EFFECTIVE COMPUTATION OF MAASS CUSP FORMS

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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 on cofinite Fuchsian groups with cusps, and the details necessary to implement it in high precision. This algorithm is heuristic and does not prove the existence of cusp forms. In Section 3 we turn to the question of *rigorously verifying* that a proposed eigenvalue, together with a proposed set of Fourier coefficients, indeed correspond to a true Maass cusp form. We will use standard methods to show that the putative eigenfunction has almost all of its spectral support concentrated near the proposed eigenvalue. It is a more subtle point to show that it is close to a *cusp form* (i.e., a discrete eigenfunction). Indeed, Selberg introduced the trace formula for the precise purpose of showing that there exist cusp forms for $\mathrm{PSL}(2,\mathbb{Z})$; we shall use a trick from [22] to greatly simplify the analysis.

We apply our technique to the data which we have computed using Hejhal's algorithm: We prove that our values for the first ten eigenvalues on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ are correct to at least 100 decimal places (Theorem 1). We also prove a theoretical result (Theorem 2) stating that our algorithm will in general achieve its certification task in *polynomial time* (with respect to the eigenvalue and digits of precision), whenever it is given input data which describes a true cusp form to a sufficient accuracy.

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 on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ 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 integers of magnitude $\leq 10^7$. This uses the 100 decimal places which were certified in Theorem 1; if we assume (and there is a great deal of evidence in this direction) that the numbers computed in 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 [10] 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 [10] 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.

Finally, we remark that the methods of this paper are "local" in the sense that they treat one Maass cusp form at a time, with the main emphasis being on high precision computation. In order to certify many eigenvalues or forms of large eigenvalue, it is natural to employ global methods from the trace formula as well. We will address this topic in a sequel paper, [5].

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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. [30] and the references listed therein. In the present section we will briefly recall the method due to Hejhal [15] 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 [30] 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 [15, 25, 30, 27], as well as sections 2.3, 3 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 [25, 27].

2.1. **Hejhal's algorithm.** We start by recalling the algorithm from [15] (cf. also [16] 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 $Y_0 = \inf\{\mathrm{Im}\ z : z \in \mathcal{F}\}$ 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 [13] or [18])

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

Here we understand $\kappa_{ir}(u)$ to mean $e^{\frac{\pi}{2}r}K_{ir}(u)$, in line with the numerical convention from [14, 15]. 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 [2].

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 [3]. 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 $y \geq Y_0$.

[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 Hecke–Maass forms on $\Gamma = \mathrm{PSL}(2,\mathbb{Z})$; here one knows that the normalization $a_1 = 1$ leads to $|a_n| \leq d(|n|)|n|^{\frac{7}{64}}$ for all n (where $d(n)$ is the usual divisor function), and a similar fact is true for newforms on any congruence subgroup of $\mathrm{PSL}(2,\mathbb{Z})$, see [20]. We refer to [27] for a more detailed discussion involving cases with $d \geq 2$ and $a_1 = 0$.

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:

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

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. [25, 27, 28].) 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 [15], 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 ($|n| \le M_0$) is obtained to an accuracy of, roughly,

$$[a_n\text{-precision}] \approx \begin{cases} D \quad \text{digits} & (\text{if } 2\pi|n|Y \lesssim r) \\ \left(D - \log_{10}^{+}\left|\frac{1}{\sqrt{Y}\kappa_{ir}(2\pi|n|Y)}\right|\right) \quad \text{digits} & (\text{if } 2\pi|n|Y \gtrsim r), \end{cases} \tag{7}$$

at least if $2\pi|n|Y$ (when $\lesssim r$) is not very close to a zero u of $\kappa_{ir}(u)$. This is easy to explain heuristically in view of our remarks below (1) on the asymptotic behaviour of $\kappa_{ir}(u)$; specifically, in the case $2\pi|n|Y \gtrsim r$, note that since $\sqrt{u}\kappa_{ir}(u)$ is positive and exponentially decaying for $u \gtrsim r$, 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 $y \ge Y_0$, since the exponential decay of $\kappa_{ir}(2\pi|n|y)$ in (2) sets in already at $|n| \approx r/(2\pi y) < r/(2\pi Y)$. Hence the coefficients a_n may be obtained to precision $\sim D$, also for $|n| > M_0$, by running a *second* computation, namely

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

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 $2\pi|n|Y' \gg r$ so that $\sqrt{Y'}\kappa_{ir}(2\pi|n|Y')$ 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 [25, 27] 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 [27, §2.8] as well as [10].

