frac{k+n}{2Q}} h_\infty(k,m) \\ &= h_\infty(n,m) + \sum_{j=1}^{\infty} (-1)^j \left[h_\infty(2jQ+n,m) + h_\infty(2jQ-n,m)\right] \qquad (4.10) \\ &= O_{r,Y}(n^{-2}e^{-\delta m}). \end{aligned}$$

Now consider pairs $(N_1,Q_1),(N_2,Q_2)$ with $N_2 \ge N_1$. Let $\widetilde{H}_{N_1,Q_1}$ be the $(N_2-1)\times(N_2-1)$ block diagonal matrix which contains H_{N_1,Q_1} in the upper left and the $(N_2-N_1)\times(N_2-N_1)$ identity matrix in the lower right. Set $X = H_{N_2,Q_2} - \widetilde{H}_{N_1,Q_1}$. Then the (n,m) entry of X is $O_{r,Y}(\min(Q_1,Q_2)^{-2}e^{-\delta m})$ if $\max(n,m) \le N_1$ and $O_{r,Y}(n^{-2}e^{-\delta m})$ otherwise. Thus, $\|X\| = O_{r,Y}(N_1^{-3/2})$, that is $\|X\| \le C(r,Y)N_1^{-3/2}$ for some effectively computable constant $C(r,Y)$ (details on how to compute this constant shall be given in Section 4.4). Consider

$$\begin{aligned} H_{N_2,Q_2}^{-1} - I_{N_2-1} &= \left(I_{N_2-1} + \widetilde{H}_{N_1,Q_1}^{-1} X\right)^{-1} \widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1} \\ &= (I_{N_2-1} + T)^{-1} \left(I_{N_2-1} + \left(\widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1}\right)\right) - I_{N_2-1}, \end{aligned}$$

where $T = \left(\widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1}\right) X + X$. Suppose that $1 + \|H_{N_1,Q_1}^{-1} - I_{N_1-1}\| < \frac{N_1^{3/2}}{C(r,Y)}$, so that $1 + \|H_{N_1,Q_1}^{-1} - I_{N_1-1}\| = (1-\varepsilon)\frac{N_1^{3/2}}{C(r,Y)}$, for some $\varepsilon > 0$. Then T has norm at most $1-\varepsilon$, and $Z = (I_{N_2-1} + T)^{-1} - I_{N_2-1}$ has norm at most $\varepsilon^{-1} - 1$, by using the fact that $Z = -T + T^2 - T^3 + \ldots$. Thus,

$$\begin{aligned} H_{N_2,Q_2}^{-1} - I_{N_2-1} &= (I_{N_2-1} + Z)(I_{N_2-1} + (\widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1})) - I_{N_2-1} \\ &= Z + (\widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1}) + Z(\widetilde{H}_{N_1,Q_1}^{-1} - I_{N_2-1}), \end{aligned}$$

has norm at most $\varepsilon^{-1}(1 + \|H_{N_1,Q_1}^{-1} - I_{N_1-1}\|) - 1$, so that $\|H_{N,Q}^{-1} - I_{N-1}\|$ is bounded for $N \geq N_1$. If this conclusion does not hold for any N_1 then we must have $1 + \|H_{N,Q}^{-1} - I_{N-1}\| \geq \frac{N^{3/2}}{C(r,Y)}$ for all $Q > N > 1$. $\square$

4.4 Explicitly finding the O-constant

The goal of this section is to make the constant $C(r,Y)$ given in the proof of Theorem 4.3.1 explicit for computation. For convenience we shall restrict $\frac{1}{2\sqrt{3}} \leq Y < \frac{\sqrt{3}}{2}$. The reason for this, is that when we compute the pullback of $z(t)$ we only need to apply the transformation $z \mapsto -1/z$ once, meaning we can write down an explicit form of the pullback easier. Then, to get into $\overline{\mathcal{F}}$ we only need to apply the maps $z \mapsto z+1$ and $z \mapsto -\overline{z}$, which only affect the real part of z. Thus, using the fact that $\cos(2\pi m x^*)$ only depends on x^* mod $\mathbb{Z}$ and that it is even, we get that

$$f_m(t) = \frac{W_{ir}(2\pi m y^*(t))}{W_{ir}(2\pi m Y)} \cos(2\pi m x^*(t)) = \frac{W_{ir}\left(\frac{2\pi m Y}{t^2+Y^2}\right)}{W_{ir}(2\pi m Y)} \cos\left(\frac{2\pi m t}{t^2+Y^2}\right), \tag{4.11}$$

for all $t \in [0, 1/2]$ and $\frac{1}{2\sqrt{3}} \leq Y < \frac{\sqrt{3}}{2}$.

In the proof of Theorem 4.3.1 we did integration by parts to get a big-O bound on the matrix coefficients of the Hejhal system, which then gives us a bound on the full matrix. Here we shall make the implied constants in all of this explicit and computable. For small m we shall actually do integration by parts three times and explicitly compute the bounds numerically. For large m we shall do integration by parts twice and bound it analytically.

4.4.1 Derivatives of f_m

Before we begin getting the explicit constant, we shall need explicit formulas for the first and second derivatives of $f_m(t)$. For this, we have

$$\begin{aligned}\frac{d}{dt}\left(\frac{2\pi mY}{t^2+Y^2}\right) &= -\frac{4\pi mYt}{(t^2+Y^2)^2},\\ \frac{d}{dt}\left(\frac{2\pi mt}{t^2+Y^2}\right) &= -\frac{2\pi m(t^2-Y^2)}{(t^2+Y^2)^2}.\end{aligned}$$

Hence,

$$\begin{aligned}\frac{\partial}{\partial t}f_m(t) &= \frac{1}{W_{ir}(2\pi mY)}\frac{\partial}{\partial t}W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\cos\left(\frac{2\pi mt}{t^2+Y^2}\right)\\ &= \frac{1}{W_{ir}(2\pi mY)}\left[-\frac{4\pi mYt}{(t^2+Y^2)^2}W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\cos\left(\frac{2\pi mt}{t^2+Y^2}\right)\right.\\ &\left.+\frac{2\pi m(t^2-Y^2)}{(t^2+Y^2)^2}W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\sin\left(\frac{2\pi mt}{t^2+Y^2}\right)\right].\end{aligned}$$

For the second derivative we have

$$\begin{aligned}\frac{d}{dt}\left(\frac{-4\pi mYt}{(t^2+Y^2)^2}\right) &= -\frac{-4\pi mY(Y^2-3t^2)}{(t^2+Y^2)^3},\\ \frac{d}{dt}\left(\frac{2\pi m(t^2-Y^2)}{(t^2+Y^2)^2}\right) &= -\frac{4\pi mt(t^2-3Y^2)}{(t^2+Y^2)^3}.\end{aligned}$$

Hence

$$\begin{aligned}\frac{\partial^2}{\partial t^2}f_m(t) = \frac{1}{W_{ir}(2\pi mY)}&\left[\frac{4\pi mY(3t^2-Y^2)}{(t^2+Y^2)^3}W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\cos\left(\frac{2\pi mt}{t^2+Y^2}\right)\right. \qquad (4.12)\\ &+\frac{16\pi^2m^2Y^2t^2}{(t^2+Y^2)^4}W''_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\cos\left(\frac{2\pi mt}{t^2+Y^2}\right)\\ &+\frac{16\pi^2m^2tY(Y^2-t^2)}{(t^2+Y^2)^4}W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\sin\left(\frac{2\pi mt}{t^2+Y^2}\right)\\ &+\frac{4\pi mt(3Y^2-t^2)}{(t^2+Y^2)^3}W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\sin\left(\frac{2\pi mt}{t^2+Y^2}\right)\\ &\left.-\frac{4\pi^2m^2(t^2-Y^2)^2}{(t^2+Y^2)^4}W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\cos\left(\frac{2\pi mt}{t^2+Y^2}\right)\right].\end{aligned}$$

4.4.2 Large m

Here we shall explicitly do the integration by parts that we did to achieve (4.9). We have, for $n > 0$, that

$$\begin{aligned} h_\infty(n,m) &= 4\int_0^{1/2} f_m(t)\cos(2\pi nt)\,dt \\ &= -\frac{2}{\pi n}\int_0^{1/2} f_m'(t)\sin(2\pi nt)\,dt \\ &= \frac{1}{(\pi n)^2}\left((-1)^n f_m'\left(\frac{1}{2}\right) - \int_0^{1/2} f_m''(t)\cos(2\pi nt)\,dt\right), \end{aligned}$$

where $f_m'(t) = \frac{\partial}{\partial t} f_m(t)$ and noting that $f_m'(0) = 0$. Hence we can bound the $h_\infty(n,m)$ terms by

$$|h_\infty(n,m)| \leq \frac{U_m}{(\pi n)^2}, \tag{4.13}$$

where

$$U_m := \left|f_m'\left(\frac{1}{2}\right)\right| + \int_0^{1/2} |f_m''(t)|\,dt.$$

For the following calculations, we shall need the following lemma.

