EFFECTIVE COMPUTATION OF MAASS CUSP FORMS

ANDREW BOOKER, ANDREAS STRÖMBERGSSON AND AKSHAY VENKATESH

1. Preliminary

The aim of this paper is to address theoretical and practical aspects of high-precision computation of Maass forms. Namely, we compute to over 1000 decimal places the Laplacian and Hecke eigenvalues for the first few Maass forms on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$, and certify the Laplacian eigenvalues correct to 100 places. We then use these computations to test certain algebraicity properties of the coefficients.

The outline of the paper is as follows. In Section 2, we discuss Hejhal's algorithm for computation of Maass forms and the details necessary to implement it in high precision. As this algorithm is heuristic and does not prove the existence of cusp forms, in Section 3 we turn to the question of *rigorously verifying* the numerical computation. In fact, it will be quite easy to show (by the "quasi-mode construction") that the putative eigenfunctions produced in Section 2 are close, in an appropriate topology, to genuine eigenfunctions. It is a more subtle point to show that they are close to cusp forms. Indeed, Selberg introduced the trace formula for the precise purpose of showing there existed cusp forms for $\mathrm{PSL}(2,\mathbb{Z})$; we shall use a trick from [17] to greatly simplify the analysis. The high precision to which we compute the forms turns out to be essential to our approach; there is an implicit loss of precision in proving an eigenfunction correct, so it seems important to have a heuristic method of computing the eigenfunction to higher precision than the desired certifiable precision.

In Section 4 we test some algebraicity properties of coefficients of Maass forms. It is generally believed that the Laplacian and Hecke eigenvalues of Maass forms are transcendental; we provide (to our knowledge, the first published) evidence in this direction. For instance, we show that the first eigenvalue of $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ is not the solution of any algebraic equation with degree ≤ 10, all of whose coefficients are $\leq 10^7$ in magnitude. This uses the results of Section 3 to provably verify this eigenvalue to 100 decimal places; if we assume (and there is a great deal of evidence in this direction) that the computations of Section 2 are correct to 1000 decimal places, we obtain much stronger results yet.

Moreover, we also test for algebraic relations *between coefficients* that generalize those that exist for eigenvalue $\frac{1}{4}$ forms or for dihedral forms. Stark has informed us that he tested for relations of a similar nature in the early 1980s, but the data he had available was less accurate.

Related problems and other applications. Farmer and Lemurell have recently found [7] that Maass forms persist when deforming lattices along certain (special) curves in Teichmüller space. The theoretical aspects of this are not fully understood; in particular, rigorously proving this persistence seems like an interesting question. The high precision algorithm which we outline in Section 2 might be a valuable tool when studying this question, at least from an experimental perspective: For example, we have used it to refine some points on the curves of [7] to more than 200 decimal places.

In this vein, it seems natural to propose the following (challenging) problem in rigorous computation of spectra: Find practical algorithms which for given numbers $\Lambda > 0$ and $\varepsilon_0 > 0$ and a given region U in Teichmüller space, determine—with proofs, and to within an error bounded by ε_0—the complete set of submanifolds in $U \times [0, \Lambda]$ described by the $\{\lambda < \Lambda\}$-part of the discrete spectra on the hyperbolic surfaces corresponding to the points in U.

Acknowledgements. We would like to thank Dennis Hejhal, Peter Sarnak, Kannan Soundararajan, and Fredrik Strömberg for helpful discussions. The first author was supported by an NSF postdoctoral fellowship. The third author was supported by a CMI Research Fellowship and NSF Grant DMS-0245606.

2. Computation

The problem of computing Maass waveforms on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ numerically has been considered by a number of authors, starting in the 1970s; cf. [25] and the references listed therein. In the present section we will briefly recall the method due to Hejhal [12] for computation of Maass waveforms, and then describe how we adapt this algorithm in order to carry out the computations in very high accuracy. Hejhal's algorithm represents a major step forward compared to earlier existing methods, regarding both numerical stability and range of applicability. For example, this algorithm was used by H. Then in [25] to compute eigenvalues of size $\lambda > 1.6 \cdot 10^9$ on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$, which is the current record.

As stressed in the introduction, the method is (at present) *non-rigorous.* It seems quite reasonable to expect that when implemented with sufficiently sharp parameters M_0, Q, Y (see below), the algorithm should succeed in finding correct data for all existing cusp forms, and that it should never indicate existence of "false" cusp forms—this is also corroborated by all experiments carried out so far (see [12, 20, 25, 22], as well as sections 2.3, 3.4 below). However, we do not attempt to prove either of these assertions here.

The algorithm of Hejhal applies to the computation of Maass waveforms on any cofinite Fuchsian group Γ such that $\Gamma\backslash\mathbb{H}$ has exactly one cusp. It has recently been extended to the case when $\Gamma\backslash\mathbb{H}$ has several cusps, see [20, 22].

2.1. Hejhal's algorithm.

We start by recalling the algorithm from [12] (cf. also [13] for more details). Let $\Gamma \subset \mathrm{PSL}(2,\mathbb{R})$ be a cofinite Fuchsian group. For simplicity we will assume that $\Gamma\backslash\mathbb{H}$ has exactly one cusp (the modifications necessary in the case with several cusps are mentioned very briefly at the end). Without loss of generality we may take this cusp to be positioned at ∞, and to have width 1, i.e. we assume that Γ_∞, the stabilizer of ∞ in Γ, is generated by $\left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$. We fix a (closed) fundamental domain $\mathcal{F} \subset \mathbb{H}$ of Γ; since $\Gamma\backslash\mathbb{H}$ has only one cusp we may assume that $Y_0 = \inf \{\text{Im } z : z \in \mathcal{F}\}$ is a *positive* number.

We also fix an integer D (say $D \geq 10$), indicating that we are optimally aiming for a precision of about D decimal digits in our results.

Let us consider any fixed Maass cusp form $f(z)$ of eigenvalue $\lambda = \frac{1}{4} + r^2$ ($r \in \mathbb{R}$) on $\Gamma\backslash\mathbb{H}$. Take its Fourier expansion at ∞ to be (see [10] or [14])

$$f(z) = \sum_{n \neq 0} a_n \sqrt{y}\, \kappa_{ir}(2\pi |n| y)\, e(nx), \qquad (z = x + iy). \tag{1}$$

Here we understand $\kappa_{ir}(u)$ to mean $e^{\frac{\pi}{2} r} K_{ir}(u)$, in line with the numerical convention from [11, 12]. This ensures that $\kappa_{ir}(u)$ is an oscillating function of u when $0 < u \lesssim r$ with amplitude roughly of order of magnitude ~ 1, and then decays exponentially for $u \gtrsim r$, see [1].

It is known in general that the coefficients a_n are bounded by $a_n = O(|n|^{\frac{1}{3}+\varepsilon})$, for all n, see [2]. We will assume from the start that the cusp form $f(z)$ has been singled out in the λ-eigenspace by a legitimate normalization $a_{n_1} = 1$, $a_{n_2} = a_{n_3} = \ldots = a_{n_d} = 0$ where d is the dimension of the λ-eigenspace and $n_1, \ldots, n_d$ are some small distinct indices. We will also assume that this normalization makes $a_n = O(|n|^{\frac{1}{3}+\varepsilon})$ hold with a *modest implied constant.*[1]

Under this assumption, one can choose a sensible (decreasing) function $M(y)$ so that, for each $z = x + iy \in \mathbb{H}$, one has

$$f(z) = \sum_{0 < |n| \leq M(y)} a_n \sqrt{y}\, \kappa_{ir}(2\pi |n| y)\, e(nx) + [[10^{-D}]], \tag{2}$$

where $[[10^{-D}]]$ is shorthand for a quantity of absolute value less than 10^{-D}. Let us declare $M(y) = M(Y_0) := M_0$ for all $y \geq Y_0$.

Thus, by (2), for every $y > 0$ we are now viewing $f(x + iy)$ as a finite Fourier series in x. We fix any number Y such that $0 < Y < Y_0$ and then take an integer Q with $Q > M(Y)$. We introduce the following $2Q$ points, evenly spaced along a closed horocycle:

$$z_j = x_j + iY = \frac{1}{2Q}\left(j - \frac{1}{2}\right) + iY \in \mathbb{H}, \qquad 1 - Q \leq j \leq Q. \tag{3}$$

[1]In all experiments known to us it has been possible to find a good a_n-normalization of this type without too much effort, although some trial and error might be necessary, especially when d is not known. The most common case is $d = 1$ and here the normalization $a_1 = 1$ very often turns out to fulfill our assumptions; for instance this is certainly true in the case of newforms with $d = 1$ when Γ is a congruence subgroup of $\mathrm{PSL}(2, \mathbb{Z})$, see [15]. We refer to [22] for a more detailed discussion involving cases with $d \geq 2$ and $a_1 = 0$.

By taking appropriate linear combinations of relation (2) over all these points, we obtain, for each $|n| \le M(Y)$:

$$a_n \sqrt{Y} \kappa_{ir}(2\pi|n|Y) = \frac{1}{2Q} \sum_{j=1-Q}^{Q} f(z_j)\, e\big(-nx_j\big) + [[10^{-D}]]. \tag{4}$$

We will now utilize the fact that f is Γ-automorphic. For each j we compute the $\mathcal{F}$-pullback of z_j, that is, we find a map $T_j \in \Gamma$ such that $z_j^* = x_j^* + iy_j^* := T_j(z_j) \in \mathcal{F}$. (There is in general a very quick way to find this map T_j; the natural algorithm to use depends on whether Γ is a "generic" cofinite subgroup of $\mathrm{PSL}(2,\mathbb{R})$, or a congruence or non-congruence subgroup of $\mathrm{PSL}(2,\mathbb{Z})$, see, e.g. [20, 22, 23].) Using the automorphy relations $f(z_j) = f(z_j^*)$ in (4) we now have

$$a_n \sqrt{Y} \kappa_{ir}(2\pi|n|Y) = \sum_{0<|\ell|\le M_0} a_\ell V_{n\ell} + 2[[10^{-D}]], \tag{5}$$

with

$$V_{n\ell} = \frac{1}{2Q} \sum_{j=1-Q}^{Q} \sqrt{y_j^*} \kappa_{ir}(2\pi|\ell|y_j^*)\, e(\ell x_j^* - nx_j). \tag{6}$$

Relation (5) holds for all $|n| \le M(Y)$, for any given Maass cusp form $f(z)$ of eigenvalue $\lambda = \frac{1}{4} + r^2$. Since $\mathrm{Im}\ z_j = Y < Y_0 \le \mathrm{Im}\ z_j^*$ we have $T_j \notin \Gamma_\infty$ for all j, and hence the system (5) should be far from a tautology.

Restricting (5) to $1 \le |n| \le M_0$, we obtain a system of $2M_0$ linear (homogeneous) equations for the $2M_0$ unknowns $\{a_n\}_{1\le|n|\le M_0}$. Of course, the eigenvalue $\lambda = \frac{1}{4} + r^2$ will not be known from the start. To get a hold of r the above linear system is repeatedly solved for two different Y-values, successively adjusting r to make the two solution vectors $\{a_n'\}_{1\le|n|\le M_0}$ and $\{a_n''\}_{1\le|n|\le M_0}$ as nearly equal as possible. (In cases of congruence groups Γ one can instead adjust r so as to satisfy Hecke multiplicative relations among the first few a_n.)

As pointed out in [12], it is not evident *a priori* that the linear system (5) will be well-conditioned as hoped, and this would indeed be one of the key issues in any attempt to *prove* that the above algorithm always achieves its goal.