2.2. **Adaptations to computations in high accuracy.** We carried out our computations using the PARI/GP programming language [29], 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 ($r \le 25$, 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 $y \ge Y_0$, using e.g. the bounds in [20] and careful estimates of the K-Bessel function. See footnote 1 on p. 3.) 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 approximately 436 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 [27]), and for $D = 525$, $r \le 10$, 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 $|n| \le 455$ we may use $Y' = 0.11$ and $Q' = 3540 > M(Y')$, and this should give all $\{a_n\}_{1\le|n|\le 455}$ 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 [14] and [30]). 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 $1 - Q \le j \le Q$ and $\ell = 1, 2, \dots, M_0$, as well as for $u = 2\pi n Y$, $n = 1, 2, \dots, M_0$. We start by pre-tabulating all these values in a decreasing list, $u_1 \ge u_2 \ge \dots \ge u_N$. In practice, with M_0 adapted to high precision $D \ge 500$, 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 $K_{ir}^{(n)}(u_m)$, $n \ge 2$, can be computed fairly quickly using the differential equation

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

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.

The advantage of this method is that for all intermediate $u_{m'}$ the above computation is *very* fast. Note that the method is particularly suitable when the list $u_1 \geq u_2 \geq \cdots \geq u_N$ is densely packed, and this becomes more and more the case the larger D we aim for.

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, but this is not a problem since such an evaluation is only done *once* per analyzed r-value.

We refer to [6] 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 rigorous error estimates for our K-Bessel values, but this would be a bit beside the point here, since the computation of Maass forms using (5) is heuristic anyway. (However, rigorous error estimates are essential later when we use (13) in Section 3.2.)

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 (partially heuristic) algorithm described above we have obtained the following main results. Our data files with eigenvalues and Fourier coefficients are available at [6], 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, [27].

(C) We have studied a few examples from Farmer and Lemurell [10] 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 [10] 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 [10] 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 [6] 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 [10]. The computations carried out in [10] 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, fulfilling tests as mentioned above, adds to this evidence.

3. Certification

In this section we present a technique for certifying the Laplacian eigenvalues computed by Hejhal's algorithms. We apply the technique to the first ten eigenfunctions on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ to prove the following theorem.

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.*

The proof will be achieved in several steps. First, in Section 3.1 we give an effective result (Proposition 1) that reduces the problem to checking approximate automorphy of a 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 Theorem 1 in Section 3.3. In Section 3.4 we analyze the complexity of the algorithm; in particular, we prove that when given correct coefficients, the certification can always be achieved in time bounded by a polynomial function of the eigenvalue and number of digits.

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 $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$

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

$$f(z) = \sum_{n=1}^{M} \frac{a_n}{\sqrt{n}} W_{ir}(2\pi n y) \cos^{(\epsilon)}(2\pi n x), \tag{14}$$

where f has eigenvalue

$$\lambda := \frac{1}{4} + r^2 \geq \frac{1}{4}, \tag{15}$$

$\epsilon \in \{0,1\}$ 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 different by a factor $e^{\frac{\pi}{2}r}$.)

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 $\cosh(d(z,w)) = 1 + 2u(z,w)$ [18, 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 $\frac{1}{4} + r^2$ [18, Theorem 1.14], that is

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

With f as in (14), we define:

$$\tilde{f} = [\text{the } \Gamma\text{-periodic extension of } f \text{ from } \mathcal{F} \text{ to } \mathbb{H}] \qquad \text{and} \qquad \tilde{f}_S = \tilde{f} \star k. \tag{17}$$

Thus $\tilde{f}_S$ is a smoothed version of $\tilde{f}$, and is Γ-periodic. Note that $\tilde{f}(z) = f(z)$ for $\operatorname{Im} z \geq 1$ and thus $\tilde{f}_S(z) = \hat{k}(r)\tilde{f}(z)$ for $\operatorname{Im} z \geq e^\delta$. 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 1 (see p. 15). In words, it states that given a finite series of the type (14), 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" (cf., e.g., [8]): In a slightly more general setting, let M be a finite-volume Riemannian manifold and f a smooth function on M. Let $\Delta = -\mathrm{div} \circ \mathrm{grad}$ be the positive Laplace 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 has almost all its spectral support concentrated near λ. However, in our context, we must implement this type of idea in a computationally efficient way. Moreover, we must show that f is actually close to a *discrete eigenfunction* of the Laplacian.