Lemma 4.4.1. *Let $n \geq 2$ be an integer and $x > 1$ be a real number. Then we have*

$$1 + \sum_{j=1}^{\infty}\left(\frac{1}{(2jx-1)^n} + \frac{1}{(2jx+1)^n}\right) \leq \zeta(n)\frac{2^n - 1}{2^{n-1}},$$

and

$$\sum_{j=1}^{\infty}\left(\left(\frac{2x-1}{2jx+1}\right)^n + \left(\frac{2x-1}{2jx-1}\right)^n\right) \leq 2\zeta(n).$$

Proof. For the first identity, we have that $2jx \pm 1 \geq 2j \pm 1$ for all $x > 1$. Hence,

$$
\begin{aligned}
1 + \sum_{j=1}^{\infty}\left(\frac{1}{(2jx-1)^n} + \frac{1}{(2jx+1)^n}\right) &\leq 1 + \sum_{j=1}^{\infty}\left(\frac{1}{(2j-1)^n} + \frac{1}{(2j+1)^n}\right) \\
&= 2\sum_{j=1}^{\infty}\frac{1}{(2j-1)^n} \\
&= 2\left(\sum_{j=1}^{\infty}\frac{1}{j^n} - \sum_{j=1}^{\infty}\frac{1}{(2j)^n}\right) \\
&= \zeta(n)\frac{2^n-1}{2^{n-1}}.
\end{aligned}
$$

For the second identity, we have that

$$
\frac{2x-1}{2jx \pm 1} = \frac{2x \pm \frac{1}{j} - \left(1 \pm \frac{1}{j}\right)}{2jx \pm 1} = \frac{1}{j} - \frac{1 \pm \frac{1}{j}}{2jx \pm 1} \leq \frac{1}{j},
$$

for all $x > 1$ and $j \geq 1$. Hence,

$$
\sum_{j=1}^{\infty}\left(\left(\frac{2x-1}{2jx+1}\right)^n + \left(\frac{2x-1}{2jx-1}\right)^n\right) \leq 2\sum_{j=1}^{\infty}\frac{1}{j^n} = 2\zeta(n).
$$

□

We recall, from (4.10), we have

$$
h_Q(n,m) = h_\infty(n,m) + \sum_{j=1}^{\infty}(-1)^j\left[h_\infty(2jQ+n,m) + h_\infty(2jQ-n,m)\right].
$$

Hence using the bound (4.13) and Lemma 4.4.1 we get, for all $n < Q$, that

$$
\begin{aligned}
|h_Q(n,m)| &\leq |h_\infty(n,m)| + \sum_{j=1}^{\infty}(-1)^j\left[|h_\infty(2jQ+n,m)| + |h_\infty(2jQ-n,m)|\right] \\
&\leq \frac{U_m}{\pi^2}\left(\frac{1}{n^2} + \frac{1}{(2Q-n)^2} + \frac{1}{(2Q+n)^2} + \frac{1}{(4Q-n)^2} + \dots\right) \\
&\leq \frac{U_m}{4n^2}.
\end{aligned}
$$

Furthermore, also using Lemma 4.4.1, we get for all $0 < Q_1 < Q_2$ that

$$\begin{aligned}
|h_{Q_1}(n,m) - h_{Q_2}(n,m)| &\leq \sum_{v\in\{1,2\}} \sum_{j=1}^{\infty} \left(|h_\infty(2jQ_v + n, m)| + |h_\infty(2jQ_v - n, m)|\right) \\
&\leq \frac{U_m}{\pi^2} \sum_{v\in\{1,2\}} \sum_{j=1}^{\infty} \left(\frac{1}{(2jQ_v + n)^2} + \frac{1}{(2jQ_v - n)^2}\right) \\
&= \frac{U_m}{\pi^2} \sum_{v\in\{1,2\}} \frac{1}{(2Q_v - n)^2} \sum_{j=1}^{\infty} \left(\left(\frac{2Q_v - n}{2jQ_v + n}\right)^2 + \left(\frac{2Q_v - n}{2jQ_v - n}\right)^2\right) \\
&\leq \frac{U_m}{3} \left(\frac{1}{(2Q_1 - n)^2} + \frac{1}{(2Q_2 - n)^2}\right).
\end{aligned}$$

Our goal now is to get an upper bound on U_m that depends only on r and Y. To do this we shall recall our bounds for W_{ir} from Appendix A in the following proposition.

Proposition 4.4.2. *We have*

$$\begin{aligned}
&|W_{ir}(x)| \leq \sqrt{\frac{\pi}{2}} e^{-x} \text{ for all } x > 0 \text{ and } r > 0, \\
&|W'_{ir}(x)| \leq \sqrt{\frac{\pi}{2}} e^{-x} \text{ for all } x \geq 1 \text{ and } r \geq 5, \\
&|W''_{ir}(x)| \leq \sqrt{\frac{\pi}{2}} e^{-x} \text{ for all } x \geq 1 \text{ and } r \geq 5, \\
&|W_{ir}(x)| \geq e^{x_0 - x} W_{ir}(x_0) > 0 \text{ for all } x \geq x_0 \geq \sqrt{\lambda}.
\end{aligned}$$

For level 1, we know the smallest even eigenvalue is $r \approx 13.77975\ldots$ [BSV06], so these bounds are valid for us. We also recall we have the bounds of $0 \leq t \leq 1/2$ and $\frac{1}{2\sqrt{3}} \leq Y < \frac{\sqrt{3}}{2}$. To begin, we note that for $x \geq x_0 \geq \sqrt{\lambda}$, we have that

$$\frac{1}{|W_{ir}(2\pi mY)|} \leq \frac{\exp(2\pi mY)}{e^{x_0} W_{ir}(x_0)} \leq \frac{\exp(2\pi mY)}{e^{\sqrt{\lambda}} W_{ir}(\sqrt{\lambda})} \tag{4.14}$$

For the first derivative of $f_m(t)$ at $t = 1/2$, we have that

$$\begin{aligned}
&\frac{2\pi mY}{\left(\frac{1}{4}+Y^2\right)^2}\left|W'_{ir}\left(\frac{2\pi mY}{\left(\frac{1}{4}+Y^2\right)}\right)\right| + \frac{2\pi m\left|\frac{1}{4}-Y^2\right|}{\left(\frac{1}{4}+Y^2\right)^2}\left|W_{ir}\left(\frac{2\pi mY}{\left(\frac{1}{4}+Y^2\right)}\right)\right| \\
&\leq \sqrt{\frac{\pi}{2}}\exp\left(-\frac{2\pi mY}{\left(\frac{1}{4}+Y^2\right)}\right)\left(2\pi m\frac{Y+\left|\frac{1}{4}-Y^2\right|}{\left(\frac{1}{4}+Y^2\right)^2}\right) \\
&\leq 3\pi m(1+\sqrt{3})\sqrt{\frac{\pi}{2}}\exp\left(-\frac{2\pi mY}{\left(\frac{1}{4}+Y^2\right)}\right).
\end{aligned}$$

Hence, combining the above two results, we see that

$$\left|f'_m\left(\frac{1}{2}\right)\right| \leq \sqrt{\frac{\pi}{2}}\exp\left(m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4}+Y^2}\right)\right)\frac{3\pi m(1+\sqrt{3})}{e^{\sqrt{\lambda}}W_{ir}(\sqrt{\lambda})}.$$