Our experiments consistently indicate that when solving (5) for a correct r-value, each coefficient a_n with $2\pi|n|Y \gg r$ (and $|n| \le M_0$) is obtained to an accuracy of, roughly,

$$[a_n\text{-precision}] \approx \left(D - \log_{10}^{+} \left| \frac{1}{\sqrt{Y}\kappa_{ir}(2\pi|n|Y)} \right| \right) \quad \text{digits.} \tag{7}$$

This is easy to explain heuristically: Note that since $\sqrt{u}\kappa_{ir}(u)$ is positive and exponentially decaying for $u \gg r$, and $y_j^* \ge Y_0 > Y$ for all j, all coefficients in the column corresponding to a_n in our system (5) will have absolute size $\lesssim \sqrt{Y}\kappa_{ir}(2\pi|n|Y)$.

It follows from (7) that the $\{a_n\}_{1\le|n|\le M_0}$ are sufficiently accurate for formula (2) to give $f(x+iy)$ to $\sim D$ digits precision whenever $y \ge Y_0$. Hence the coefficients a_n may be obtained to precision $\sim D$, also for $|n| > M_0$, by running a *second* computation, namely

$$a_n^{(new)} = \frac{\sum_{0<|\ell|\leq M_0} a_\ell V_{n\ell}}{\sqrt{Y'}\kappa_{ir}(2\pi|n|Y')} \tag{8}$$

for some $Y' < Y$ such that $\sqrt{Y'}\kappa_{ir}(2\pi|n|Y')$ is not extremely small, using $Q' > M(Y')$ in place of Q in (6) to compute each $V_{n\ell}$. In fact, even if $\sqrt{Y'}\kappa_{ir}(2\pi|n|Y')$ is very small we may still expect (8) to give a_n to an accuracy as in (7), with Y' in place of Y.

Note that in the particular case of $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$ (or more generally if $J\Gamma J = \Gamma$ where $J : \mathbb{H} \ni z \mapsto -\overline{z} \in \mathbb{H}$) we may assume each eigenfunction f to be either *even* (viz., $a_{-n} = a_n$, $\forall n$) or *odd* (viz., $a_{-n} = -a_n$, $\forall n$). This of course allows us to reduce the number of unknowns in our system (5) by a factor 2.

In the case when $\Gamma\backslash\mathbb{H}$ has several cusps, the only approach which has so far been found to work well in general is to solve simultaneously for the Fourier coefficients at *all* cusps. Then for *each* cusp η one introduces a set of evenly spaced points $z_j^{(\eta)}$ around a closed horocycle encircling η, and forms linear combinations analogous to (4). We refer to [20, 22] for more details. It should be noted that in many cases, in particular when Γ is a congruence group, the linear system can be reduced to involve fewer cusps, because of the existence of Hecke-type symmetries (Fricke involutions) which connect the Fourier expansions at various cusps. See [22, §2.8] as well as [7].

2.2. **Adaptations to computations in high accuracy.** We carried out our computations using the PARI/GP programming language [24], making use of its capacity to do numerics in any given precision D (decimal digits). As we let D increase, we also need to increase the size of the system of equations (5), because of $M_0 = M(Y_0)$ and the definition of $M(Y)$ in (2). For example, for $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$ one has $Y_0 = \sqrt{3}/2$, and tests on the size of $K_{ir}(u)$ suggest that for modest r ($r \leq 25$, say), the smallest admissible choices of $M_0 = M(Y_0)$ in (2) are roughly as follows:

D	50	100	200	525	1050
M_0	30	55	95	235	455

(In the case $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$ it would be possible to *prove* that (2) holds for these choices of M_0 and $y \geq Y_0$, using e.g. the bounds in [15] and careful estimates of the K-Bessel function. See footnote 1.) Hence for $D = 1050$ our system will be of size $\sim 455 \times 455$. This makes both time and memory very serious issues (note that 112 bytes are required to store a single real number in precision $D = 1050$).

On $\Gamma_0(5)$ (which has two cusps) one has $Y_0 = \sqrt{3}/10$ (see [22]), and for $D = 525$, $r \leq 10$, we need to take M_0 as large as ~ 1135 ($D = 1050$ would require $M_0 \sim 2240$; we have not carried this out). We remark that due to symmetries the system of equations used for $\Gamma_0(5)$ need not be of dimension larger than $M_0 \times M_0$.

In the second computation, (8), the main problem is time, as the number of terms involved is often quite large (recall that in (8) we are to use (6) with $Q' > M(Y')$ in place of Q). It is useful to note that we may sacrifice accuracy in a controlled way, allowing for a much larger choice of Y'. For example, for $r \approx 13.77$ on $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$, we may allow $2\pi|n|Y'$ to be as large as 315 and still only lose ~ 130 digits according to (7); hence for $|n| \leq 455$ we may use $Y' = 0.11$ and $Q' = 3540 > M(Y')$, and this should give all $\{a_n\}_{1\leq|n|\leq 455}$ to more than 900 digits precision. However, if we would only allow a loss of ~ 5 digits in (8), then for $|n| = 455$ we would need to take $Y' \sim 0.0097$ and $Q' > M(Y') \gtrsim 40000$, and the computation would be more than ten times as long.

When implementing the algorithm outlined in Section 2.1 on a computer, the most time-consuming task is, by far, that of computing the values of the K-Bessel function $K_{ir}(u)$ (see [11] and [25]). Our approach to computing $K_{ir}(u)$ (for $u, r > 0$) to very high accuracy is quite elementary, and builds on recursive use of Taylor power series.

From (5) and (6) we see that our task will always involve computing $K_{ir}(u)$ for a *fixed* r and a large set of different u-values, namely, $u = 2\pi\ell y_j^*$ with $1 - Q \leq j \leq Q$ and $\ell = 1, 2, \ldots, M_0$, as well as for $u = 2\pi nY$, $n = 1, 2, \ldots, M_0$. We start by pre-tabulating all these values in a decreasing list, $u_1 \geq u_2 \geq \ldots \geq u_N$. In practice, with M_0 adapted to high precision $D \geq 500$, the number N is well beyond 10^5, and the vast majority of gaps $u_m - u_{m+1}$ are found to be much smaller than $\frac{1}{10}$. We then use the fact that once $K_{ir}(u_m)$ together with $K'_{ir}(u_m)$ have been calculated for some m, all the higher derivatives $K_{ir}^{(n)}(u_m)$, $n \geq 2$, can be computed fairly quickly using the differential equation

$$u^2 K''_{ir}(u) + uK'_{ir}(u) + (r^2 - u^2)K_{ir}(u) = 0. \tag{9}$$

Thus we obtain the coefficients of the Taylor expansion of $K_{ir}(u)$ about $u = u_m$, and this can be used to quickly compute $K_{ir}(u_{m'})$ for all points $u_{m'}$ in our list lying sufficiently close to u_m.

Specifically, using (9) we find that

$$u^n K_{ir}^{(n)}(u) = P_n(u)K_{ir}(u) + Q_n(u)uK'_{ir}(u) \tag{10}$$

where $P_n(u)$ and $Q_n(u)$ are polynomials which satisfy $P_0(u) = 1$, $Q_0(u) = 0$ and the recursion relations

$$\begin{cases} P_{n+1}(u) = uP'_n(u) - nP_n(u) + (u^2 - r^2)Q_n(u) \\ Q_{n+1}(u) = uQ'_n(u) - nQ_n(u) + P_n(u). \end{cases} \tag{11}$$

In particular, we see that $P_n(u)$ and $Q_n(u)$ are polynomials of degree $\leq n$ (more precisely, $\deg P_n = 2[n/2]$ and $\deg Q_n = 2[(n-1)/2]$ for $n \geq 2$), the coefficients of which only depend on n and r. Hence the coefficients of these polynomials can be computed explicitly once and for all as soon as r is given. The Taylor expansion of $K_{ir}(u)$ at $u = u_m$ is then given by

$$K_{ir}(u) = \sum_{n=0}^{\infty} \frac{P_n(u_m)K_{ir}(u_m) + Q_n(u_m)u_m K'_{ir}(u_m)}{n!}(u - u_m)^n. \tag{12}$$

Note that the coefficients of this series may be computed and stored once u_m is given (along with $K_{ir}(u_m)$, $K'_{ir}(u_m)$). Our approach now is to truncate (12) at some finite n, and use this sum to compute $K_{ir}(u_{m'})$ for all $m' > m$ such that $u_{m'}$ lies sufficiently close to u_m, say $u_m - L \leq u_{m'} \leq u_m$ for some $L > 0$. When we reach the last m', i.e. $u_{m'+1} < u_m - L \leq u_{m'}$, we use the differentiated version of (12) to compute $K'_{ir}(u_{m'})$, and use $K_{ir}(u_{m'})$ and $K'_{ir}(u_{m'})$ to evaluate the Taylor polynomial for $K_{ir}(u)$ about $u = u_{m'}$, that is, we return to the start of the above procedure but with m' in place of m.

Since $K_{ir}(u)$ is exponentially decreasing in u for $u \gg r$, it is essential to work with *decreasing* u-values, $u_1 \geq u_2 \geq \ldots \geq u_N$ as above, in order to make the recursive procedure numerically stable.

In order to compute $K_{ir}(u)$, $K'_{ir}(u)$ at some initial point $u = u_m$ as well as for small u, we use the power series about the point $u = 0$, viz.

$$K_{ir}(u) = \frac{-\pi \operatorname{Im} I_{ir}(u)}{\sinh(\pi r)} = -\frac{\pi}{\sinh(\pi r)} \cdot \operatorname{Im}\left(\sum_{n=0}^{\infty} \frac{(u/2)^{ir+2n}}{n!\,\Gamma(n+ir+1)}\right). \tag{13}$$

When using this formula one encounters a catastrophic cancellation of significant digits unless u is quite small. To remedy for this fact we compute the sum using an internal precision much larger than D. For example, for $r \approx 13.77$ (the first even eigenvalue on $\mathrm{PSL}(2,\mathbb{Z})$) and $u = 3400$, the maximum absolute value of an individual term in $\sum_{n=0}^{\infty} \frac{(u/2)^{ir+2n}}{n!\,\Gamma(n+ir+1)}$ is slightly larger than $3.9 \cdot 10^{1472}$ (attained for $n = 1699$), whereas the total sum has imaginary part $\approx -5.3 \cdot 10^{-1461}$; to achieve the final precision $D = 1050$ for $3 \leq r \leq 25$ and u in the range $1000 \leq u \leq 3400$, we added the terms using an internal precision of 5000 digits, and cutting the sum off at $n = 8500$. Of course this computation is rather time-consuming; for large u it takes several *minutes* to compute one single $K_{ir}(u)$-value using (13) (on a 1.5 GHz PC).

We refer to [4] for information on our precise choices of parameters such as the maximum interval length L and n-cutoff to use in (12), and the cutoff and internal precision in (13). These choices were made using trial and error, and tested by computing long series of K-Bessel values and checking against the result obtained using (13) with extra precision and longer cutoff. Note that it would in principle not be difficult to work out more rigorous error estimates for our K-Bessel values, but this would be a bit beside the point since the computation of Maass forms using (5) is heuristic anyway.

We also compared our method for $K_{ir}(u)$ with the PARI (version 2.1.5) built-in function `besselk` (which treats $K_{ir}(u)$ as a special case of the confluent hypergeometric function, computed using a recursion relation combined with an asymptotic expansion for large z). In precision $D = 50$ our approach was found to be more than 5 times as fast as the built-in function (when considering the total time for a whole series $u_1 \geq \ldots \geq u_N$ from (5)). For $D = 200$ the corresponding speed gain was a factor > 20, and for larger values of D we ran into cases where the built-in function seems to enter an infinite loop.