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

$$T_p f(z) = \frac{1}{\sqrt{p}} \left(f(pz) + \sum_{b=0}^{p-1} f\left(\frac{z+b}{p}\right) \right). \tag{18}$$

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

Lemma 1. *Let $f(z)$ be any finite Fourier series as in* (14). *Put*

$$C_{f,p} = \frac{2(p^{1/2}+p^{-1/2})}{|p^{ir}+p^{-ir}-a_p|} \text{ for } p \text{ prime}, \qquad C_{f,1}=1. \tag{19}$$

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 $\mathbb{Q}$ (viz., S is a finite subset of $\{\infty,2,3,5,7,11,\dots\}$), 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

$$\sum_{v\in S}\left|\tilde\lambda_v-\lambda_v\right|^2 \le \frac{2C_{f,p}^2\sum_{v\in S}\left\|(T_v-\lambda_v)\tilde f_S\right\|_2^2}{\left|\hat k(r)\right|^2\int_{pe^\delta}^\infty W_{ir}(2\pi y)^2\frac{dy}{y^2}}. \tag{20}$$

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

$$\Diamond = 2\cos\left(\log p\sqrt{\Delta-\frac14}\right)-T_p \tag{21}$$

in the general case. This operator was introduced in [22] and is engineered to annihilate the part of the spectrum of the Laplacian which comes from the Eisenstein series. Here $\clubsuit := \cos\left(\log p\sqrt{\Delta-\frac14}\right)$ 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

$$\clubsuit f(z) = \int_{\mathbb{H}}\mathcal{L}(z,w)f(w)d\mu(w). \tag{22}$$

Moreover, $\mathcal{L}(z,w)$ is supported in the region $d(z,w)\le\log(p)$. The operator $\Diamond$ has norm $\le 2(p^{1/2}+p^{-1/2})$ 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 [22] for a further discussion.

For $p>1$ (and prime), $\Diamond$ maps into the space of *cusp* forms, by [22]. In any case, we see that $g=\Diamond(\tilde f_S)$ is cuspidal. Assume now that $p>1$, the case $p=1$ following similarly. Since $\Diamond$ commutes with $T_v-\lambda_v$ for each $v\in S$, and in view of the bound on its operator norm, we have

$$\|(T_v-\lambda_v)g\|_2 \le 2\big(p^{1/2}+p^{-1/2}\big)\big\|(T_v-\lambda_v)\tilde f_S\big\|_2. \tag{23}$$

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 $\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2\le H$ (note that this span may be empty). Then

$$\begin{aligned}\|\mathrm{Pr}_H g\|_2^2 &= \|g\|_2^2 - \sum_{j:\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2>H}|\epsilon_j|^2 \ge \|g\|_2^2-\sum_{j=1}^\infty|\epsilon_j|^2\frac{\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2}{H}\\ &= \|g\|_2^2 - H^{-1}\sum_{v\in S}\|(T_v-\lambda_v)g\|_2^2,\end{aligned} \tag{24}$$

and we even have strict inequality here unless $\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2 = H$ or 0 for all j with $\epsilon_j \neq 0$. Consequently, there is a j such that $\sum_{v\in S}|\lambda_{j,v}-\lambda_v|^2 \le H$ as long as

$$H \ge \frac{\sum_{v\in S}\|(T_v-\lambda_v)g\|_2^2}{\|g\|_2^2}. \tag{25}$$

By (23), this will always be the case if

$$H \ge 4\big(p^{1/2}+p^{-1/2}\big)^2\,\frac{\sum_{v\in S}\big\|(T_v-\lambda_v)\tilde f_S\big\|_2^2}{\|g\|_2^2}. \tag{26}$$