Now we consider the second derivative of $f_m(t)$. To do this we shall bound each of the terms in (4.12) and integrate them separately over $0 \leq t \leq 1/2$ and add these up. To begin, consider

$$\frac{4\pi mY|3t^2-Y^2|}{(t^2+Y^2)}\left|W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| \leq \frac{4m\pi\sqrt{\pi/2}}{Y^3}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right).$$

Hence,

$$\begin{aligned}
\int_0^{1/2}\frac{4\pi mY|3t^2-Y^2|}{(t^2+Y^2)}\left|W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| dt &\leq \frac{4m\pi\sqrt{\pi/2}}{Y^3}\int_0^{1/2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right) dt \\
&\leq \frac{4m\pi\sqrt{\pi/2}}{Y^3}\exp\left(-\frac{2\pi mY}{\frac{1}{4}+Y^2}\right)\int_0^{1/2} dt \\
&= \frac{2m\pi\sqrt{\pi/2}}{Y^3}\exp\left(-\frac{2\pi mY}{\frac{1}{4}+Y^2}\right).
\end{aligned}$$

Next, we consider

$$\begin{aligned}
\frac{(4\pi mYt)^2}{(t^2+Y^2)^4}\left|W''_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| &\leq \frac{16\pi^2m^2Y^2t^2\sqrt{\pi/2}}{(t^2+Y^2)^4}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right) \\
&\leq \frac{2\pi m\sqrt{\pi/2}}{Y^3}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right).
\end{aligned}$$

Hence,

$$\int_0^{1/2} \frac{(4\pi mYt)^2}{(t^2+Y^2)^4}\left|W''_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| dt \le \frac{2\pi m\sqrt{\pi/2}}{Y^3}\int_0^{1/2}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right)dt$$
$$\le \frac{2\pi m\sqrt{\pi/2}}{Y^3}\exp\left(-\frac{2\pi mY}{\frac{1}{4}+Y^2}\right).$$

Now, consider

$$\frac{(4\pi m)^2tY|Y^2-t^2|}{(t^2+Y^2)^4}\left|W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| \le \frac{16\pi^2m^2tY|Y^2-t^2|\sqrt{\pi/2}}{(t^2+Y^2)^4}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right)$$
$$\le \frac{4\pi m\sqrt{\pi/2}}{Y^2}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right).$$

Hence,

$$\int_0^{1/2}\frac{(4\pi m)^2tY|Y^2-t^2|}{(t^2+Y^2)^4}\left|W'_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| dt \le \frac{4\pi m\sqrt{\pi/2}}{Y^2}$$
$$\cdot\int_0^{1/2}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right)dt$$
$$\le \frac{4\pi m\sqrt{\pi/2}}{Y^2}\exp\left(-\frac{2\pi mY}{\frac{1}{4}+Y^2}\right).$$

Next, consider

$$\frac{4\pi mt|3Y^2-t^2|}{(t^2+Y^2)^3}\left|W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| \le \frac{4\pi mt|3Y^2-t^2|\sqrt{\pi/2}}{(t^2+Y^2)^3}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right)$$
$$\le \frac{3\sqrt{\pi/2}}{Y}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right).$$

Hence,

$$\int_0^{1/2}\frac{4\pi mt|3Y^2-t^2|}{(t^2+Y^2)^3}\left|W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)\right| dt \le \frac{3\sqrt{\pi/2}}{Y}$$
$$\cdot\int_0^{1/2}\frac{4\pi mYt}{(t^2+Y^2)^2}\exp\left(-\frac{2\pi mY}{t^2+Y^2}\right)dt$$
$$\le \frac{3\sqrt{\pi/2}}{Y}\exp\left(-\frac{2\pi mY}{\frac{1}{4}+Y^2}\right).$$

Finally, consider

$$\frac{4\pi^2 m^2 (t^2 - Y^2)^2}{(t^2+Y^2)^4} \left| W_{ir}\left(\frac{2\pi m Y}{t^2+Y^2}\right)\right| \leq \frac{4\pi^2 m^2 \sqrt{\pi/2}}{Y^4} \exp\left(-\frac{2\pi m Y}{t^2+Y^2}\right).$$

Hence,

$$\begin{aligned}\int_0^{1/2} \frac{4\pi^2 m^2 (t^2 - Y^2)^2}{(t^2+Y^2)^4} \left| W_{ir}\left(\frac{2\pi m Y}{t^2+Y^2}\right)\right| dt &\leq \frac{4\pi^2 m^2 \sqrt{\pi/2}}{Y^4} \int_0^{1/2} \exp\left(-\frac{2\pi m Y}{t^2+Y^2}\right) dt \\ &\leq \frac{4\pi^2 m^2 \sqrt{\pi/2}}{Y^4} \exp\left(-\frac{2\pi m Y}{\frac{1}{4}+Y^2}\right) \int_0^{1/2} dt \\ &\leq \frac{2\pi^2 m^2 \sqrt{\pi/2}}{Y^4} \exp\left(-\frac{2\pi m Y}{\frac{1}{4}+Y^2}\right).\end{aligned}$$

Combining each of these and (4.14), we see that

$$\int_0^{1/2} |f_m''(t)|\, dt \leq \exp\left(m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4}+Y^2}\right)\right) \frac{\frac{3}{Y} + m\left(\frac{4\pi}{Y^2} + \frac{4\pi}{Y^3}\right) + m^2 \frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}} W_{ir}(\sqrt{\lambda})}.$$

Thus, overall we get that

$$|U_m| \leq \sqrt{\frac{\pi}{2}} \exp\left(m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4}+Y^2}\right)\right) \frac{\frac{3}{Y} + m\left(3\pi(1+\sqrt{3}) + \frac{4\pi}{Y^2} + \frac{4\pi}{Y^3}\right) + m^2 \frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}} W_{ir}(\sqrt{\lambda})}. \tag{4.15}$$

4.4.3 Small m

For small m, we shall do a similar treatment to what we did for large m, however we shall not find upper bounds for the f_m terms, and instead numerically compute them. To begin we shall perform integration by parts three times to achieve

$$\begin{aligned} h_\infty(n,m) &= 4\int_0^{1/2} f_m(t)\cos(2\pi n t)\, dt \\ &= \frac{(-1)^n}{(\pi n)^2} f_m'(1/2) + \frac{1}{2(\pi n)^3} \int_0^{1/2} f_m'''(t) \sin(2\pi n t)\, dt.\end{aligned}$$

Now, using the Cauchy–Schwartz inequality, we can bound the integral by

$$\left(\int_0^{1/2} f_m'''(t)\sin(2\pi n t)\, dt\right)^2 \leq \int_0^{1/2} f_m'''(t)^2\, dt \int_0^{1/2} \sin^2(2\pi n t)\, dt = \frac{1}{4}\int_0^{1/2} f_m'''(t)^2\, dt.$$

Hence,

$$h_\infty(n,m) \le \frac{(-1)^n}{(\pi n)^2} f_m'(1/2) + \frac{1}{4(\pi n)^3}\left(\int_0^{1/2} f_m'''(t)^2\,dt\right)^{1/2}.$$

Thus,

$$|h_\infty(n,m)| \le \frac{a_m}{(\pi n)^2} + \frac{b_m}{(\pi n)^3},$$

where,

$$a_m = \left| f_m'\left(\frac{1}{2}\right)\right| \quad \text{and} \quad b_m = \frac{1}{4}\left(\int_0^{1/2} f_m'''(t)^2\,dt\right)^{1/2}.$$

From the definition of $h_Q(n,m)$ (4.8) and using Lemma 4.4.1, we get that

$$\begin{aligned} |h_Q(n,m)| &\le \left(\frac{a_m}{(\pi n)^2} + \frac{b_m}{(\pi n)^3}\right) \\ &\quad + \sum_{j=1}^{\infty}\left(\frac{a_m}{\pi^2}\left(\frac{1}{(2jQ+n)^2} + \frac{1}{(2jQ-n)^2}\right)\right. \\ &\qquad \left. + \frac{b_m}{\pi^3}\left(\frac{1}{(2jQ+n)^3} + \frac{1}{(2jQ-n)^3}\right)\right) \\ &\le \frac{a_m}{4n^2} + \frac{7\zeta(3) b_m}{4\pi^3 n^3}. \end{aligned}$$