2.3. **Results.** Using the algorithm described above we have obtained the following main results. Our data files with eigenvalues and Fourier coefficients are available on [4], where each value is printed only to the number of decimals which we are certain (empirically) are correct.

(A) We have computed the first ten eigenvalues on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ (viz., $r \approx 9.5337$, 12.1730, 13.7798, 14.3585, 16.1381, 16.6443, 17.7386, 18.1809, 19.4235, 19.4847) to a precision of more than 1000 decimal digits, together with the first 455 Fourier coefficients $a_1, \ldots, a_{455}$ to 900 digits (at least the first 50 of these were actually obtained to more than 1000 digits).

(B) We have computed a few examples of (newform) eigenvalues on congruence subgroups of low level, namely

- the first eigenvalue on $\Gamma_0(5)\backslash\mathbb{H}$: $r \approx 5.4362$;
- the first two eigenvalues for $\Gamma_0(5)$ with nontrivial nebentypus character $\chi = (5/\cdot)$: $r \approx 3.2643$ (a CM-form) and $r \approx 4.8938$ (a double eigenvalue);
- the first eigenvalue on $\Gamma_0(6)\backslash\mathbb{H}$: $r \approx 2.5924$.

In each case the eigenvalue and the first 50 Fourier coefficients were obtained to a precision of more than 480 digits, and all the first 1050 Fourier coefficients were obtained to a precision decaying with the index roughly as suggested by (7) (with $Y = 0.171$ for $\Gamma_0(5)$, $Y = 0.143$ for $\Gamma_0(6)$, and $D = 525$). As initial data for the eigenvalues we used data from the work of Fredrik Strömberg, [22].

(C) We have studied a few examples from Farmer and Lemurell [7] of (what appear to be) Maass cusp form eigenvalues on deformations of an arithmetic surface, and refined the precision from about 8 decimal digits as given in [7] to more than 200 digits (for both the eigenvalue r and the deformation parameters). More specifically, our examples lie along the curves in the 2-dimensional Teichmüller space $T(\Gamma_0(5))$ which were found in [7] when deforming the Maass forms with eigenvalues $r \approx 4.1324$, 5.4362 and 6.8235 on $\Gamma_0(5)\backslash\mathbb{H}$.

The computer time required was between one and three weeks per example in (A) and (B) (on a 1.5 GHz PC).

In each of these cases, we have performed a number of tests to make certain (empirically) that the data obtained is correct to the expected accuracy. Specifically, in all cases the system of equations (5) was solved *twice*, using different Y-values, and the eigenvalues and the coefficients were consistently seen to agree to the expected accuracy (i.e. in accordance with (7)). In cases (A) and (C) we also used (8) to obtain the higher coefficients to better precision, each time using two different Y'-values, and in cases (A) and (B) all Hecke multiplicativity relations involving the calculated coefficients were tested; all these tests consistently indicated agreement to the expected accuracy. (See [4] for more details.)

Furthermore the eigenvalues and the Fourier coefficients of the CM-form in (B) are in fact known explicitly (see Section 4.1; in particular $r = \pi/\log((3+\sqrt{5})/2) \approx 3.2643$) and hence this provides an excellent test of the computational algorithm; we verified that the calculated eigenvalue and all the Fourier coefficients agreed with the known explicit values to the expected accuracy.

Regarding the examples in (C) we note that it is an open problem to *prove* that Maass forms can truly be deformed along submanifolds in Teichmüller space, as suggested in [7]. The computations carried out in [7] provide strong evidence for this, however, and the fact found here that these examples could be refined (in each case tried) to more than 200 digits' precision, fulfulling tests as mentioned above, adds to this evidence.

3. Verification

In this section we prove the following proposition.

Proposition 1. *Let* $\tilde{\lambda} = \frac{1}{4} + \tilde{r}^2$ *and* $\{\tilde{a}_n\}$ *be the Laplacian and Hecke eigenvalues of a Maass cusp form on* $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$*. There is an algorithm with the following properties: For any* $\varepsilon > 0$ *there is a number* $D_0 = D_0(\varepsilon) \ll_{\varepsilon,\eta} \tilde{\lambda}^{1+\eta}\ \forall\eta > 0$ *such that whenever* $\lambda \geq \frac{1}{4}$ *and* $\{a_n\}_{n=1}^{M}$ *are numbers approximating* $\tilde{\lambda}$ *and* $\tilde{a}_n$ *to* D *decimal places, i.e.*

$$|\lambda - \tilde{\lambda}| < 10^{-D} \quad \text{and} \quad |a_n - \tilde{a}_n| < 10^{-D} \text{ for all } n \leq M, \tag{14}$$

with $D_0 \leq D \leq M$*, the algorithm certifies in polynomial time* $O(D^A)$ *(with both the implied constant and* $A > 0$ *absolute) the existence of a cusp form of eigenvalue* $\tilde{\lambda}'$ *such that* $|\lambda - \tilde{\lambda}'| < 10^{-(1-\varepsilon)D}$*.*

Remarks.

(1) The existence of an algorithm to certify the eigenvalue of a Maass form to any given number of digits is not surprising; one could, after all, use the trace formula for this purpose. (In fact, low precision eigenvalue computations have been rigorously carried out using the trace formula for congruence subgroups; see [3].) The key feature of Proposition 1 is the polynomial running time in the eigenvalue and number of digits.

(2) The algorithm does not guarantee the *uniqueness* of the eigenvalue, i.e. that $\tilde{\lambda} = \tilde{\lambda}'$. To do that would require checking the Hecke eigenvalues as well, which could be done by generalizing the results below using Hecke operators; see Lemma 1 for the first steps in this direction. Certification of the Hecke eigenvalues is computationally more difficult (although still polynomial) for reasons that are explained below; see the remarks after Lemma 3. We give full details only for the Laplacian eigenvalue.

(3) Proposition 1 may also be extended to congruence subgroups, with the running time depending polynomially on the level. However, there are many technical considerations in doing so. To avoid these complications, we restrict to the case of level 1.

    An interesting question (cf. discussion of [7], end of Section 1) is whether there is an effective method to determine the discrete spectrum for a non-arithmetic lattice $\Gamma\backslash\mathrm{SL}(2,\mathbb{R})$. (See also [13, §5(i)]).

(4) There is an implicit *loss of precision*: that is, to prove correct $(1-\varepsilon)D$ decimal places we need a heuristic method of finding a cusp form to D decimal places. Thus,

even to verify the first few digits of a cusp form, it is necessary to work to higher precision.

The proof will be achieved in several steps. First, in Section 3.1 we give an effective result (Proposition 2) that reduces the problem to checking approximate automorphy of the conjectured form in a small neighborhood of the boundary of the fundamental domain, and is well suited to implementation on a computer. We provide details of the implementation in Section 3.2 and complete the proof of Proposition 1 in Section 3.3. In Section 3.4 we discuss in more detail the complexity of the algorithm and some numerical results.

First, we set some notation to be used in this section. Let $W_\nu(y) := \sqrt{y}K_\nu(y)$; this shorthand will be useful when it comes to taking derivatives with respect to y. Since we work with $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$ throughout, we may assume from the outset that all forms are eigenfunctions of $J : z \mapsto -\overline{z}$, i.e. we consider Fourier expansions of the form

$$f(z) = \sum_{n=1}^{M} \frac{a_n}{\sqrt{n}} W_{ir}(2\pi ny)\cos^{(\epsilon)}(2\pi nx), \tag{15}$$

where f has eigenvalue $\lambda := 1/4 + r^2$, $\epsilon \in \{0,1\}$ indicates the parity and $\cos^{(\epsilon)}(t)$ is the ϵ^{th} derivative of $\cos(t)$, i.e. it equals $\cos(t)$ for $\epsilon = 0$ and $-\sin(t)$ for $\epsilon = 1$. We shall moreover normalize f so that $a_1 = 1$. (Thus the normalization of the coefficients coincides with that of the Section 2.1, but that of f itself is somewhat different, owing to the slightly different normalization of the Bessel function. This is done for convenience in stating the estimates in Lemma 6 and (75); note that since Proposition 1 is stated in terms of Hecke eigenvalues, any constant scaling factor cancels out in the end and does not influence the result.)

Let $\mathcal{F} = \left\{z \in \mathbb{H} : |z| \geq 1, |\mathrm{Re}\ z| \leq \frac{1}{2}\right\}$ be the (closure of) the "standard" fundamental domain for Γ. For $z, w \in \mathbb{H}$, set $u(z,w) := \frac{|z-w|^2}{4\mathrm{Im}\ z\,\mathrm{Im}\ w}$. Recall that, if d denotes the hyperbolic distance, then $\cosh(d(z,w)) = 1 + 2u(z,w)$ [14, Section 1.3]. If for $z \in \mathbb{H}$ we define $u_z := u(z,i)$ and $\varphi_z \in [0,\pi)$ to be the hyperbolic angle of z (*loc. cit.*) then the measure $d\mu(z) := \frac{dx\,dy}{y^2}$ on $\mathbb{H}$ may be expressed in "polar coordinates" as $4\,du_z\,d\varphi_z$.

Let ϕ be a non-negative, twice differentiable function on $[0,\infty)$, with support contained in $[0,1]$, such that $\int_0^\infty \phi(x)\,dx = 1$. Let $\delta > 0$ be given, and assume that Y is such that the point-pair invariant $k(z,w) = \phi(u(z,w)Y)$ vanishes for $d(z,w) \geq \delta$. We denote by $\hat{k}(r)$ the scalar by which k acts on any Laplacian eigenfunction of eigenvalue $\frac{1}{4} + r^2$ [14, Theorem 1.14], that is

$$\hat{k}(r) = \int_{\mathbb{H}} k(z,i) y^{1/2+ir} d\mu(z). \tag{16}$$

Let $\tilde{f}, \tilde{f}_S$ be (respectively) the Γ-periodic extension of f from $\mathcal{F}$ to $\mathbb{H}$ and the Γ-periodic smoothed extension, defined via $\tilde{f}_S = \tilde{f} \star k$. Note that $\tilde{f}_S(z) = \hat{k}(r)\tilde{f}(z)$ for $\mathrm{Im}\ z \geq e^\delta$. Evidently there is an issue (at least for odd f) regarding the definition of $\tilde{f}(z)$ for those $z \in \mathbb{H}$ that are in the Γ-orbit of the boundary of $\mathcal{F}$. However, in all our bounds below, it is only necessary for $\tilde{f}$ to be defined *off a set of measure* 0. In particular, one should interpret

L^∞ bounds as referring to the *essential* supremum of a function. Thus this ambiguity is irrelevant to our proceedings.

3.1. **An effective bound.** The eventual aim of this section is to prove Proposition 2 (see p. 14). In words, it states that given a finite series of the type (15), we can bound how close it is to a cusp form by checking that it is "almost automorphic", i.e. almost invariant by certain fixed generators of $\mathrm{PSL}(2,\mathbb{Z})$. Moreover, to measure closeness of the eigenvalue, the "almost invariance" need only be checked on a very small region around the boundary of the standard fundamental domain.

The idea is the usual "quasimode construction." In a slightly more general setting, let M be a finite-volume Riemannian manifold and f a smooth function on M. Let Δ be the Laplacian operator on M, and suppose that $(\Delta-\lambda)f$ has small L^2 norm. Then by making a spectral expansion, we conclude at once that f is close to a genuine Laplacian eigenfunction, whose eigenvalue is near λ. However, in our context, we must implement this type of idea in a computationally efficient way. Moreover, we must show not only that f is near a Laplacian eigenfunction, but that it is near a *cusp form*.