Now, for $\operatorname{Im} z \ge pe^\delta$ 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 (18) and the comments after (22).) We thus have the lower bound

$$\|g\|_2^2 \ge \frac{|c_1|^2}{2}\int_{pe^\delta}^\infty W_{ir}(2\pi y)^2\frac{dy}{y^2}. \tag{27}$$

The conclusion follows. □

Lemma 2.

$$\big|\hat k(r)\big| > \frac{4\pi}{Y}\left(1-4\sqrt{\frac{\lambda}{Y}}\right). \tag{28}$$

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

$$\int_{z\in\mathbb H} k(z,i)\,d\mu(z) = \frac{4\pi}{Y}. \tag{29}$$

Hence

$$\left|\hat k(r)-\frac{4\pi}{Y}\right| \le \frac{4\pi}{Y}\sup_{u(z,i)\le 1/Y}\big|y^{1/2+ir}-1\big|. \tag{30}$$

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

$$\begin{aligned}\big|y^{1/2+ir}-1\big| &= \left|\int_1^y\left(\frac12+ir\right)t^{-1/2+ir}\,dt\right| \le 2\sqrt{\lambda}\big|y^{1/2}-1\big| \\ &\le 4\sqrt{\frac{\lambda}{Y}}\frac{y^{1/2}}{y^{1/2}+1} < 4\sqrt{\frac{\lambda}{Y}}.\end{aligned} \tag{31}$$

□

Lemma 3. *Put $A=\int_{\mathbb H}\big|(\Delta-\lambda)k(z,i)\big|\,d\mu(z)$, and let $B(\delta)$ be a hyperbolic δ-neighborhood of the arc $\big\{z\in\mathbb H : |z|=1, |\operatorname{Re} z|\le\frac12\big\}$. Then*

$$\big\|(\Delta-\lambda)\tilde f_S\big\|_2 \le A\sqrt{\operatorname{vol}(B(\delta)\cap\mathcal F)}\,\operatorname{ess.sup}_{z\in B(\delta)}\big|\tilde f(z)-f(z)\big|. \tag{32}$$

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

$$(\Delta-\lambda)\tilde{f}_S = \tilde{f}\star(\Delta-\lambda)k - f\star(\Delta-\lambda)k = (\tilde{f}-f)\star(\Delta-\lambda)k. \tag{33}$$

From this we see that

$$\begin{aligned}\left\|(\Delta-\lambda)\tilde{f}_S\right\|_2^2 &\le \mathrm{vol}(B(\delta)\cap\mathcal{F})\left\|(\Delta-\lambda)\tilde{f}_S\right\|_\infty^2 \\ &\le \mathrm{vol}(B(\delta)\cap\mathcal{F})\left(\left\|f-\tilde{f}\right\|_{\infty,B(\delta)}\int_{\mathbb{H}}|(\Delta-\lambda)k(z,i)|\,d\mu(z)\right)^2.\end{aligned} \tag{34}$$

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 $w\pm1$ 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. Then*

$$A\le 4\pi\left[\int_0^1\left|x\phi''(x)+\phi'(x)\right|dx+\frac{1}{Y}\left(\lambda+\int_0^1\left|x^2\phi''(x)+2x\phi'(x)\right|dx\right)\right]. \tag{35}$$

Proof. [18, 1.21] shows that $-\Delta$ corresponds, in (u,φ) coordinates, to the operator $u(u+1)\frac{\partial^2}{\partial u^2}+(2u+1)\frac{\partial}{\partial u}+\frac{1}{16u(u+1)}\frac{\partial^2}{\partial\varphi^2}$. Hence since $k(z,w)=\phi(u(z,w)Y)$ we get

$$A=4\pi\int_0^{1/Y}\left|u(u+1)Y^2\phi''(Yu)+(2u+1)Y\phi'(Yu)+\lambda\phi(Yu)\right|du. \tag{36}$$

The inequality now follows by substituting $u=x/Y$ and using $\int_0^1\phi(x)\,dx=1$. □

Lemma 5.

$$\mathrm{vol}(B(\delta)\cap\mathcal{F})<\frac{2}{\sqrt{3}}\delta. \tag{37}$$

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

$$B(\delta)\cap\mathcal{F}\subset\mathcal{F}\setminus e^\delta\mathcal{F}=\left\{z\in\mathcal{F}:1\le|z|<e^\delta\right\}. \tag{38}$$