Similarly, also using Lemma 4.4.1, we have that

$$\begin{aligned} |h_{Q_1}(n,m) - h_{Q_2}(n,m)| &\le \sum_{v\in\{1,2\}}\sum_{j=1}^{\infty}\left(\frac{a_m}{\pi^2}\left(\frac{1}{(2jQ_v+n)^2} + \frac{1}{(2jQ_v-n)^2}\right)\right. \\ &\qquad \left. + \frac{b_m}{\pi^3}\left(\frac{1}{(2jQ_v+n)^3} + \frac{1}{(2jQ_v-n)^3}\right)\right) \\ &\le \frac{2a_m}{3(2Q_1-n)^2} + \frac{2\zeta(3) b_m}{\pi^3(2Q_1-n)^3}. \end{aligned}$$

4.4.4 Explicit bound on size of $\|X\|$

Recall we defined $X = H_{N_2,Q_2} - \widetilde{H}_{N_1,Q_1}$. Entrywise this is

$$X = (x_{nm})_{2\le n,m\le N_2} = \begin{cases} h_{Q_1}(n,m) - h_{Q_2}(n,m) & \text{if } 2 \le n,m \le N_1, \\ -h_{Q_2}(n,m) & \text{otherwise.} \end{cases}$$

Hence, we have

$$\begin{aligned}
\|X\|^2 &= \sum_{n=2}^{N_2}\sum_{m=2}^{N_2} x_{nm}^2 \\
&= \sum_{m=2}^{N_1}\left(\sum_{n=2}^{N_1}(h_{Q_1}(n,m)-h_{Q_2}(n,m))^2 + \sum_{n=N_1+1}^{N_2} h_{Q_2}(n,m)^2\right) \\
&+ \sum_{m=N_1+1}^{N_2}\sum_{n=2}^{N_2} h_{Q_2}(n,m)^2.
\end{aligned}$$

Now, we want to split up the first sum over m between small and large values of m. We shall then use our bounds derived in the previous section to get a bound for $\|X\|^2$. Let $2 \le M < N_1$. Then

$$\begin{aligned}
\|X\|^2 = &\sum_{m=2}^{M}\left(\sum_{n=2}^{N_1}(h_{Q_1}(n,m)-h_{Q_2}(n,m))^2 + \sum_{n=N_1+1}^{N_2} h_{Q_2}(n,m)^2\right) \\
&+ \sum_{m=M+1}^{N_1}\left(\sum_{n=2}^{N_1}(h_{Q_1}(n,m)-h_{Q_2}(n,m))^2 + \sum_{n=N_1+1}^{N_2} h_{Q_2}(n,m)^2\right) \\
&+ \sum_{m=N_1+1}^{N_2}\sum_{n=2}^{N_2} h_{Q_2}(n,m)^2 \\
&\le \sum_{m=2}^{M}\left(\sum_{n=2}^{N_1}\left(\frac{2a_m}{3(2Q_1-n)^2}+\frac{2\zeta(3)b_m}{\pi^3(2Q_1-n)^3}\right)^2 + \sum_{n=N_1+1}^{N_2}\left(\frac{a_m}{4n^2}+\frac{7\zeta(3)b_m}{4\pi^3n^3}\right)^2\right) \\
&+ \sum_{m=M+1}^{N_1} U_m^2\left(\frac{4}{9}\sum_{n=2}^{N}\frac{1}{(2Q_1-n)^4}+\frac{1}{16}\sum_{n=N_1+1}^{N_2}\frac{1}{n^4}\right) + \sum_{m=N_1+1}^{N_2} U_m^2 \sum_{n=2}^{N_2}\frac{1}{16n^4}.
\end{aligned}$$

Here we note that, for $k > 1$,

$$\sum_{n=2}^{N_1}\frac{1}{(2Q_1-n)^k} \le \sum_{n=2}^{N_1}\frac{1}{(2N_1-n)^k} \le \int_1^{N_1}\frac{1}{(2Q_1-t)^k}\,dt \le \frac{1}{k-1}\frac{1}{N_1^{k-1}},$$

and similarly

$$\sum_{n=N_1+1}^{N_2} n^{-k} \le \sum_{n=N_1+1}^{\infty} n^{-k} \le \int_{N_1}^{\infty} t^{-k}\,dt \le \frac{1}{k-1}N_1^{k-1}.$$

Hence,

$$\begin{aligned}
\|X\|^2 \leq \sum_{m=2}^{M} \bigg(&\frac{4}{27N_1^3} a_m^2 + \frac{2\zeta(3)}{3\pi^3 N_1^4} a_m b_m + \frac{4\zeta(3)^2}{5\pi^6 N_1^5} b_m^2 \\
&+ \frac{1}{48N_1^3} a_m^2 + \frac{7\zeta(3)}{32\pi^3 N_1^4} a_m b_m + \frac{49\zeta(3)^2}{80\pi^6 N_1^5} b_m^2 \bigg) \\
&+ \left(\frac{4}{27} + \frac{1}{48} \right) \frac{1}{N_1^3} \sum_{m=M+1}^{N_1} U_m^2 + \frac{\zeta(4)-1}{16} \sum_{m=N_1+1}^{N_2} U_m^2 \\
&= \frac{73}{432N_1^3} \sum_{m=2}^{M} a_m^2 + \frac{85\zeta(3)}{96\pi^3 N_1^4} \sum_{m=2}^{M} a_m b_m + \frac{113\zeta(3)^2}{80\pi^6 N_1^5} \sum_{m=2}^{M} b_m^2 \\
&+ \frac{73}{432N_1^3} \sum_{m=M+1}^{N_1} U_m^2 + \frac{\zeta(4)-1}{16} \sum_{m=N_1+1}^{N_2} U_m^2.
\end{aligned}$$

To bound the sums of U_m, we shall use our bound (4.15) and majorise the sums by a geometric series. Taking our bound from (4.15) and squaring we have

$$|U_m|^2 \leq d_m$$

where

$$d_m := \frac{\pi}{2} \exp\left(2m \left(2\pi Y - \frac{2\pi Y}{\frac{1}{4} + Y^2} \right) \right) \left(\frac{\frac{3}{Y} + m\left(3\pi(1+\sqrt{3}) + \frac{4\pi}{Y^2} + \frac{4\pi}{Y^3}\right) + m^2 \frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}} W_{ir}(\sqrt{\lambda})} \right)^2.$$

Hence, for some $M, N \in \mathbb{N}$ with $M < N$, we have

$$\sum_{m=M}^{N} |U_m|^2 \leq \sum_{m=M}^{\infty} |U_m|^2 \leq \sum_{m=M}^{\infty} d_m \leq d_M \sum_{k=0}^{\infty} \left(\frac{d_{M+1}}{d_M} \right)^k \leq \frac{d_M^2}{d_M - d_{M+1}}.$$

Thus combining all this, we obtain the final bound of

$$\begin{aligned}
\|X\|^2 \leq &\frac{73}{432N_1^3} \sum_{m=2}^{M} a_m^2 + \frac{85\zeta(3)}{96\pi^3 N_1^4} \sum_{m=2}^{M} a_m b_m + \frac{113\zeta(3)^2}{80\pi^6 N_1^5} \sum_{m=2}^{M} b_m^2 \\
&+ \frac{73}{432N_1^3} \frac{d_{M+1}^2}{d_{M+1} - d_{M+2}} + \frac{\pi^4 - 90}{1440} \frac{d_{N_1+1}^2}{d_{N_1+1} - d_{N_1+2}},
\end{aligned}$$

where

$$a_m := \left| f_m'\left(\frac{1}{2}\right) \right|,$$

$$b_m := \frac{1}{4}\left(\int_0^{1/2} f_m'''(t)^2\, dt\right)^{1/2},$$

$$d_m := \frac{\pi}{2}\exp\left(2m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4}+Y^2}\right)\right)\left(\frac{\frac{3}{Y} + m\left(3\pi(1+\sqrt{3}) + \frac{4\pi}{Y^2} + \frac{4\pi}{Y^3}\right) + m^2\frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}}W_{ir}(\sqrt{\lambda})}\right)^2.$$

We see that this is of the required form for Theorem 4.3.1. In practice, when implementing this as part of Hejhal's algorithm, we numerically compute the a_m and b_m for $2 \le m \le M$ in interval arithmetic.