For p a prime number, we define the p^{th} Hecke operator T_p as the endomorphism of $C^\infty(\Gamma\backslash\mathbb{H})$ defined by

$$T_p f(z) = \frac{1}{\sqrt{p}}\left(f(pz) + \sum_{b=0}^{p-1} f\left(\frac{z+b}{p}\right)\right). \tag{17}$$

The notation $\|\cdot\|_q$ will mean, unless otherwise indicated, the L^q norm on $\Gamma\backslash\mathbb{H}$.

Lemma 1. *Put*

$$C_{f,p} = \frac{2(p^{1/2}+p^{-1/2})}{|p^{ir}+p^{-ir}-a_p|} \text{ for } p \text{ prime}, \qquad C_{f,1}=1. \tag{18}$$

Let p be a prime number if f is even, and 1 if f is odd. Let S be a finite set of places of $\mathbb{Q}$, and let numbers λ_v be given for each $v\in S$. Let T_v be the Hecke operator for each finite place v, and set $T_\infty=\Delta$. Then there exists a cusp form on $\Gamma\backslash\mathbb{H}$ with T_v-eigenvalues $\tilde{\lambda}_v$ satisfying

$$\sum_{v\in S}\left|\tilde{\lambda}_v-\lambda_v\right|^2 \le \frac{2C_{f,p}^2\sum_{v\in S}\left\|(T_v-\lambda_v)\tilde{f}_S\right\|_2^2}{\left|\hat{k}(r)\right|^2\int_{pe^\delta}^\infty W_{ir}(2\pi y)^2\frac{dy}{y^2}}. \tag{19}$$

Proof. Let $\lozenge$ be the identity endomorphism of $C^\infty(\Gamma\backslash\mathbb{H})$ if $p=1$, and set

$$\lozenge = 2\cos\left(\log p\sqrt{\Delta-\frac{1}{4}}\right) - T_p \tag{20}$$

in the general case. Here $\clubsuit := \cos\left(\log p\sqrt{\Delta-\frac{1}{4}}\right)$ may be given a rigorous interpretation, either by using the spectral decomposition of Δ, or by regarding it as the operation of convolution with a certain compactly supported distributional point-pair invariant $\mathcal{L}(z,w)$, that is to say

$$\clubsuit f(z) = \int_{\mathbb{H}} \mathcal{L}(z,w) f(w) d\mu(w). \tag{21}$$

Moreover, $\mathcal{L}(z,w)$ is supported in the region $d(z,w) \leq \log(p)$. The operator $\diamondsuit$ has norm $\leq 2(p^{1/2}+p^{-1/2})$ w.r.t. the L^2 norm on $C^\infty(\Gamma\backslash\mathbb{H})$, and commutes with T_v for all v. We refer to [17] for a further discussion.

For $p > 1$, $\diamondsuit$ maps into the space of cusp forms, by [17]. In any case, we see that $g = \diamondsuit\big(\tilde{f}_S\big)$ is cuspidal. Assume now that $p > 1$, the case $p = 1$ following similarly.

Since $\diamondsuit$ commutes with $T_v - \lambda_v$ for each $v \in S$, and in view of the bound on its operator norm, we have

$$\|(T_v - \lambda_v)g\|_2 \leq 2\big(p^{1/2}+p^{-1/2}\big)\big\|(T_v-\lambda_v)\tilde{f}_S\big\|_2. \tag{22}$$

Next, let $\{f_j\}_{j=1}^\infty$ be an L^2-basis of eigenforms for the cuspidal spectrum, with T_v-eigenvalues $\lambda_{j,v}$, and put $g = \sum_{j=1}^\infty \epsilon_j f_j$. Let Pr_H denote the orthogonal projection onto the span of f_j such that $\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2 \leq H$. Then

$$\begin{aligned}\|\mathrm{Pr}_H g\|_2^2 &= \|g\|_2^2 - \sum_{j:\sum_{v\in S}|\lambda_{j,v}-\lambda|^2 > H} |\epsilon_j|^2 \geq \|g\|_2^2 - \sum_{j=1}^\infty |\epsilon_j|^2 \frac{\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2}{H} \\ &= \|g\|_2^2 - H^{-1}\sum_{v\in S}\|(T_v-\lambda_v)g\|_2^2.\end{aligned} \tag{23}$$

Consequently, there is a j such that $\sum_{v\in S}|\lambda_{j,v}-\lambda|^2 \leq H$ as long as

$$H \geq \frac{\sum_{v\in S}\|(T_v-\lambda_v)g\|_2^2}{\|g\|_2^2} \tag{24}$$

By (22), this will always be the case if

$$H \geq 4\big(p^{1/2}+p^{-1/2}\big)^2 \frac{\sum_{v\in S}\big\|(T_v-\lambda_v)\tilde{f}_S\big\|_2^2}{\|g\|_2^2}. \tag{25}$$

Now, for $\mathrm{Im}\ z \geq pe^\delta$ we have $g(z) = \sum_{n=1}^\infty \frac{c_n}{\sqrt{n}} W_{ir}(2\pi ny)\cos^{(\epsilon)}(2\pi nx)$, with $c_1 = \hat{k}(r)\big(p^{ir} + p^{-ir} - a_p\big)$. (To see this, use (17) and the comments after (21).) We thus have the lower bound

$$\|g\|_2^2 \geq \frac{|c_1|^2}{2}\int_{pe^\delta}^\infty W_{ir}(2\pi y)^2 \frac{dy}{y^2}. \tag{26}$$

The conclusion follows. □

Lemma 2.

$$\big|\hat{k}(r)\big| > \frac{4\pi}{Y}\left(1 - 4\sqrt{\frac{\lambda}{Y}}\right). \tag{27}$$

Proof. Recall that $\hat{k}(r) = \int_{\mathbb{H}} y^{1/2+ir} k(z,i)\, d\mu(z)$. In view of the "polar coordinates" expression of $d\mu$, we obtain

$$\int_{z\in\mathbb{H}} k(z,i)\, d\mu(z) = \frac{4\pi}{Y}. \tag{28}$$

Hence

$$\left|\hat{k}(r) - \frac{4\pi}{Y}\right| \le \frac{4\pi}{Y} \sup_{u(z,i)\le 1/Y} \left|y^{1/2+ir} - 1\right|. \tag{29}$$

Now for $z = x + iy$, if $u(z,i) \le 1/Y$ then $|z-i|^2 \le 4y/Y$. Thus

$$\begin{aligned} \left|y^{1/2+ir} - 1\right| &= \left|\int_1^y \left(\frac{1}{2} + ir\right) t^{-1/2+ir}\, dt\right| \le 2\sqrt{\lambda}\left|y^{1/2} - 1\right| \\ &\le 4\sqrt{\frac{\lambda}{Y}}\frac{y^{1/2}}{y^{1/2}+1} < 4\sqrt{\frac{\lambda}{Y}}. \end{aligned} \tag{30}$$

□

Lemma 3. *Put $A = \int_{\mathbb{H}} \left|(\Delta - \lambda)k(z,i)\right| d\mu(z)$, and let $B(\delta)$ be a hyperbolic δ-neighborhood of the arc $\left\{z \in \mathbb{H} : |z| = 1, |\mathrm{Re}\, z| \le \frac{1}{2}\right\}$. Then*

$$\left\|(\Delta - \lambda)\tilde{f}_S\right\|_2 \le A\sqrt{\mathrm{vol}(B(\delta)\cap\mathcal{F})}\ \mathrm{ess.sup}_{z\in B(\delta)}\left|\tilde{f}(z) - f(z)\right|. \tag{31}$$

Proof. Note that on $\mathcal{F}$, $\tilde{f}_S$ agrees with $\hat{k}(r)\tilde{f}$ except on $B(\delta)$. Consequently, $(\Delta-\lambda)\tilde{f}_S$ vanishes away from $B(\delta)$. One has

$$(\Delta - \lambda)\tilde{f}_S = \tilde{f} \star (\Delta - \lambda)k - f \star (\Delta - \lambda)k = (\tilde{f} - f) \star (\Delta - \lambda)k. \tag{32}$$

From this we see that

$$\begin{aligned} \left\|(\Delta - \lambda)\tilde{f}_S\right\|_2^2 &\le \mathrm{vol}(B(\delta)\cap\mathcal{F})\left\|(\Delta - \lambda)\tilde{f}_S\right\|_\infty^2 \\ &\le \mathrm{vol}(B(\delta)\cap\mathcal{F})\left(\left\|f - \tilde{f}\right\|_{\infty,B(\delta)} \int_{\mathbb{H}} |(\Delta - \lambda)k(z,i)|\, d\mu(z)\right)^2. \end{aligned} \tag{33}$$

The last inequality holds since $z \in \mathcal{F}\cap B(\delta)$ and $d(z,w) < \delta$ imply that one of the points w or $w \pm 1$ belongs to $\mathcal{F}\cup B(\delta)$, while $f - \tilde{f}$ is invariant under translation by $\mathbb{Z}$ and vanishes on $\mathcal{F}$. □

Remark. Lemma 3 reduces the estimation of $\left\|(\Delta-\lambda)\tilde{f}_S\right\|_2$ to bounding $\tilde{f} - f$ in a "thin" set around the arc at the bottom of the fundamental domain. A similar technique may be used to estimate $\left\|(T_p - a_p)\tilde{f}_S\right\|_2$, but will involve $\tilde{f} - f$ on the larger (genuinely 2-dimensional) set $\left\{z \in \mathbb{H} : |\mathrm{Re}\, z| \le \frac{1}{2}, \mathrm{Im}\, z \ge \frac{\sqrt{3}}{2p}\right\}$; thus, this is computationally more complex, and becomes increasingly difficult as p increases.

Lemma 4. *Let A be as in Lemma 3.*

$$A \le 4\pi\left[\int_0^1 \left|x\phi''(x) + \phi'(x)\right| dx + \frac{1}{Y}\left(\lambda + \int_0^1 \left|x^2\phi''(x) + 2x\phi'(x)\right| dx\right)\right]. \tag{34}$$

Proof. [14, 1.21] shows that Δ corresponds, in (u,φ) coordinates, to the operator $u(u+1)\frac{\partial^2}{\partial u^2} + (2u+1)\frac{\partial}{\partial u} + \frac{1}{16u(u+1)}\frac{\partial^2}{\partial \varphi^2}$. The result follows by direct computation. ☐

Lemma 5.

$$\operatorname{vol}(B(\delta) \cap \mathcal{F}) < \frac{2}{\sqrt{3}}\delta. \tag{35}$$

Proof. Note that $B(\delta) \subset \{z \in \mathbb{H} : |z| < e^{\delta}\}$. Thus,

$$B(\delta) \cap \mathcal{F} \subset \mathcal{F} \setminus e^{\delta}\mathcal{F} = \{z \in \mathcal{F} : 1 \leq |z| < e^{\delta}\}. \tag{36}$$

By the invariance of the hyperbolic measure under scaling, this set has the same volume as

$$e^{\delta}\mathcal{F} \setminus \mathcal{F} \subset \left\{ x+iy : \frac{1}{2} < |x| \leq \frac{e^{\delta}}{2}, y \geq \frac{\sqrt{3}}{2}e^{\delta} \right\}. \tag{37}$$

The volume is therefore bounded by $\frac{e^{\delta}-1}{\frac{\sqrt{3}}{2}e^{\delta}} < \frac{2}{\sqrt{3}}\delta$. ☐

We can now prove our first main result, which gives an effective bound on how far the eigenvalue of a putative cusp form is to that of a genuine cusp form.