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

$$e^\delta\mathcal{F}\setminus\mathcal{F}\subset\left\{x+iy:\frac{1}{2}<|x|\le\frac{e^\delta}{2},y\ge\frac{\sqrt{3}}{2}e^\delta\right\}. \tag{39}$$

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

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

Proof. The point-pair invariant $k(z,i)$ vanishes when $u(z,i) \ge 1/Y$, i.e. for $d(z,i) \ge \cosh^{-1}(1+2/Y)$. 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

$$\phi(x) = \begin{cases} 3(1-x)^2 & \text{if } x \le 1, \\ 0 & \text{else.} \end{cases} \tag{41}$$

Then, by Lemma 4,

$$A \le 12\pi + \pi\delta^2 \left(\lambda + \frac{16}{9}\right). \tag{42}$$

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

Next, by Lemma 2 we have

$$\frac{1}{\left|\hat{k}(r)\right|} < \frac{1}{\pi\delta^2} \cdot \frac{1}{1-2\delta\sqrt{\lambda}} \le \frac{2}{\pi\delta^2}. \tag{43}$$

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

3.2. **Implementation.** Proposition 1 reduces our problem to bounding $\left|f(z)-\tilde{f}(z)\right|$ (in L^∞ norm) on a hyperbolic δ-neighborhood $B(\delta)$ of the arc $\left\{z \in \mathbb{H} : |z| = 1, |\operatorname{Re} z| \le \frac{1}{2}\right\}$. Here we describe an algorithm, based on Taylor's theorem, for obtaining such a bound on a computer.

Because of the symmetry of f in the x variable, it suffices to bound $\left|f(z)-\tilde{f}(z)\right|$ for $x \ge 0$. If δ is sufficiently small then the only Γ-translates of the fundamental domain intersecting $B(\delta)$ 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:

$$\begin{aligned} z \in S\mathcal{F}: &\ f(z)-\tilde{f}(z) = f(z) - f(Sz); \\ z \in ST^{-1}\mathcal{F}: &\ f(z)-\tilde{f}(z) = f(z) - f(TSz) = f(z) - f(Sz); \\ z \in TS\mathcal{F}: &\ f(z)-\tilde{f}(z) = f(z) - f(ST^{-1}z) = f(T^{-1}z) - f(ST^{-1}z); \\ z \in TST\mathcal{F}: &\ f(z)-\tilde{f}(z) = f(z) - f(T^{-1}ST^{-1}z) = f(T^{-1}z) - f(ST^{-1}z). \end{aligned} \tag{44}$$

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

$$\big(B(\delta) \cap (S\mathcal{F} \cup ST^{-1}\mathcal{F})\big) \cup T^{-1}\big(B(\delta) \cap (TS\mathcal{F} \cup TST\mathcal{F})\big). \tag{45}$$

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

$$\big(B(\delta) \cap (S\mathcal{F} \cup ST^{-1}\mathcal{F})\big) \cup JT^{-1}\big(B(\delta) \cap (TS\mathcal{F} \cup TST\mathcal{F})\big). \tag{46}$$

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 $x \geq 0$ is contained in the Euclidean δ-neighborhood of the arc $\{e^{i\theta} : \frac{\pi}{3} \leq \theta \leq \frac{\pi}{2}\}$.

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

$$\begin{aligned} f(z) - f(-1/z) &= f(e^t \cos\theta, e^t \sin\theta) - f(e^{-t}\cos(\pi - \theta), e^{-t}\sin(\pi - \theta)) \\ &= f(e^t \cos\theta, e^t \sin\theta) - (-1)^\epsilon f(e^{-t}\cos\theta, e^{-t}\sin\theta). \end{aligned} \tag{47}$$

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

$$\frac{F^{(i)}(u)}{i!} = \sum_{r+s=i} \frac{(t_1 - t_0)^r}{r!} \frac{(\theta_1 - \theta_0)^s}{s!} \frac{\partial^{r+s} E}{\partial t^r \partial \theta^s}(t_0 + (t_1 - t_0)u, \theta_0 + (\theta_1 - \theta_0)u). \tag{48}$$