We choose M such that we can use our lower bound effectively in Proposition 4.4.2. Explicitly, we need make sure our input values are greater than $\sqrt{\lambda}$, hence we choose M such that

$$M = \left\lceil \frac{\sqrt{\lambda}}{2\pi Y} \right\rceil.$$

4.4.5 Computing b_m

To numerically compute the integral appearing in the definition of b_m, we shall use the quadrature method described in Appendix B. As stated we shall implement this in interval arithmetic. We recall the error bound for the quadrature method is

$$\exp\left(4 - \frac{5n}{\log(5n)}\right) \sup_{z\in D(0,2)} |f(z)|, \tag{4.16}$$

where f is a holomorphic function on $D(0,2) = \{z \in \mathbb{C} : |z| \le 2\}$. By the maximum modulus principle, we know that f attains its maximum on the boundary of $D(0,2)$, i.e all $z \in \mathbb{C}$ such that $|z| = 2$. We recall we have

$$f_m(t) = \frac{W_{ir}\left(\frac{2\pi mY}{t^2+Y^2}\right)}{W_{ir}(2\pi mY)}\cos\left(\frac{2\pi mt}{t^2+Y^2}\right),$$

for $m > 0$. We also recall that $W_{ir}(y) = \sqrt{y}K_{ir}(y)$. In the definition of b_m, we will be integrating the third derivative of this function. To numerically compute the third derivative, we replace t by the polynomial $\widetilde{t} = x + t$. We first compute the power series of

$$\sqrt{\frac{2\pi mY}{\widetilde{t}^2+Y^2}},\, K_{ir}\left(\frac{2\pi mY}{\widetilde{t}^2+Y^2}\right) \text{ and } \cos\left(\frac{2\pi m\widetilde{t}}{\widetilde{t}^2+Y^2}\right)$$

separately and then multiply them together. Then, after scaling by 3!, the term for the z^3 term will give a numerical answer for the third derivative at t.

Now, using this to compute the error bound for the integral would be very slow, so we should bound the error analytically. To begin, let $\varepsilon > 0$ and $C_\varepsilon = \{z \in \mathbb{C} \mid |z - z_0| < \varepsilon\}$, that is, the circle of radius ε and centred at $z_0 \in \mathbb{C}$. We have by Cauchy's theorem that

$$f^{(k)}(z_0) = \frac{k!}{2\pi i}\oint_{C_\varepsilon(z_0)} \frac{f(z)}{(z-z_0)^{k+1}}\, dz$$

for some nice analytic f. Then we have the bound

$$\left|\frac{f^{(k)}(z_0)}{k!}\right| \le \sup_{z\in C_\varepsilon(z_0)} |f(z)|\varepsilon^{-k}.$$

To bound the supremum, we first fix a value for ε. For us $f(z) = W_{ir}(2\pi mY)f_m(z)$.

To begin, using the bound of $W_{ir}(z)$ for complex z from Appendix A, we have

$$|\cos(z)| \le \cosh(\operatorname{Im}(z)) \text{ and}$$
$$|W_{ir}(z)| \le \sqrt{\frac{\pi|z|}{2\operatorname{Re}(z)}}e^{-\operatorname{Re}(z)},$$

for $z \in \mathbb{C}$ with $\operatorname{Re}(z) > 0$. Hence,

$$\begin{aligned}
|f(z)| &= \left|W_{ir}\left(\frac{2\pi m}{Y((z/Y)^2+1)}\right)\right|\left|\cos\left(\frac{2\pi mz}{Y((z/Y)^2+1)}\right)\right| \\
&\le \sqrt{\frac{\pi/2}{|(\frac{z}{Y})^2+1|\operatorname{Re}(\frac{1}{(\frac{z}{Y})^2+1})}}\exp\left(-\operatorname{Re}\left(\frac{1}{(\frac{z}{Y})^2+1}\right)\right)\cosh\left(\operatorname{Im}\left(\frac{2\pi mz}{Y((\frac{z}{Y})^2+1)}\right)\right) \\
&= \frac{1}{2}\sqrt{\frac{\pi/2}{|(\frac{z}{Y})^2+1|\operatorname{Re}(\frac{1}{(\frac{z}{Y})^2+1})}}\left(\exp\left(\frac{2\pi m\operatorname{Im}\left(\frac{1}{\frac{z}{Y}+i}\right)}{Y}\right)+\exp\left(\frac{2\pi m\operatorname{Im}\left(\frac{1}{-\frac{z}{Y}+i}\right)}{Y}\right)\right).
\end{aligned}$$

We could further try to refine this bound, but for our case this will be sufficient.

Thus, to compute the error bound, we first split up the circle centred at 0 of radius 2 into N intervals around the circle, where N is chosen such that

$$4 - \frac{5N}{\log(5N)} < B \log 2,$$

where B is the number of bits of precision desired. We then bound our integrand on each interval but choosing z_0 to be the centre of each interval and ε to be half the length of the interval. We just compute the above bound in interval arithmetic with z_0 being interpreted as a complex ball of radius ε centred at z_0.

Note, we actually implemented this in `Arb` which technically represents complex numbers in rectangles rather than balls, but this distinction will not affect the result drastically.

We also note that the error bound (4.16) is for integrals taken between -1 and 1. In order to treat generic bounds, we need to scale and move the disk centred at 0 and of radius 2 to the disk centred at $b-a$ and of radius $\frac{a+b}{2}$ where we now integrate from a to b.

4.5 Odd case

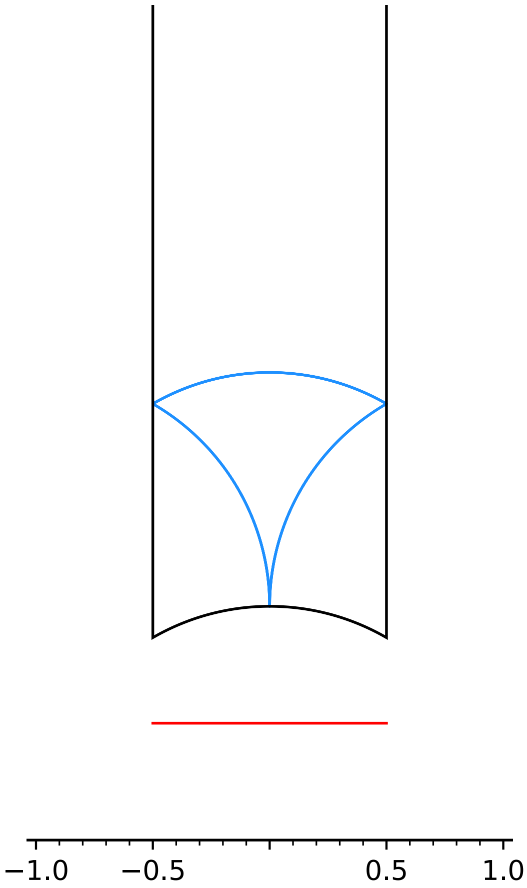
The above analysis was concerned with looking at even Maass cusp forms, we can generalise this for odd forms as well. Fix Y and Q. Let $z(t) = x(t) + iY$ be a horocycle below the fundamental domain, now with $t \in [-1/2, 1/2]$. We then let $z^*(t) = x^*(t) + iy^*(t)$ to be the $\mathrm{PSL}(2,\mathbb{Z})$-pullback into the full fundamental domain $\mathcal{F}$ of $\mathrm{PSL}(2,\mathbb{Z})$. We then define, for $m \in \mathbb{Z}$,