Proposition 2. *Suppose $\delta \leq \frac{1}{4\sqrt{\lambda}}$, and let notations be as above. Then there exists a cusp form on $\Gamma\backslash\mathbb{H}$ with Laplacian eigenvalue $\tilde{\lambda}$ satisfying*

$$\left|\tilde{\lambda} - \lambda\right| < 40\delta^{-3/2} C_{f,p} \frac{\operatorname{ess.sup}_{z \in B(\delta)} \left|\tilde{f}(z) - f(z)\right|}{\left(\int_{pe^{\delta}}^{\infty} W_{ir}(2\pi y)^2 \frac{dy}{y^2}\right)^{1/2}}, \tag{38}$$

where $C_{f,p}$ is as in Lemma 1.

Proof. The point-pair invariant $k(z,i)$ vanishes when $u(z,i) \geq 1/Y$, i.e. for $d(z,i) \geq \cosh^{-1}(1+2/Y)$. Taking $Y = 4\delta^{-2}$, we see that $k(z,i)$ is supported within a δ-neighborhood of i.

We choose the point-pair invariant given by

$$\phi(x) = \begin{cases} 3(1-x)^2 & \text{if } x \leq 1, \\ 0 & \text{else.} \end{cases} \tag{39}$$

Then, by Lemma 4,

$$A \leq 12\pi + \pi\delta^2\left(\lambda + \frac{16}{9}\right). \tag{40}$$

The hypothesis on δ, together with the bound $\lambda \geq \frac{1}{4}$, yields $A \leq 12\pi + \pi\left(\frac{1}{16} + \frac{4}{9}\right)$.

Next, by Lemma 2 we have

$$\frac{1}{\left|\hat{k}(r)\right|} < \frac{1}{\pi\delta^2} \cdot \frac{1}{1 - 2\delta\sqrt{\lambda}} \leq \frac{2}{\pi\delta^2}. \tag{41}$$

Combining these estimates with Lemmas 3 and 5, we apply Lemma 1 with the set $S = \{\infty\}$. The proposition follows. ☐

3.2. **Implementation.** Proposition 2 reduces our problem to bounding (in L^∞ norm) $\left|f-\tilde{f}\right|$ on a hyperbolic δ-neighborhood of the arc $\left\{z\in\mathbb{H}:|z|=1,|\mathrm{Re}\ z|\le\frac{1}{2}\right\}$. Because of the symmetry of f in the x variable, it suffices to do this for $x\ge 0$. If δ is sufficiently small then the only Γ-translates of the fundamental domain intersecting the neighborhood for $x\ge 0$ are $\gamma\mathcal{F}$ for $\gamma\in\{1,T,S,ST^{-1},TS,TST\}$, where $S=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)$ and $T=\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)$. For $z\in\mathcal{F}\cup T\mathcal{F}$ we evidently have $f(z)-\tilde{f}(z)=0$. For the others we have:

$$\begin{aligned}
z\in S\mathcal{F}:&\ f(z)-\tilde{f}(z)=f(z)-f(Sz);\\
z\in ST^{-1}\mathcal{F}:&\ f(z)-\tilde{f}(z)=f(z)-f(TSz)=f(z)-f(Sz);\\
z\in TS\mathcal{F}:&\ f(z)-\tilde{f}(z)=f(z)-f(ST^{-1}z)=f(T^{-1}z)-f(ST^{-1}z);\\
z\in TST\mathcal{F}:&\ f(z)-\tilde{f}(z)=f(z)-f(T^{-1}ST^{-1}z)=f(T^{-1}z)-f(ST^{-1}z).
\end{aligned}\tag{42}$$

Thus it suffices to bound simply $|f(z)-f(Sz)|$ for z in the set

$$\big(B(\delta)\cap(S\mathcal{F}\cup ST^{-1}\mathcal{F})\big)\cup T^{-1}\big(B(\delta)\cap(TS\mathcal{F}\cup TST\mathcal{F})\big).\tag{43}$$

Again by parity, we may replace this by (recall $J(z):=-\overline{z}$)

$$\big(B(\delta)\cap(S\mathcal{F}\cup ST^{-1}\mathcal{F})\big)\cup JT^{-1}\big(B(\delta)\cap(TS\mathcal{F}\cup TST\mathcal{F})\big).\tag{44}$$

In words, this amounts to reflecting the portion of $B(\delta)$ contained in $TS\mathcal{F}\cup TST\mathcal{F}$ across the line $x=\frac{1}{2}$. Note that in this region, the outer edge of $B(\delta)$ is not a sharp corner, but rather a hyperbolic circle around the point $\frac{1}{2}+i\frac{\sqrt{3}}{2}$. The reflection of the circle across $x=\frac{1}{2}$ is itself, and hence it suffices to obtain a bound just on $B(\delta)\cap(S\mathcal{F}\cup ST^{-1}\mathcal{F})$. The part of this for $x\ge 0$ is contained in the Euclidean δ-neighborhood of the arc $\{e^{i\theta}:\frac{\pi}{3}\le\theta\le\frac{\pi}{2}\}$.

It is convenient to introduce polar coordinates $x=e^t\cos\theta, y=e^t\sin\theta$. Then the function we want to bound is

$$\begin{aligned}
f(z)-f(-1/z)&=f(e^t\cos\theta,e^t\sin\theta)-f(e^{-t}\cos(\pi-\theta),e^{-t}\sin(\pi-\theta))\\
&=f(e^t\cos\theta,e^t\sin\theta)-(-1)^\epsilon f(e^{-t}\cos\theta,e^{-t}\sin\theta).
\end{aligned}\tag{45}$$

We write $E(t,\theta)$ for this final expression. By abuse of notation, we may also write $f(t,\theta)$ for $f(e^t\cos\theta,e^t\sin\theta)$; the choice of coordinates will be clear from context.

We bound $E(t,\theta)$ by computing derivatives with respect to t and θ and using Taylor's theorem. Suppose that we compute derivatives of E at some reference point (t_0,θ_0) and we wish to bound it at (t_1,θ_1). Set $F(u)=E(t_0+(t_1-t_0)u,\theta_0+(\theta_1-\theta_0)u)$. Then

$$\frac{F^{(i)}(u)}{i!}=\sum_{r+s=i}\frac{(t_1-t_0)^r}{r!}\frac{(\theta_1-\theta_0)^s}{s!}\frac{\partial^{r+s}E}{\partial t^r\partial\theta^s}(t_0+(t_1-t_0)u,\theta_0+(\theta_1-\theta_0)u).\tag{46}$$

Note that in the case $t_0=0$ this simplifies to

$$2\sum_{\substack{r+s=i\\ r\equiv\epsilon+1\ (\mathrm{mod}\ 2)}}\frac{t_1^r}{r!}\frac{(\theta_1-\theta_0)^s}{s!}\frac{\partial^{r+s}f}{\partial t^r\partial\theta^s}(t_1u,\theta_0+(\theta_1-\theta_0)u).\tag{47}$$

Now Taylor's theorem says that for any $d \geq 0$,

$$E(t_1, \theta_1) = F(1) = \sum_{i=0}^{d-1} \frac{F^{(i)}(0)}{i!} + \frac{F^{(d)}(u^*)}{d!}, \tag{48}$$

for some $u^* \in [0, 1]$.

We choose $N+1$ equally spaced sample points along the arc, i.e. $t_0 = 0, \theta_0 = \frac{\pi}{3} + \frac{\pi}{6}\frac{j}{N}$, for $j = 0, 1, \ldots, N$. We choose δ in Proposition 2 so that the maximum displacement from a sample point is at most $\frac{\pi}{12N}$ in each variable. This means taking δ proportional to N^{-1}, so the constant on the right-hand side of (38) will be large. However, it is only polynomially large in N; this is an acceptable error since eventually the other factors will be of size $e^{-\sqrt{N}}$.

We bound each term of (47) individually assuming the maximum displacement. Under the hypotheses of the theorem, the terms of (47) will be miraculously small for $u = 0$, and the main contribution to (48) will come from a trivial bound for $F^{(d)}(u^*)/d!$. Taking d and N sufficiently large, we may control this term as well.

The form of f makes it convenient to compute derivatives in rectangular coordinates. To compute the derivatives in (47), we therefore have to convert. The conversion takes the general form

$$\frac{\partial^{r+s} f}{\partial t^r \partial \theta^s}(x, y) = \sum_{k+\ell \leq r+s} P(x, y; r, s, k, \ell) \frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x, y), \tag{49}$$

where $P(x, y; r, s, k, \ell)$ is a homogeneous polynomial with integer coefficients, of degree $k+\ell$ in x and y. Using the formulas

$$\frac{\partial}{\partial t} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \qquad \frac{\partial}{\partial \theta} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}, \tag{50}$$

we see that P satisfies the recurrence relations

$$\begin{aligned} P(x, y; r+1, s, k, \ell) &= x\frac{\partial P}{\partial x}(x, y; r, s, k, \ell) + y\frac{\partial P}{\partial y}(x, y; r, s, k, \ell) \\ &\quad + xP(x, y; r, s, k-1, \ell) + yP(x, y; r, s, k, \ell-1), \\ P(x, y; r, s+1, k, \ell) &= x\frac{\partial P}{\partial y}(x, y; r, s, k, \ell) - y\frac{\partial P}{\partial x}(x, y; r, s, k, \ell) \\ &\quad + xP(x, y; r, s, k, \ell-1) - yP(x, y; r, s, k-1, \ell). \end{aligned} \tag{51}$$

We compute P recursively from these formulas as we compute the derivatives.

We have now reduced everything to the computation of $\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x, y)$ at or near each of the sample points. Note that

$$\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x, y) = \sum_{n=1}^{M} \frac{a_n}{\sqrt{n}} \frac{\partial^\ell}{\partial y^\ell} W_{ir}(2\pi n y) \frac{\partial^k}{\partial x^k} \cos^{(\epsilon)}(2\pi n x). \tag{52}$$

The difficult part of that is the computation of $W_{ir}^{(\ell)}(2\pi ny)$, for each ℓ and each $n = 1, 2, \dots, M$. In practical terms, we may use any method for $\ell = 0, 1$ since the number of evaluations is limited. For example, in our implementation we used the power series (13); this has the advantage that the error is easy to control, e.g. for $n \geq u/\sqrt{2}$, the tail of the series (from term $n+1$ onward) is bounded by the magnitude of the n^{th} term.

Computing the higher derivatives is another simple recursion: For $\ell \geq 2$ we have

$$W_{ir}^{(\ell)}(y) = W_{ir}^{(\ell-2)}(y) + \lambda \sum_{j=0}^{\ell-2} c_{\ell j} y^{j-\ell} W_{ir}^{(j)}(y), \tag{53}$$

for certain integer coefficients $c_{\ell j}$, defined by the recurrence

$$c_{\ell+1,j} = \begin{cases} (j-\ell)c_{\ell j} + c_{\ell,j-1}, & j \leq \ell - 2 \\ -1, & j = \ell - 1. \end{cases} \tag{54}$$

(Note that this is essentially the same as the expansion (10) for $K^{(n)}$.)

Since the coefficients $c_{\ell j}$ and those of $P(x, y; r, s, k, \ell)$ grow quite large, some care must be taken to ensure that the computations are accurate. To that end, one could determine a sufficient fixed point precision (roughly proportional to $D \log D$), using the bounds for $c_{\ell j}$ and $P(x, y; r, s, k, \ell)$ given in the next section. In practice, it is much easier and more efficient to work with, say, $3D/2$ digits of floating point precision, and use interval arithmetic. (Also note that we only need to know the final bound to leading order to see that it is small, i.e. significant precision loss is both acceptable and expected.) For our implementation we used the MPFI package [18] for arbitrary precision interval arithmetic, based on the MPFR and GMP libraries [19, 8].