Note that when $u = t_0 = 0$ this simplifies to

$$\frac{F^{(i)}(0)}{i!} = 2 \sum_{\substack{r+s=i \\ r \equiv \epsilon + 1 \pmod 2}} \frac{t_1^r}{r!} \frac{(\theta_1 - \theta_0)^s}{s!} \frac{\partial^{r+s} f}{\partial t^r \partial \theta^s}(0, \theta_0). \tag{49}$$

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

$$E(t_1, \theta_1) = F(1) = \sum_{i=0}^{d-1} \frac{F^{(i)}(0)}{i!} + \frac{F^{(d)}(u^*)}{d!}, \tag{50}$$

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

The basic outline of our implementation is as follows. 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 1 so that the maximum displacement from a sample point is at most $\frac{\pi}{12N}$ in each variable. For each sample point $(0, \theta_0)$ we evaluate $\frac{\partial^{r+s} f}{\partial t^r \partial \theta^s}(0, \theta_0)$ for all r, s with $r + s = i < d$, $r \equiv \epsilon + 1 \pmod 2$. If it happens that f is close to a Maass form then all these derivatives will be small, and we obtain from (49) a good bound $\left|F^{(i)}(0)/i!\right| \leq 2(\frac{\pi}{12N})^i \sum (r!s!)^{-1} \left|\frac{\partial^{r+s} f}{\partial t^r \partial \theta^s}(0, \theta_0)\right|$ valid for all (t_1, θ_1) with $|t_1|, |\theta_1 - \theta_0| \leq \frac{\pi}{12N}$. For each sample

point $(0,\theta_0)$ we also compute a trivial bound for $\left|F^{(d)}(u)/d!\right|$ valid for all $u \in [0,1]$ and all (t_1,θ_1) with $|t_1|, |\theta_1-\theta_0| \le \frac{\pi}{12N}$. Via (50) this gives an upper bound for $|E(t_1,\theta_1)|$ valid for all (t_1,θ_1) with $|t_1|, |\theta_1-\theta_0| \le \frac{\pi}{12N}$. Taking the supremum of these bounds over all $N+1$ sample points $(0,\theta_0)$ we finally obtain the desired upper bound for $\operatorname{ess.sup}_{z\in B(\delta)}\left|\tilde{f}(z)-f(z)\right|$, which we use in Proposition 1.

It now remains to describe how we compute the derivatives $\frac{\partial^{r+s} f}{\partial t^r \partial\theta^s}$ occurring in (49). The form of f makes it more convenient to compute derivatives in rectangular coordinates, and we therefore have to convert. The conversion takes the general form

$$\frac{\partial^{r+s} f}{\partial t^r \partial\theta^s}(x,y) = \sum_{k+\ell\le r+s} P(x,y;r,s,k,\ell)\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x,y), \tag{51}$$

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

$$\frac{\partial}{\partial t} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \qquad \frac{\partial}{\partial\theta} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}, \tag{52}$$

we see that P satisfies the recurrence relations

$$\begin{aligned} P(x,y;r+1,s,k,\ell) &= x\frac{\partial P}{\partial x}(x,y;r,s,k,\ell) + y\frac{\partial P}{\partial y}(x,y;r,s,k,\ell) \\ &\quad + xP(x,y;r,s,k-1,\ell) + yP(x,y;r,s,k,\ell-1), \\ P(x,y;r,s+1,k,\ell) &= x\frac{\partial P}{\partial y}(x,y;r,s,k,\ell) - y\frac{\partial P}{\partial x}(x,y;r,s,k,\ell) \\ &\quad + xP(x,y;r,s,k,\ell-1) - yP(x,y;r,s,k-1,\ell). \end{aligned} \tag{53}$$

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

$$\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x,y) = \sum_{n=1}^{M} \frac{a_n}{\sqrt{n}} \frac{\partial^\ell}{\partial y^\ell} W_{ir}(2\pi n y) \frac{\partial^k}{\partial x^k} \cos^{(\epsilon)}(2\pi n x). \tag{54}$$