$$f_m(t) = \frac{W_{ir}(2\pi m y^*(t))}{W_{ir}(2\pi m Y)} \sin(2\pi m x^*(t)).$$

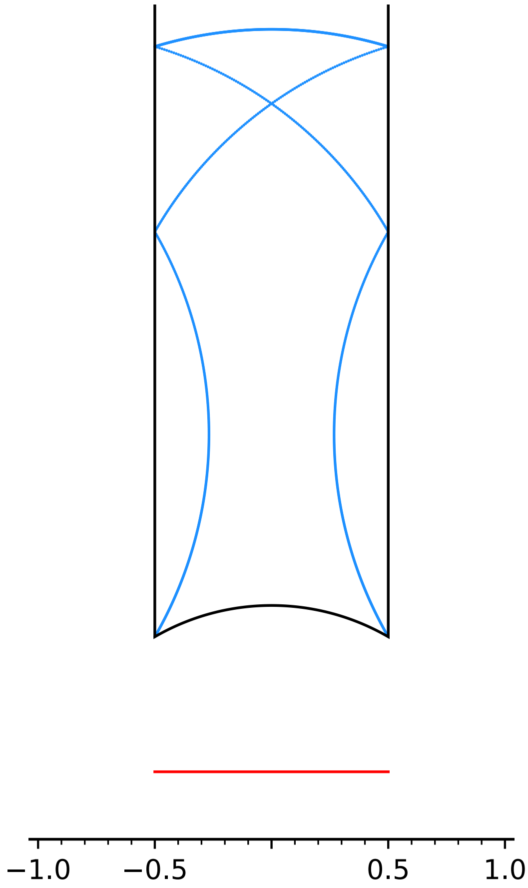
Since we are dealing with the whole fundamental domain F, the pullback of the horocycle is not continuous which means our definition of $f_m(t)$ is not continuous for all $0 < Y < \sqrt{3}/2$. Not all is lost however, since we will show there are specific values of Y that will give us continuity. To begin, similar to the even case, restrict $\frac{1}{2\sqrt{3}} \leq Y < \frac{\sqrt{3}}{2}$, then we can write

$$f_m(t) = \frac{W_{ir}(2\pi m y^*(t))}{W_{ir}(2\pi m Y)} \sin(2\pi m x^*(t)) = -\frac{W_{ir}\left(\frac{2\pi m Y}{t^2+Y^2}\right)}{W_{ir}(2\pi m Y)} \sin\left(\frac{2\pi m t}{t^2+Y^2}\right). \tag{4.17}$$

We observe that if we now choose $Y = \frac{1}{2}$ or $Y = \frac{1}{2\sqrt{3}}$, then $f_m(\pm 1/2) = 0$ for all m, that is it vanishes at the endpoints of the horocycle. Since $f_m(t)$ will also vanish



$Y = \frac{1}{2}$



$Y = \frac{1}{2\sqrt{3}}$

Figure 4.1: Plot of horocycles $z(t) = t + iY$ with the values of $Y = \frac{1}{2}$ and $Y = \frac{1}{2\sqrt{3}}$ that make the odd case work. The red line is the horocyle and the blue line is its pullback. We note that these figures were made by computing $z(t)$ and its pullback on a certain number of points, which means it does not illustrate the Pac-Man-like crossings of the boundaries of the fundamental domain.

when crossing over the fundamental domain, we get that we have continuity of the pullback and f_m for these values. Plots of these horocycles with their pullbacks are given in Figure 4.1. This will allow us to perform integration by parts again. From now on, we shall assume $Y = \frac{1}{2}$ or $Y = \frac{1}{2\sqrt{3}}$.

Next, define for $n \in \mathbb{Z}_{\geq 0}$,

$$h_Q(n,m) = \begin{cases} \dfrac{2}{Q}\displaystyle\sum_{j=1}^{Q} f_m\left(\frac{j-\frac{1}{2}}{2Q}\right)\sin\left(2\pi n\frac{j-\frac{1}{2}}{2Q}\right) & \text{if } n > 0, \\ \dfrac{1}{Q}\displaystyle\sum_{j=1}^{Q} f_m\left(\frac{j-\frac{1}{2}}{2Q}\right) & \text{if } n = 0. \end{cases} \tag{4.18}$$

Further defining

$$H_{N,Q} = (\delta_{nm} - h_Q(n,m))_{2\le n,m\le N} \quad \text{and} \quad b_{N,Q} = (h_Q(n,1))_{2\le n\le N},$$

we can set up the Hejhal system as follows,

$$H_{N,Q}\begin{pmatrix} x_2 \\ \vdots \\ x_N \end{pmatrix} = b_{N,Q}.$$

Define

$$h_\infty(n,m) = \lim_{Q\to\infty} h_Q(n,m) = \begin{cases} 4\displaystyle\int_0^{1/2} f_m(t)\sin(2\pi nt)\,dt & \text{if } n>0, \\ 2\displaystyle\int_0^{1/2} f_m(t)\,dt & \text{if } n=0, \end{cases} \tag{4.19}$$

so that

$$f_m(t) = \sum_{n=0}^{\infty} h_\infty(n,m)\sin(2\pi nt).$$

For any t at which $f_m(t)$ is smooth, we have

$$\frac{\partial^k}{\partial t^k} f_m(t) \ll_{r,Y,k} m^k e^{-2\pi m\left(\frac{\sqrt{3}}{2}-Y\right)} \ll_{r,Y,k} e^{-\delta m},$$

for any fixed $\delta \in (0, 2\pi(\frac{\sqrt{3}}{2} - Y))$.

Since $f_m(t)$ is continuous, we can again perform integration by parts twice to the integral above to obtain

$$\int_0^{1/2} f_m(t)\sin(2\pi nt)dt = \frac{f_m(0)}{2\pi n} - \frac{f_m(1/2)}{2\pi n}\cos(\pi n) - \frac{1}{(2\pi n)^2}\int_0^{1/2} f_m''(t)\sin(2\pi nt)dt.$$

We now note that $f_m(0) = 0$, since the pullback of $z(0) = iY$ is just the map $S(z) = -1/z$. Hence $z^*(0) = S(iY) = i/Y$, which is always in the fundamental domain for all $Y \in (0, \sqrt{3}/2)$. We see that $\mathrm{Re}(z^*(0)) = 0$, thus the sin term vanishes in the definition of $f_m(t)$. Using this, we actually obtain

$$\int_0^{1/2} f_m(t)\sin(2\pi nt)dt = -\frac{f_m(1/2)}{2\pi n}\cos(\pi n) - \frac{1}{(2\pi n)^2}\int_0^{1/2} f_m''(t)\sin(2\pi nt)dt.$$

To get the $O(n^{-2})$ required, we note the fact that for our choices for Y, we have that $f_m(1/2) = 0$ for all m. Thus, we get that

$$\int_0^{1/2} f_m(t)\sin(2\pi nt)dt = -\frac{1}{(2\pi n)^2}\int_0^{1/2} f_m''(t)\sin(2\pi nt)dt, \tag{4.20}$$

giving us the $O(n^{-2})$ required. Similar to the even case, we shall use (4.20) for large m and the bound from applying integration by parts a third time for small m. In fact, we can apply integration by parts a third time and get $O(n^{-3})$ overall, however we do not do this since we can re-use the bounds derived in Section 4.4 for $O(n^{-2})$.