For the final term of (48) we must produce a bound for $W_{ir}^{(\ell)}(2\pi ny)$, for each n and ℓ, and y in a neighborhood of a given sample point. This could in principle be done very accurately, i.e. with bounds very close to the truth, in polynomial time. However, as will be clear from the next section, such precision is not necessary; any bound correct up to an exponential factor in ℓ will do. We again relied on the recurrence (53) and interval arithmetic.

3.3. **Proof of Proposition 1.** The algorithm described above derives an upper bound for the distance from a number λ to the nearest eigenvalue of a Maass form on $\Gamma\backslash\mathbb{H}$, based on the parameters d, M and N. The essence of the proof in this section is to show that *if λ and a_n are close to the true data for a Maass form* then there is a choice of parameters (that one could in principle write down in advance) for which the upper bound is good. The proof ultimately relies on the bounds for Bessel functions given in Lemma 6 below. (Note that these estimates are only needed in the proof; in practice one uses trial and error combined with the more direct computational methods described above. See Section 3.4 below for further remarks.)

Lemma 6. *Let $\varepsilon > 0$. There is a number $C = C(\varepsilon) > 0$ such that, for all $\ell \geq 0$ and $r \in \mathbb{R}$,*

(1) $W_{ir}^{(\ell)}(y) \ll_\varepsilon \big[C(1+\ell)\big]^\ell \quad \forall y \geq \varepsilon$;

(2) $\frac{d}{d\lambda} W_{ir}^{(\ell)}(y) \ll_\varepsilon \big[C(1+\ell)\big]^\ell \quad \forall y \geq \varepsilon$;

(3) $W_{ir}^{(\ell)}(y) \ll C^\ell e^{-y} \quad \forall y \geq \max(\ell, \lambda)$.

Here, as usual, $\lambda = \frac{1}{4} + r^2$.

Proof. 1. We have the integral representation (apply Mellin inversion to the equations preceding B.37 in [14])

$$W_{ir}^{(\ell)}(y) = \frac{1}{2\pi i} \int_{\text{Re } s=1} 2^{s-2} \Gamma\left(\frac{s+ir}{2}\right) \Gamma\left(\frac{s-ir}{2}\right) (1/2-s)\cdots(1/2-s-(\ell-1)) y^{1/2-s-\ell}\, ds. \tag{55}$$

Applying Stirling's formula, we have for $s = 1 + it$,

$$\Gamma\left(\frac{s+ir}{2}\right) \Gamma\left(\frac{s-ir}{2}\right) \ll e^{-\frac{\pi}{4}|t+r|} e^{-\frac{\pi}{4}|t-r|}. \tag{56}$$

Using the elementary inequality $|t+r| + |t-r| \geq 2|t|$, we get the estimate

$$\begin{aligned} W_{ir}^{(\ell)}(y) &\ll \int_{-\infty}^{\infty} e^{-\pi|t|/2} (1/2+|t|)\cdots(\ell-1/2+|t|) y^{-(\ell+1/2)}\, dt \\ &\ll_\varepsilon \varepsilon^{-\ell} \int_0^\infty e^{-\pi t/2} (t+1+\ell)^\ell\, dt. \end{aligned} \tag{57}$$

Next note that

$$(t+1+\ell)^\ell \leq 2^\ell \big(t^\ell + (1+\ell)^\ell\big). \tag{58}$$

Substituting this into the above, we get the bound

$$\big(2\varepsilon^{-1}\big)^\ell \int_0^\infty e^{-\pi t/2} \big(t^\ell + (1+\ell)^\ell\big)\, dt \ll \big(2\varepsilon^{-1}\big)^\ell (1+\ell)^\ell. \tag{59}$$

2. We repeat the above argument with the Γ factors replaced by

$$\begin{aligned} \frac{1}{2r}\frac{d}{dr} \Gamma\left(\frac{s+ir}{2}\right) \Gamma\left(\frac{s-ir}{2}\right) &= \frac{i}{4r} \left[\Gamma'\left(\frac{s+ir}{2}\right) \Gamma\left(\frac{s-ir}{2}\right) - \Gamma\left(\frac{s+ir}{2}\right) \Gamma'\left(\frac{s-ir}{2}\right)\right] \\ &\ll \log^2(2+|t|) e^{-\frac{\pi}{4}|t+r|} e^{-\frac{\pi}{4}|t-r|}. \end{aligned} \tag{60}$$

The extra factor of $\log^2(2+|t|)$ does not affect the quality of the final bound.

3. The result for $\ell = 0$ follows from the asymptotic [14, B.36]

$$K_\nu(y) = \sqrt{\frac{\pi}{2y}} e^{-y} \left[1 + O\left(\frac{1+|\nu|^2}{y}\right)\right]. \tag{61}$$

The case $\ell = 1$ follows from (61) and the recurrence $-2K_\nu'(y) = K_{\nu+1}(y) + K_{\nu-1}(y)$. (In fact, by a different method one can see that the result holds without the restriction $y \geq \lambda$; we will not make use of this.)

Note that $|c_{\ell j}| \le (\ell-1)!/j!$, by induction from (54). Hence, for $\ell \ge 2$,

$$\big|W_{ir}^{(\ell)}(y)\big| \le \big|W_{ir}^{(\ell-2)}(y)\big| + \lambda \sum_{j=0}^{\ell-2} \frac{(\ell-1)!}{j!} y^{j-\ell} \big|W_{ir}^{(j)}(y)\big|. \tag{62}$$

Suppose that $\big|W_{ir}^{(j)}(y)\big| \le AC^j e^{-y}$ for $j < \ell$ and $y \ge \max(j,\lambda)$. Then, for $y \ge \max(\ell,\lambda)$ the above becomes

$$\big|W_{ir}^{(\ell)}(y)\big| \le AC^{\ell-2}e^{-y} + \lambda \sum_{j=0}^{\ell-2} \frac{(\ell-1)!}{j!} y^{j-\ell} AC^j e^{-y}. \tag{63}$$

The final term (with $j = \ell-2$) is $\lambda(\ell-1)y^{-2}AC^{\ell-2}e^{-y}$, and to pass from term j to term $j-1$ we multiply by j/Cy. Assume $C \ge 2$, so that $Cy \ge 2\ell$; then the sum is majorized by

$$\lambda\ell y^{-2}AC^{\ell-2}e^{-y}\sum_{n=0}^{\infty} 2^{-n} = 2\lambda\ell y^{-2}AC^{\ell-2}e^{-y}. \tag{64}$$

Altogether we get

$$\big|W_{ir}^{(\ell)}(y)\big| \le AC^{\ell-2}e^{-y}\big(1+2\lambda\ell y^{-2}\big) \le AC^{\ell}e^{-y}. \tag{65}$$

□

Lemma 7. *For $r+s \le d$,*

$$|P(x,y;r,s,k,\ell)| \le (d+4)!\big[1+\max(|x|,|y|)\big]^d. \tag{66}$$

Proof. From (51), we see by induction that the coefficients of $P(x,y;r,s,k,\ell)$ are bounded by $(r+s+3)!$. The result follows by homogeneity of P. □

With these estimates in hand, we may complete the proof. Let notation be as in section 3.2. For convenience, we introduce the notation $x \prec^d y$ to mean there exist absolute positive constants A and B such that $|x| \le AB^d y$.

We treat first the final term $F^{(d)}(u^*)/d!$ of (48). From (47) we must estimate $\frac{\partial^{r+s}f}{\partial t^r \partial\theta^s}(t^*,\theta^*)$ for $r+s=d$, where (t^*,θ^*) lies on the line segment between (t_0,θ_0) and (t_1,θ_1). These are handled, using (49), by estimates for $\frac{\partial^{k+\ell}f}{\partial x^k \partial y^\ell}(x^*,y^*)$ at the corresponding point (x^*,y^*). We have

$$\frac{\partial^{k+\ell}f}{\partial x^k \partial y^\ell}(x^*,y^*) = \sum_{n=1}^{M} \frac{a_n}{\sqrt{n}}(2\pi n)^{k+\ell} W_{ir}^{(\ell)}(2\pi n y^*)\cos^{(k+\epsilon)}(2\pi n x^*). \tag{67}$$

Since the a_n are close to Hecke eigenvalues of a Maass form, we have that $a_n/\sqrt{n} \ll 1$, with implied constant universal. Since y^* is bounded away from 0, Lemma 6 part 1 yields

$$\frac{\partial^{k+\ell}f}{\partial x^k \partial y^\ell}(x^*,y^*) \prec^d M\big[M(1+d)\big]^d. \tag{68}$$

Since x^* and y^* are bounded, Lemma 7 says that $P(x^*,y^*;r,s,k,\ell) \prec^d (1+d)^d$. Combining this with (49), we get

$$\frac{\partial^{r+s} f}{\partial t^r \partial\theta^s}(t^*,\theta^*) \prec^d M\big[M(1+d)^2\big]^d. \tag{69}$$

Finally, from (47) and the bounds $t_1, \theta_1-\theta_0 \ll N^{-1}$, we have

$$\frac{F^{(d)}(u^*)}{d!} \prec^d M\big[N^{-1}M(1+d)\big]^d. \tag{70}$$

Next we estimate the terms of (48) for $i<d$. For that we compare f to the true Maass form f^*, with coefficients $\tilde{a}_n$, for which the analogous expression vanishes. In other words, we replace f by $f-f^*$ and compute (46). There are two parts to consider, corresponding to the terms $n\le M$ and $n>M$, respectively. (The latter terms are introduced when we pass from f to $f-f^*$.) First, from (14), Lemma 6 parts 1 and 2, and the mean value theorem, we have, for (x_0,y_0) a point on the arc $\big\{z\in\mathbb{H} : |z|=1, |\mathrm{Re}\, z|\le \frac{1}{2}\big\}$,

$$\begin{aligned}
&\frac{a_n}{\sqrt{n}}W_{ir}^{(\ell)}(2\pi n y_0) - \frac{\tilde{a}_n}{\sqrt{n}}W_{i\tilde{r}}^{(\ell)}(2\pi n y_0)\\
&\qquad = \left(\frac{a_n}{\sqrt{n}}-\frac{\tilde{a}_n}{\sqrt{n}}\right)W_{ir}^{(\ell)}(2\pi n y_0) + \frac{\tilde{a}_n}{\sqrt{n}}\Big(W_{ir}^{(\ell)}(2\pi n y_0) - W_{i\tilde{r}}^{(\ell)}(2\pi n y_0)\Big)\\
&\qquad \prec^\ell 10^{-D}(1+\ell)^\ell.
\end{aligned} \tag{71}$$

Proceeding as above, we see that the contribution of the terms $n\le M$ to $F^{(i)}(0)/i!$ is

$$\prec^i 10^{-D}M\big[N^{-1}M(1+i)\big]^i. \tag{72}$$

For the terms $n>M$ we apply Lemma 6 part 3 to obtain the estimate

$$\sum_{n>M}\frac{\tilde{a}_n}{\sqrt{n}}(2\pi n)^{k+\ell}W_{i\tilde{r}}^{(\ell)}(2\pi n y_0)\cos^{(k+\epsilon)}(2\pi n x_0) \prec^{k+\ell} \sum_{n>M} n^{k+\ell}e^{-2\pi n y_0}, \tag{73}$$

valid provided that $M\ge C_1\max(k+\ell,\lambda)$, for some absolute constant $C_1<1$. Since $y_0\ge\sqrt{3}/2$, the above is $\prec^{k+\ell} M^{k+\ell}10^{-M}$. We deduce in the same manner as the foregoing computations that the contribution of the terms $n>M$ to $F^{(i)}(0)/i!$ is $\prec^i \big[N^{-1}M\big]^i 10^{-M}$.