The difficult part of that is the computation of $W_{ir}^{(\ell)}(2\pi n y)$, 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 $n \ge u/\sqrt{2}$, 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 $\ell \ge 2$ we have

$$W_{ir}^{(\ell)}(y) = W_{ir}^{(\ell-2)}(y) + \lambda \sum_{j=0}^{\ell-2} c_{\ell j} y^{j-\ell} W_{ir}^{(j)}(y), \tag{55}$$

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

$$c_{\ell+1,j} = \begin{cases} (j-\ell)c_{\ell j} + c_{\ell,j-1}, & j \le \ell - 2 \\ -1, & j = \ell - 1. \end{cases} \tag{56}$$

(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. In practice, an efficient way to do this rigorously is to use floating point precision and interval arithmetic (cf., e.g., [1]). For our implementation we used the MPFI package [23] for arbitrary precision interval arithmetic, based on the MPFR and GMP libraries [24, 11]. See Section 3.3 below for specific data on which precision we used.

For the final term of (50) 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. For this we again relied on the recurrence (55) and crude use of interval arithmetic. (It will be clear from Section 3.4 that it is acceptable to overshoot by an exponential factor in ℓ when computing these bounds for $W_{ir}^{(\ell)}(2\pi ny)$.)

3.3. **Results.** We may now complete the proof of Theorem 1. We implemented the algorithm descibed above using the MPFI library on a 3 GHz PC; see [6, verify.c]. In addition to the expansion (14), our program takes as input the parameters d, N, and the number of bits of precision; it outputs the bound on the distance to the nearest eigenvalue given by Proposition 1. Table 2 shows the running time and bound obtained with various choices of the parameters, for the Maass form of smallest eigenvalue $\lambda = 91.1413\ldots$ computed in Section 2. Note that we already get a non-trivial estimate for the eigenvalue using double precision (53 bits). On the other hand, roughly 6–8 decimal places of precision are consistently lost; thus it is important that we compute the form to higher precision than the desired certification.

Table 3 shows the parameter values used for each of the first ten forms in order to certify the eigenvalues to 100 decimal places. That establishes Theorem 1, except for the assertion that the list in Table 1 is complete. In principle, this should be possible to prove by making the linear algebra used in Hejhal's algorithms rigorous (cf. [16, §5]). However, taking advantage of the fact that we now know the eigenvalues to high precision, a much simpler method is to bound their number using the trace formula. This is carried out in [4, Prop. 4.4].

3.4. **Complexity.** In this section, we show that from a theoretical point of view, the certification procedure described above will always work when given sufficiently accurate numbers, and can be performed in polynomial time. Precisely, we have the following.

M (coefficients used)	d	N	precision	λ correct within	running time
5	12	8	24 ($D \approx 7$)	5.7×10^{-2}	< 1 second
8	16	16	53 ($D \approx 16$)	2.2×10^{-10}	2.9 seconds
14	22	32	100 ($D \approx 30$)	4.3×10^{-24}	21 seconds
27	35	64	200 ($D \approx 60$)	1.1×10^{-53}	6.7 minutes
54	58	128	400 ($D \approx 120$)	6.0×10^{-112}	4.0 hours

TABLE 2. Eigenvalue bound and running time with various choices of parameters for the form of eigenvalue $\lambda = 91.1413\ldots$ (The precision is given in bits, and D is the corresponding number of decimal digits.)

λ	M	d	N	precision	λ correct within	running time
$91.14\ldots$	50	54	120	368 ($D \approx 111$)	4.0×10^{-102}	2.4 hours
$148.43\ldots$	50	55	122	368	3.8×10^{-103}	2.6 hours
$190.13\ldots$	50	55	122	368	1.4×10^{-101}	2.6 hours
$206.41\ldots$	50	55	122	368	8.3×10^{-102}	2.6 hours
$260.68\ldots$	50	56	124	368	8.9×10^{-103}	2.9 hours
$277.28\ldots$	50	56	124	368	1.4×10^{-102}	2.9 hours
$314.90\ldots$	50	56	124	368	1.7×10^{-101}	2.9 hours
$330.79\ldots$	50	56	124	368	1.4×10^{-101}	2.9 hours
$377.52\ldots$	50	57	126	368	2.1×10^{-102}	3.1 hours
$379.90\ldots$	50	57	126	368	8.2×10^{-103}	3.2 hours