4.5.1 Large m

From the definition of $h_\infty(n,m)$ and (4.20), we have

$$h_\infty(n,m) = -\frac{1}{(\pi n)^2}\int_0^{1/2} f_m''(t)\sin(2\pi nt)dt.$$

Hence,

$$|h_\infty(n,m)| \le \frac{U_m}{(\pi n)^2},$$

where

$$U_m := \int_0^{1/2} |f_m''(t)|dt.$$

Here we note that we can just directly use our bound from Section 4.4.2 to this integral, since the only differences are the sines instead of cosines and some minus signs from this, all of which get removed when we crash through with absolute values. Hence,

$$|U_m| \le \sqrt{\frac{\pi}{2}}\exp\left(m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4}+Y^2}\right)\right)\frac{\frac{3}{Y} + m\left(\frac{4\pi}{Y^2}+\frac{4\pi}{Y^3}\right) + m^2\frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}}W_{ir}(\sqrt{\lambda})}.$$

4.5.2 Small m

For small m, we shall do integration by parts a third time to (4.20), noting that $f_m''(0) = 0$ by similar reasoning to before, to get

$$\begin{aligned} h_\infty(n,m) &= \int_0^{1/2} f_m(t)\sin(2\pi nt)dt \\ &= \frac{f_m''(1/2)}{2(\pi n)^3}(-1)^n - \frac{1}{2(\pi n)^3}\int_0^{1/2} f_m'''(t)\cos(2\pi nt)dt. \end{aligned}$$

Now, using the Cauchy–Schwartz inequality, we can bound the integral by

$$\left(\int_0^{1/2} f_m'''(t)\cos(2\pi nt)dt\right)^2 \le \int_0^{1/2} f_m'''(t)^2 dt \int_0^{1/2} \cos^2(2\pi nt)dt = \frac{1}{4}\int_0^{1/2} f_m'''(t)^2 dt.$$

Hence, we can bound

$$|h_\infty(n,m)| \le \frac{b_m}{(\pi n)^3},$$

where

$$b_m := \frac{|f_m''(1/2)|}{2} + \frac{1}{4}\left(\int_0^{1/2} |f_m'''(t)|dt\right)^{1/2}.$$

Now, we can just apply the same bounds derived in Section 4.4.3, with $a_m = 0$ for all m and the b_m choosen above.

4.5.3 Explicit bound for $\|X\|$

Applying the exact same idea from Section 4.4.4, we get that

$$\|X\|^2 \le \frac{73}{432N_1^3}\frac{d_{M+1}^2}{d_{M+1} - d_{M+2}} + \frac{\pi^4 - 90}{1440}\frac{d_{N_1+1}^2}{d_{N_1+1} - d_{N_1+2}} + \frac{113\zeta(3)^2}{80\pi^6 N_1^5}\sum_{m=2}^{M} b_m^2,$$

where

$$\begin{aligned} b_m &:= \frac{|f_m''(1/2)|}{2} + \frac{1}{4}\left(\int_0^{1/2} |f_m'''(t)|dt\right)^{1/2}, \\ d_m &:= \frac{\pi}{2}\exp\left(2m\left(2\pi Y - \frac{2\pi Y}{\frac{1}{4} + Y^2}\right)\right)\left(\frac{\frac{3}{Y} + m\left(\frac{4\pi}{Y^2} + \frac{4\pi}{Y^3}\right) + m^2\frac{2\pi^2}{Y^4}}{e^{\sqrt{\lambda}}W_{ir}(\sqrt{\lambda})}\right)^2. \end{aligned}$$

We note, that this is only valid for the two values $Y = \frac{1}{2}$ or $Y = \frac{1}{2\sqrt{3}}$.

4.5.4 Computational results

We implemented the test from Theorem 4.3.1 for the first 4 Laplace eigenvalues of $\mathrm{PSL}(2, \mathbb{Z})$, each with a rigorous error bound of 10^{-96}. These results are summarised in the following table. The numbers in the N_1 column denote the smallest value of N_1 such that we are in case (i) of Theorem 4.3.1.

Laplace eigenvalue R	parity	M	N_1
9.53369526135 ...	odd	6	7
12.1730083246 ...	odd	7	13
13.7797513518 ...	even	8	24
14.3585095182 ...	odd	8	19

Appendix A

K-Bessel Bounds

An important function we use throughout is the K-Bessel function and we require several bounds of this function and its derivatives. To begin, we recall the definition of the K-Bessel function.

Definition A.0.1 (K-Bessel function)**.** Let x be a positive real number and $\nu \in \mathbb{C}$. Then we define the K-Bessel function by

$$K_\nu(x) := \frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh(t)+\nu t}\,dt = \int_0^{\infty} \cosh(\nu t)e^{-x\cosh(t)}\,dt.$$

We have that $y = K_\nu(x)$ satisfies the differential equation

$$y'' + \frac{y'}{x} - \left(1 + \frac{\nu^2}{x^2}\right)y = 0. \tag{A.1}$$

We shall now assume that ν is purely imaginary, i.e. $\nu = ir$ for some real r. We shall also mainly be considering the Whittaker function of the form $W_{ir}(x) = \sqrt{x}K_{ir}(x)$. We now have the following proposition giving bounds for this function and its derivatives with respect to x.

Proposition A.0.1. *We have*

$$|W_{ir}(x)| \leq \sqrt{\frac{\pi}{2}}e^{-x} \text{ for all } x > 0 \text{ and } r > 0,$$
$$|W'_{ir}(x)| \leq \sqrt{\frac{\pi}{2}}e^{-x} \text{ for all } x \geq 1 \text{ and } r \geq 5,$$
$$|W''_{ir}(x)| \leq \sqrt{\frac{\pi}{2}}e^{-x} \text{ for all } x \geq 1 \text{ and } r \geq 5.$$

Proof. Using the fact that $\cosh(t) \geq 1 + \frac{t^2}{2}$ for all $t > 0$, we have

$$|K_{ir}(x)| = \left|\frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh(t)+irt}\,dt\right| \leq \frac{1}{2}\int_{-\infty}^{\infty} \left|e^{-x\cosh(t)+irt}\right|\,dt = \frac{1}{2}\int_{-\infty}^{\infty} e^{-x\cosh(t)}\,dt$$
$$\leq \frac{1}{2}e^{-x}\int_{-\infty}^{\infty} e^{-\frac{xt^2}{2}}\,dt = \sqrt{\frac{\pi}{2x}}e^{-x}.$$

Hence

$$|W_{ir}(x)| \leq \sqrt{\frac{\pi}{2}} e^{-x}.$$

Define $\lambda = \frac{1}{4} + r^2$. Then by (A.1) we have the following differential equation

$$W_{ir}''(x) = \left(1 - \frac{\lambda}{x^2}\right) W_{ir}(x).$$

For $x > \sqrt{\lambda/2}$ the bound is clear for the second derivative by using the bound for $|W_{ir}(x)|$. For $1 \leq x \leq \sqrt{\lambda/2}$ we use the following result from Proposition 2 in [BST13], which states that for all $1 \leq x < r$ we have

$$|K_{ir}(x)| < e^{-(\pi/2)r} \begin{cases} \dfrac{5}{\sqrt[4]{r^2 - x^2}} & \text{if } x \leq r - \dfrac{1}{2} r^{\frac{1}{3}}, \\ 4r^{-\frac{1}{3}} & \text{if } x \geq r - \dfrac{1}{2} r^{\frac{1}{3}}. \end{cases}$$

Hence

$$|W_{ir}''(x)| = \left|1 - \frac{\lambda}{x^2}\right| |W_{ir}(x)| \leq \left|\frac{\lambda}{x^2} - 1\right| \sqrt{x} \frac{5}{(r^2 - x^2)^{1/4}} e^{-(\pi/2)r}.$$

Now we want a bound of the form $|W_{ir}''(x)| \leq C \exp(-x)$ for some $C \in \mathbb{R}$. Hence, we want to bound

$$\left|\frac{\lambda}{x^2} - 1\right| \sqrt{x} \frac{5}{(r^2 - x^2)^{1/4}} e^{-(\pi/2)r} e^x = \frac{r^2 + \frac{1}{4} - x^2}{x^{3/2}} \frac{5}{(r^2 - x^2)^{1/4}} e^{-(\pi/2)r} e^x.$$

The first fraction obtains its maximum at $x = 1$ and the second fraction obtains its maximum at $x = \sqrt{\lambda/2}$. Also, note that $e^x \leq e^{\sqrt{\lambda/2}}$. Thus

$$\frac{r^2 + \frac{1}{4} - x^2}{x^{3/2}} \frac{5}{(r^2 - x^2)^{1/4}} e^{-(\pi/2)r} e^x \leq \frac{5(r^2 - 3/4)}{(r^2/2 - 1/8)^{1/4}} e^{-(\pi r/2 - \sqrt{r^2/2 + 1/8})} =: A(r).$$

This obtains its maximum of approximately 2.59009 at $r \approx 2.12008$. Notably, $A(r) \leq \sqrt{\pi/2}$ for $r \gtrsim 4.3268$. Hence,

$$|W_{ir}''(x)| \leq \sqrt{\frac{\pi}{2}} e^{-x}$$

for $x \geq 1$ and $r \geq 5$. To get a bound for the first derivative, we have that

$$W'_{ir}(x) = -\int_x^\infty W''_{ir}(y)dy.$$

Thus,

$$|W'_{ir}(x)| \leq \int_x^\infty |W''_{ir}(y)|dy \leq \sqrt{\frac{\pi}{2}} \int_x^\infty e^{-y}dy = \sqrt{\frac{\pi}{2}} e^{-x},$$

for all $x \geq 1$ and $r \geq 5$. □

We shall also need a lower bound for the Whittaker function in the exponential region.