Combining the estimates (70), (72) and (73), we have finally

$$E(t_1,\theta_1) \ll M\big[AN^{-1}M(1+d)\big]^d + 10^{-D}M\sum_{i=0}^{d-1}\big[BN^{-1}M(1+i)\big]^i + 10^{-M}\sum_{i=0}^{d-1}\big[CN^{-1}M\big]^i, \tag{74}$$

for appropriate constants A, B and C. We assume for simplicity that $D\ge\lambda$ and take $d=M=D$. We take N so that $C_2D^2\le N\le 2C_2D^2$, for a sufficiently large, absolute constant C_2. Thus, altogether we have $E(t_1,\theta_1)\ll 10^{-D}D$.

Finally, we combine this bound with Proposition 2. Recall that δ was of size N^{-1}; thus $\delta^{-3/2} \ll D^3$. From (61) we have a bound of the form

$$W_{ir}(y) \gg e^{-y} \text{ for } y \gg 1 + r^2. \tag{75}$$

Thus, for large p, we get

$$\int_{pe^\delta}^{\infty} W_{ir}(2\pi y)^2 \frac{dy}{y^2} \gg p^{-2} \exp\bigl(-4\pi p e^\delta\bigr). \tag{76}$$

By Proposition 2, there is a form of eigenvalue $\tilde{\lambda}'$ such that

$$\bigl|\lambda - \tilde{\lambda}'\bigr| \ll D^4 10^{-D} p \exp\bigl(2\pi p e^\delta\bigr) C_{f,p}. \tag{77}$$

To conclude, we need to show that for even forms f we may always find a p for which $C_{f,p}$ is not too large. (Note that in practice this is not an issue, as we can almost always take $p = 2$.) This is an application of the Rankin-Selberg method; an argument similar to that of [21] for holomorphic forms shows that there is a $p \ll_\varepsilon \lambda^{1+\varepsilon}$ such that $|p^{ir} + p^{-ir} - a_p| \gg_\varepsilon \lambda^{-\varepsilon}$. (In fact, [21] shows a corresponding result but without the restriction "p prime"; however, it is simple to see that one can restrict from general integers to primes at the cost of a factor λ^ε.)

Hence, as long as $M = D \gg \lambda^{1+\eta}$ for fixed $\eta > 0$, we have

$$\bigl|\lambda - \tilde{\lambda}'\bigr| < 10^{-(1+o(1))D}, \tag{78}$$

as required.

3.4. **Complexity and results.** Our algorithm works by first computing and storing the values of $\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x_0, y_0)$ for all k, ℓ and all sample points (x_0, y_0). If the Bessel function computations are done efficiently then the bulk of the time is spent computing (49) for each r and s and each sample point from the tabulated data. That amounts to about Nd^5 arithmetic operations. The proof above shows that it suffices to take $d = D = M$ and N of size about D^2, for a total running time of $O_\varepsilon(D^{8+\varepsilon})$, assuming arithmetic of D-digit numbers takes time $O_\varepsilon(D^{1+\varepsilon})$. Note, however, that the estimates in Lemma 6 are quite crude; in practice one may obtain much better bounds using interval arithmetic, and measure the performance of the algorithm in real time. Numerical tests indicate that the resulting bound for $E(t_1, \theta_1)$ is roughly of size N^{-d}; using this as a rule of thumb, one may choose N and d to obtain the desired result in optimal time.

We implemented the above algorithm using the MPFI library on a 1.5 GHz PC. The results for the first few eigenvalues on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ are summarized below. The running time for each was approximately one day. (To prove that there are no other small eigenvalues requires a computation with the trace formula; see [3].)

Theorem 1. *The first ten cuspidal eigenvalues on* $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ *are as given in Table 1, correct to 100 decimal places.*

λ_1	91.14134533635527808180977380712054599169397081569090
	24779657001959542423895651247275628962288096291166 . . .
λ_2	148.43213167272073721634630026099613950074024730230597
	18429528711664752493611551782064774884270840759058 . . .
λ_3	190.13154731993464754245355701518494068113589428312883
	85576731615371323200677917820840283441119667596429 . . .
λ_4	206.41679558595764086930256998274121408698217444408924
	57353424774780566562633717682316760582937054960721 . . .
λ_5	260.68740568936685449640878661876843428670512980543410
	25160896652698127129961088063918703474378409525572 . . .
λ_6	277.28136438002683115037066737081556475641461871642721
	10389795051170027636925268679261948599959882451968 . . .
λ_7	314.90663082378975395201087956594111981400929643683543
	24577475933753113883450789890543230665313679076946 . . .
λ_8	330.79577330595661811354919800716770713227919058116130
	90838441757780526911223164841141432001520297756449 . . .
λ_9	377.52163244760855963494607025104782105738237467084493
	35117196084788698571774187390792935770199066442588 . . .
λ_{10}	379.90407400113640004061759185737660211892670229631256
	52341784484968001450252766577139865937140147593072 . . .

TABLE 1. First ten eigenvalues on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$

4. TESTING ALGEBRAICITY

We shall now use these results to test for certain algebraicity properties of the coefficients of Maass forms. It is generally believed that the Laplacian eigenvalue and Hecke eigenvalues of the general Maass form are transcendental; we provide a significant amount of evidence for this below.

We have also tested more refined algebraicity questions that amount to asking: do any of the algebraic properties of *dihedral forms* generalize to general Maass forms? We formulate this question a little more precisely in Section 4.1; but in any case, we do not find any evidence that even this (much weaker) form of algebraicity extends to general Maass forms. It seems that this type of question was first considered and tested (but with much less accurate data) by H. Stark.

To be precise, recall that dihedral Maass forms are those associated to a Grössencharacter of a real quadratic field. The eigenvalue of such a form is essentially of the shape $\frac{1}{4}+\frac{\pi^2k^2}{R^2}$, where $k \in \mathbb{Z}$ and R is the regulator of the real quadratic field. Although there is no reason to believe that this is algebraic, what is still true is that, *given the eigenvalue*, the Hecke eigenvalues of a dihedral form are specified by a finite amount of algebraic data. A similar comment applies to eigenvalue $\frac{1}{4}$ Maass forms: it is believed ([16, p. 2] and discussion of (T3) therein) that any Maass form for $\Gamma_0(N)\backslash\mathbb{H}$ with eigenvalue $\frac{1}{4}$ is associated to a

2-dimensional even Galois representation. In particular, it has algebraic coefficients. We therefore might ask: is it possible that, in a more general setting, the eigenvalue λ of a Maass form controls the algebraicity of its coefficients? Although we know of no theoretical justification for such a question, it seems to be a natural one; we explain in Section 4.1 a more precise formulation, based on "interpolating" between the properties of Eisenstein series, eigenvalue $\frac{1}{4}$ forms, dihedral forms and holomorphic forms.

4.1. **Looking for algebraic relations between coefficients–a precise formulation.** Let f be a (Hecke or Maass) newform—not necessarily cuspidal—on $\mathbb{H}$ with Nebentypus χ_f. Let $t \in \mathbb{R} \cup i\mathbb{R}$ be so that the Casimir eigenvalue on the representation underlying f is $\frac{1}{4} - t^2$, i.e. $t = (k-1)/2$ if f is a holomorphic form of weight k, and $t = ir$ if f is a Maass form of eigenvalue $\frac{1}{4} + r^2$. Let p be a prime number at which f does not ramify, and let $\lambda_p(f)$ be the p^{th} Hecke eigenvalue of f; we normalize matters so that the Ramanujan conjecture corresponds to $|\lambda_p(f)| \leq 2$.

Question. Do there exist roots of unity ζ, ζ' with $\zeta\zeta' = \chi_f(p)$, and a p-integral algebraic number $\alpha \in \overline{\mathbb{Q}}$ so that

$$\lambda_p(f) = \zeta\alpha^t + \zeta'\alpha^{-t}? \tag{79}$$

Here, if α is not real, there is clearly some ambiguity as to the meaning of α^t. We shall interpret it (in the most optimistic way) to mean *any* t^{th} power of α: that is to say, any element of the form $\exp(tx)$ when $\exp(x) = \alpha$.

We note that that ζ, ζ', α are often by no means uniquely determined. We now show that, in every case when the $\lambda_p(f)$ may be written down explicitly, the answer to the question is YES.

(1) If f is a holomorphic form of weight k, the fact that $\lambda_p(f)$ has the form (79) follows from the existence of the associated Galois representation. Indeed, by [6], there are algebraic integers $\beta_1, \beta_2 \in \overline{\mathbb{Q}}$ such that all conjugates of β_1 and β_2 have absolute value $p^{(k-1)/2}$, $\beta_1\beta_2 = \chi_f(p)p^{k-1}$, and $\lambda_p(f) = \frac{\beta_1+\beta_2}{p^{(k-1)/2}}$. In this case, (79) is satisfied if we take (e.g.) $\alpha = \beta_1^{2/(k-1)}p^{-1}$, $\zeta = 1, \zeta' = \chi_f(p)$.

(2) If f is a CM-form, i.e. so that $L(s,f) = L(s,K,\chi)$ for some quadratic extension $K/\mathbb{Q}$ and some unitary Grössencharacter $\chi : \mathbb{A}_K^\times/K^\times \to \mathbb{C}^\times$, then a simple computation verifies (79).

Indeed, we may assume that K is a real quadratic field. (If K is imaginary, then f is holomorphic.) Now $\lambda_p(f) = 0$ if p does not split in K, and (79) is trivially satisfied. (Take, e.g. $\alpha = 1$ and ζ, ζ' to solve $\zeta = -\zeta', \zeta\zeta' = \chi_f(p)$.) On the other hand, suppose p splits as $\mathfrak{p}_1\mathfrak{p}_2$, and let be ω_1, ω_2 uniformizers at $\mathfrak{p}_1, \mathfrak{p}_2$ respectively; we regard ω_1, ω_2 as belonging to $\mathbb{A}_K^\times$, the ring of adeles of K. Then

$$\lambda_p(f) = \chi(\omega_1) + \chi(\omega_2). \tag{80}$$

Let $\mathbb{A}_{K,f}$ be the ring of finite adeles of K, and let $U \subset \mathbb{A}_{K,f}^\times$ be an open compact subgroup such that $\chi|_U$ is trivial. The quotient $\mathbb{A}_K^\times/K^\times K_\infty^\times U$ is finite; thus there is

$M \geq 1$ such that ω_1^M and ω_2^M belong to $K^\times K_\infty^\times U$. Here $K_\infty := K \otimes \mathbb{R} \cong \mathbb{R} \times \mathbb{R}$. Write $\omega_1^M = z^{-1} z_\infty u$ with $z \in K^\times, z_\infty \in K_\infty^\times, u \in U$. If σ_1, σ_2 are the two distinct isomorphisms of K into $\mathbb{R}$, then we can identify K_∞ with $\mathbb{R} \times \mathbb{R}$ in such a way that z_∞ corresponds to $(\sigma_1(z), \sigma_2(z))$.

With this identification, the restriction of χ to $K_\infty^\times$ takes the form

$$(x, y) \mapsto (x/|x|)^{\epsilon_1}(y/|y|)^{\epsilon_2}|x|^{ir}|y|^{-ir}, \tag{81}$$

for some $\epsilon_i \in \{0, 1\}$ and $r \in \mathbb{R}$. Then an easy computation shows that $t = ir$ (i.e. the Casimir eigenvalue of f is $\frac{1}{4} + r^2$). It follows that $\chi(\omega_1^M) = \pm(\sigma_1(z)/\sigma_2(z))^{ir}$. It is now easy to see that (79) holds with $\alpha = \left(\frac{\sigma_1(z)}{\sigma_2(z)}\right)^{1/M}$ and an appropriate choice of ζ, ζ'.