Proposition A.0.2. *For $x \geq x_0 \geq \sqrt{\lambda}$, we have*

$$W_{ir}(x) \geq W_{ir}(x_0)e^{x_0 - x} > 0.$$

Proof. By the differential equation, we have $W''_{ir}(x) = (1 - \lambda x^{-2})W_{ir}(x)$. Using this, we get that

$$W'_{ir}(y) = -\int_y^\infty (1 - \lambda x^{-2})W_{ir}(x)\, dx$$

and

$$\begin{aligned} W_{ir}(z) &= -\int_z^\infty W'_{ir}(y)\, dy = \int_z^\infty \int_y^\infty (1 - \lambda x^{-2})W_{ir}(x)\, dx\, dy \\ &= \int_z^\infty (x - z)(1 - \lambda x^{-2})W_{ir}(x)\, dx. \end{aligned} \tag{A.2}$$

Before we can continue, we shall state the following asymptotic expansion of $W_{ir}(x)$ from [GR07, 8.451 6]

$$W_{ir}(x) = \sqrt{\frac{\pi}{2}} e^{-x} \left[\sum_{k=0}^{n-1} \frac{\Gamma\left(ir + k + \frac{1}{2}\right)}{(2x)^k \Gamma\left(ir - k + \frac{1}{2}\right) k!} + O(x^{-n}) \right]. \tag{A.3}$$

First, we show that $W_{ir}(x) > 0$ for $x \geq \sqrt{\lambda}$. Suppose that is not the case. Then, by (A.3), we see that $W_{ir}(x) > 0$ for sufficiently large x. Thus, there must exist some $z \geq \sqrt{\lambda}$ such that $W_{ir}(z) = 0$ and $W_{ir}(x) > 0$ for all $x > z$. However,

$$0 = W_{ir}(z) = \int_z^\infty (x - z)(1 - \lambda x^{-2}) W_{ir}(x)\, dx > 0,$$

for all $x > z$, which is a contradiction. Hence, $W_{ir}(x) > 0$ for $x \geq \sqrt{\lambda}$.

Next, let $g(x) = e^x W_{ir}(x)$ and $h(x) = (1 - \lambda x^{-2}) g(x)$. We aim to show that $g'(x) > 0$ for all $x \geq \sqrt{\lambda}$. Again, suppose this is not the case. Using (A.3), multiplying by e^x and then differentiating with respect to x, we get that

$$g'(x) = -\sqrt{\frac{\pi}{2}} \left[\sum_{k=1}^{n-2} \frac{\Gamma\left(ir + k + \frac{1}{2}\right)}{2^k x^{k+1} \Gamma\left(ir - k + \frac{1}{2}\right)(k-1)!} + O(x^{-n}) \right].$$

We note that $\Gamma(ir + 3/2)/\Gamma(ir - 1/2) = -r^2 - 1/4$, hence the first term of this expansion is actually positive. From this asymptotic we can see that $g'(x) > 0$ for sufficiently large x. Thus, there exists some $z \geq \sqrt{\lambda}$ such that $g'(z) = 0$ and $g'(x) > 0$ for $x > z$, and it follows that $h'(x) > 0$ for $x > z$. Rewriting (A.2) in terms of g and h, we get that

$$g(z) = \int_z^\infty (x - z) e^{z-x} h(x)\, dx = \int_0^\infty t e^{-t} h(z + t)\, dt.$$

However,

$$0 = g'(z) = \int_0^\infty t e^{-t} h'(z + t)\, dt > 0,$$

which is again a contradiction. Hence $g'(x) > 0$ for all $x \geq \sqrt{\lambda}$, that is $g(x) = e^x W_{ir}(x)$ is always increasing for $x \geq \sqrt{\lambda}$. This means there exists some $x \geq x_0 \geq \sqrt{\lambda}$ such that

$$g(x) \geq g(x_0) = W_{ir}(x_0) e^{x_0},$$

which gives the result. $\square$

We can extend the definition of $K_{ir}(z)$ to $z \in \mathbb{C}$ with $\mathrm{Re}(z) > 0$, and the corresponding Whittaker function by $W_{ir}(z) = \sqrt{|z|} K_{ir}(z)$. In a similar way to the real case, we can also get an upper bound for the absolute value of this.

Proposition A.0.3. *For all $z \in \mathbb{C}$ with $\operatorname{Re}(z) > 0$ and $r > 0$ we have*

$$|W_{ir}(z)| \leq \sqrt{\frac{\pi|z|}{2\operatorname{Re}(z)}} e^{-\operatorname{Re}(z)}.$$

Proof. Similar to the real case, using the fact that $\cosh(t) \geq 1 + \frac{t^2}{2}$ for all $t > 0$ and the definition of K_{ir}, we have

$$\begin{aligned} |K_{ir}(z)| &= \left| \frac{1}{2} \int_{-\infty}^{\infty} e^{-z\cosh(t)+irt}\, dt \right| \leq \frac{1}{2} \int_{-\infty}^{\infty} \left| e^{-z\cosh(t)+irt} \right| \, dt = \frac{1}{2} \int_{-\infty}^{\infty} e^{-\operatorname{Re}(z)\cosh(t)}\, dt \\ &\leq \frac{1}{2} e^{-\operatorname{Re}(z)} \int_{-\infty}^{\infty} e^{-\frac{\operatorname{Re}(z)t^2}{2}}\, dt = \sqrt{\frac{\pi}{2\operatorname{Re}(z)}} e^{-\operatorname{Re}(z)}. \end{aligned}$$

Hence,

$$W_{ir}(z) = \sqrt{|z|} K_{ir}(z) \leq \sqrt{\frac{\pi|z|}{2\operatorname{Re}(z)}} e^{-\operatorname{Re}(z)}.$$

$\square$

Appendix B

Rigorous numerical quadrature

Throughout our work, we require the need to numerically compute integrals with rigorous error bounds. For this we use the following theorem from [Mol16].

Theorem B.0.1 (Molin)**.** *Let f be a holomorphic function on the disk $D(0,2) = \{z \in \mathbb{C} : |z| \leq 2\}$. Then we have*

$$\left| \int_0^1 f(x)\, dx - \sum_{n=-k}^{k} x_k f(a_k) \right| \leq \exp\left(4 - \frac{5n}{\log(5n)}\right) \sup_{z \in D(0,2)} |f(z)|,$$

where $h = \frac{\log(5n)}{n}$, $a_k = \frac{h\cosh(kh)}{\cosh(\sinh(kh))^2}$ and $x_k = \tanh(\sinh(kh))$.

The benefit of this method compared to others, is that it can be easily implemented in interval arithmetic due to the explicit form of the error. We note that in this setup, the supremum of $|f(z)|$ with $z \in D(0,2)$ actually occurs on the boundary of the disk when $|z| = 2$ by the maximum modulus principle. To implement the rigorous error, we either bound it analytically and use that as our error bound or we can numerically compute it in interval arithmetic.

To implement this error numerically, we first divide the interval $[0,1]$ into n intervals labelled θ_n, and then, using interval arithmetic, compute each

$$|f(2\exp(2\pi i\theta_n))|$$

and then take the maximum of these intervals. We choose n such that

$$4 - \frac{5n}{\log(5n)} < B\log 2,$$

where B is the number of bits of precision desired.

To implement this theorem with general integral limits, we first rescale the integral in the following way

$$\int_a^b f(x)\, dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}y + \frac{a+b}{2}\right) dy,$$

where $b > a$. If after rescaling the disk within the error bound has a singularity within it, we can compute the integral piecewise to help minimise the error.

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