We also note in passing that if η is the fundamental unit for the ring of integers of K, then the finite part of η lies in the maximal compact subgroup of $\mathbb{A}_{K,f}^\times$, hence $(\eta_\infty/\eta)^M \in U$ for some $M \geq 1$. Since $\chi(\eta) = 1$ and $\sigma_1(\eta)/\sigma_2(\eta) = \sigma_1(\eta^2)$, this implies

$$r = \frac{2\pi q}{\log \sigma_1(\eta^2)}, \qquad \text{for some } q \in \frac{1}{M}\mathbb{Z} + \frac{1}{2}\mathbb{Z} \subset \mathbb{Q}. \tag{82}$$

(3) Let χ be a Dirichlet character of $\mathbb{Q}$, and let f be the Eisenstein series satisfying $L(s, f) = L(s + ir, \chi)L(s - ir, \chi)$; then $\lambda_p(f) = \chi(p)p^{ir} + \chi(p)^{-1}p^{-ir}$ visibly satisfies (79), with $\zeta = \chi(p), \zeta' = \chi(p)^{-1}, \alpha = p$.

(4) Suppose $r = 0$. Then f corresponds to either a form of weight 1 (where (79) follows from a result of Deligne-Serre) or a Maass form of eigenvalue $\frac{1}{4}$, which are *believed* to all arise from Galois representations $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}) \to \mathrm{GL}(2, \mathbb{C})$. If this is indeed the case, (79) follows.

4.2. **Transcendence of coefficients–numerical results.** We performed various tests to search for algebraic relations. In order to have control on exactly what negative result was proved we used the PARI routine `lllint`(A), which performs LLL-reduction on a lattice basis given by the columns of an *integral* matrix A, using only integer operations. For this routine, precise lower bounds are available on the shortest vector in the given lattice, and it is easy to derive from these the non-existence of integer algebraic relations with certain bounds on the coefficients. See [5, 2.6.3 and 2.7.2].

Let us say a number α is $[d, H]$*-algebraic* if it satisfies some relation

$$m_d\alpha^d + m_{d-1}\alpha^{d-1} + \ldots + m_0 = 0, \tag{83}$$

where $m_0, m_1, \ldots, m_d$ are integers, not all zero, with $|m_j| \leq H$ for $j = 0, 1, \ldots, d$.

In short, *we found no unexpected algebraic relation.* In particular, from the fact that we know the first ten eigenvalues provably to 100 decimal places (Theorem 1), we obtain using lattice reduction:

Proposition 3. *If λ is one of the first ten eigenvalues on* $\mathrm{PSL}(2, \mathbb{Z})\backslash\mathbb{H}$ *(cf. Table 1), then λ is* not $[2, 10^{30}]$*-algebraic; nor is λ* $[5, 10^{14}]$*- or* $[10, 10^7]$*-algebraic.*

However, most of our searches were performed assuming that our values for the eigenvalue λ and the Fourier coefficients $\lambda_2(f)$, $\lambda_3(f)$, $\lambda_5(f)$, $\lambda_7(f)$ are correct to 1020 decimal digits (see Section 2). *Under this assumption, we found that for each of the first ten eigenvalues* λ *on* $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$, λ *is not* $[2, 10^{331}]$*-algebraic; nor is* λ $[10, 10^{89}]$-, $[30, 10^{30}]$- *or* $[50, 10^{17}]$-*algebraic. Exactly the same assertions hold for* $r = \sqrt{\lambda - \frac{1}{4}}$ *and for each of the Hecke eigenvalues* $\lambda_2(f)$, $\lambda_3(f)$, $\lambda_5(f)$, $\lambda_7(f)$.

We also checked that for each r as above, there does *not* exist any relation of the form $r = 2\pi q/\log\alpha$ where $\alpha > 0$ is $[2, 10^{104}]$- or $[10, 10^{66}]$-algebraic and q is rational with $|q| \leq 10$ and denominator $d(q) \leq 30$. (Recall that a relation of the form $r = 2\pi q/\log\alpha$ with α a unit in a real quadratic field holds whenever f is a CM-form, see (82) above.)

4.3. **Algebraic relations between coefficients–numerical results.** Furthermore, we searched for *joint relations* of the form (79) between r and $\lambda_p(f)$, using various parameters, and found the following: For each of the first ten eigenfunctions f on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$, there does *not* exist any relation

$$\lambda_p(f) = e^{i(2\pi q + r\log\alpha)} + e^{-i(2\pi q + r\log\alpha)} \tag{84}$$

with $p \in \{2, 3, 5\}$, $\alpha > 0$, $\left|2\pi q + r\log\alpha\right| \leq \pi$, q rational with denominator $d(q) \in \mathbb{Z}^+$, and α, q satisfying the conditions in any one line of the following table:

α $[2, 10^{100}]$-algebraic	$\lvert q\rvert \leq 30$	$d(q) \leq 100$
α $[10, 10^{66}]$-algebraic	$\lvert q\rvert \leq 30$	$d(q) \leq 10$
α $[30, 10^{22}]$-algebraic	$\lvert q\rvert \leq 4$	$d(q) \leq 10$

For comparison we note that for the Ramanujan Delta function, $\Delta(z) = e^{2\pi iz}\prod_{n=1}^{\infty}(1 - e^{2\pi inz})^{24} = \sum_{n=1}^{\infty}\tau_n e^{2\pi inz}$, which is the holomorphic cusp form of level 1 and lowest weight ($k = 12$), the Hecke eigenvalue $\lambda_2(\Delta) = \tau_2/2^{11/2} = -24/2^{11/2}$ satisfies the relation (79) with $\zeta = \zeta' = 1$ and α algebraic with $32\alpha^{22} + 55\alpha^{11} + 32 = 0$, i.e. α is $[22, 100]$-algebraic.

All transcendence tests described above were carried out also for the three non-CM Maass forms on $\Gamma_0(5)\backslash\mathbb{H}$ and $\Gamma_0(6)\backslash\mathbb{H}$ listed in Section 2.3(B). We refer to [4] for the precise statements of our (negative) results in these cases.

4.4. **Comments.** The tests above are clearly not comprehensive. We invite the reader to carry out their own tests using the numbers from [4]!

References

[1] Charles B. Balogh. Asymptotic expansions of the modified Bessel function of the third kind of imaginary order. *SIAM J. Appl. Math.*, 15:1315–1323, 1967.

[2] Joseph Bernstein and Andre Reznikov. Analytic continuation of representations and estimates of automorphic forms. *Ann. of Math. (2)*, 150(1):329–352, 1999.

[3] A. Booker and A. Strömbergsson. Numerical computations with the trace formula and the Selberg eigenvalue conjecture. *in preparation.*

[4] A. Booker, A. Strömbergsson, and A. Venkatesh. web page containing data files of eigenvalues and Fourier coefficients. `http://www.math.uu.se/~astrombe/emaass/emaass.html`.

[5] Henri Cohen. *A course in computational algebraic number theory*, volume 138 of *Graduate Texts in Mathematics*. Springer-Verlag, Berlin, 1993.

[6] P. Deligne. Formes modulaires et représentations ℓ-adiques. *Séminaire Bourbaki*, 355.

[7] D. Farmer and S. Lemurell. Deformations of Maass forms. *Math. Comp.*, to appear.

[8] *GMP, version* `4.1.4`, 2004. available from `http://www.swox.com/gmp/`.

[9] V. V. Golovchanskiĭ and M. N. Smotrov, Calculation of first Fourier coefficients of eigenfunctions of the Laplace operator on the fundamental domain of a modular group. (Russian) *Numerical methods in algebra and analysis (Russian)*, 15–19, 85, Akad. Nauk SSSR, Dal′nevostochn. Nauchn. Tsentr, Vladivostok, 1984.

[10] Dennis A. Hejhal. *The Selberg trace formula for* $\mathrm{PSL}(2, \mathbf{R})$*. Vol. 2*, volume 1001 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1983.

[11] Dennis A. Hejhal. On eigenvalues of the Laplacian for Hecke triangle groups. In *Zeta functions in geometry (Tokyo, 1990)*, volume 21 of *Adv. Stud. Pure Math.*, pages 359–408. Kinokuniya, Tokyo, 1992.

[12] Dennis A. Hejhal. On eigenfunctions of the Laplacian for Hecke triangle groups. In *Emerging applications of number theory (Minneapolis, MN, 1996)*, volume 109 of *IMA Vol. Math. Appl.*, pages 291–315. Springer, New York, 1999.

[13] Dennis A. Hejhal. On the calculation of maass cusp forms. to appear in Proceedings of the International School on Mathematical Aspects of Quantum Chaos II (Reisensburg, 2003).

[14] Henryk Iwaniec. *Introduction to the spectral theory of automorphic forms*. Biblioteca de la Revista Matemática Iberoamericana. [Library of the Revista Matemática Iberoamericana]. Revista Matemática Iberoamericana, Madrid, 1995.

[15] Henry H. Kim. Functoriality for the exterior square of GL_4 and the symmetric fourth of GL_2. *J. Amer. Math. Soc.*, 16(1):139–183 (electronic), 2003. With appendix 1 by Dinakar Ramakrishnan and appendix 2 by Kim and Peter Sarnak.

[16] Robert P. Langlands. Beyond endoscopy. In *Contributions to automorphic forms, geometry, and number theory*, pages 611–697. Johns Hopkins Univ. Press, Baltimore, MD, 2004.

[17] E. Lindenstrauss and A. Venkatesh. Existence and Weyl's law for spherical cusp forms. *preprint*.

[18] *MPFI, version* `1.3.2`, 2004. available from `http://perso.ens-lyon.fr/nathalie.revol/software.html#download`.

[19] *MPFR, version* `2.1.0`, 2004. available from `http://www.mpfr.org/mpfr-current/`.

[20] B. Selander and A. Strömbergsson. Sextic coverings of genus two which are branched at three points. `http://www.math.uu.se/~astrombe/papers.html`, preprint, 2002.

[21] J. Sengupta. Distinguishing Hecke eigenvalues of primitive cusp forms. *Acta Arith.*, 114(1):23–34, 2004.

[22] F. Strömberg. Maass waveforms on $(\Gamma_0(N), \chi)$ (computational aspects). to appear in Proceedings of the International School on Mathematical Aspects of Quantum Chaos II (Reisensburg, 2003).

[23] A. Strömbergsson. A pullback algorithm for general (cofinite) fuchsian groups, technical note. `http://www.math.uu.se/~astrombe/papers.html`.

[24] The PARI Group, Bordeaux. *PARI/GP, version* `2.1.5`, 2004. available from `http://pari.math.u-bordeaux.fr/`.

[25] Holger Then. Maass cusp forms for large eigenvalues. *Math. Comp.*, 74(249):363–381 (electronic), 2005.

Andrew Booker, Dept. Of Mathematics, University of Michigan, Ann Arbor, MI 48109-1109. email: `arbooker@umich.edu`

Andreas Strömbergsson, Dept. of Mathematics, Box 480, Uppsala Univ., S-75106 Uppsala, Sweden. email: `astrombe@math.uu.se`

Akshay Venkatesh, Courant Institute of Mathematical Sciences, New York University, 251 Mercer St., New York NY 10012. email: `venkatesh@cims.nyu.edu`