TABLE 3. Eigenvalue bound and running time for each of the first ten forms on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$

Theorem 2. *There is a function $D_0(\varepsilon, \lambda)$, satisfying $D_0(\varepsilon, \lambda) \ll_{\varepsilon,\eta} \lambda^{1/2+\eta}$ for all $\eta > 0$, and an algorithm with the following specifications:*

INPUT: *An integer ("target accuracy") D, a constant $0 < \varepsilon < 1$ ("allowable accuracy loss") and a sequence of numbers ("purported cusp form data") $\{a_n\}_{n=1}^{M}$ and $\lambda \geq \frac{1}{4}$. These input data must satisfy $D \geq D_0(\varepsilon, \lambda)$ and $M \geq \frac{\log 10}{\pi\sqrt{3}} D$.*

RUNNING TIME: *$O(D^A)$, where A and the implied constant are absolute.*

OUTPUT: `YES` *or* `INCONCLUSIVE`.

The algorithm has the following properties:

(1) *If* `YES`*, then "λ is correct to $(1-\varepsilon)D$ digits": there exists a cusp form on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ of eigenvalue $\tilde{\lambda}'$ satisfying $\left|\lambda - \tilde{\lambda}'\right| < 10^{-(1-\varepsilon)D}$.*

(2) *Moreover, the algorithm will* always *return* `YES` *if there exists a Hecke-Maass cusp form f^* on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ with Laplacian and Hecke eigenvalues $\tilde{\lambda}, \{\tilde{a}_n\}$ satisfying*

$$\left|\lambda - \tilde{\lambda}\right| < 10^{-D} \quad \text{and} \quad \left|a_n - \tilde{a}_n\right| < 10^{-D} \text{ for all } n \leq M. \tag{57}$$

Remarks.

(1) The key feature of Theorem 2 is the *polynomial running time* in the eigenvalue and number of digits. The mere 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 [4].)

(2) The assumption $M \geq \frac{\log 10}{\pi\sqrt{3}} D$ is a natural one; it corresponds to the value $Y_0 = \sqrt{3}/2$ in Section 2.1, so that (14) approximates the true cusp form f^* to roughly D decimal places uniformly throughout the fundamental domain. On the other hand, using more intricate estimates for the K-Bessel function than we employ here, Theorem 2 can be extended to allow *much smaller* values of D w.r.t. λ. This is important for studying the large λ aspect of Maass form computations, which we will address in [5].

(3) The algorithm as presented does not guarantee the *uniqueness* of the eigenvalue, i.e. that $\tilde{\lambda} = \tilde{\lambda}'$. One way to do so would be to certify the first several Hecke eigenvalues as well, by generalizing the results above using Hecke operators; see Lemma 1 for the first steps in this direction. However, it turns out to be more efficient to use global information coming from the trace formula (e.g. to bound the eigenvalue counting function, cf. [4, Prop. 4.4]) in conjunction with the methods presented here; we will follow this approach in [5].

In this vein, note that we do not need to assume any *a priori* bound on the multiplicity of $\tilde{\lambda}$ in Theorem 2; the reason is that we make the strong assumption that the true cusp form f^* is also an eigenfunction of all Hecke operators. If there did exist eigenvalues $\tilde{\lambda}$ on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ of very large multiplicity, then this would likely cause problems to any algorithm (heuristic or not) used for the actual computation of λ, $\{a_n\}_{n=1}^M$ which are given as input in Theorem 2. (Of course it is *believed* that all eigenvalues on $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$ are simple.)

(4) Theorem 2 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 $\mathrm{PSL}(2,\mathbb{Z})\backslash\mathbb{H}$.

An interesting question (cf. our discussion of [10], 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 [16, §5(i)]).

(5) 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. This was visible in the results of Section 3.3.

The algorithm described in Sections 3.1–3.2 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 and N. The essence of the proof of Theorem 2 in this section is to show that *if* λ *and* a_n *are close to the true data for a Hecke-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 the following lemma.

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) $\frac{\partial}{\partial\lambda} W_{ir}^{(\ell)}(y) \ll_\varepsilon \big[C(1+\ell)\big]^\ell \quad \forall y \geq \varepsilon$;
(3) $W_{ir}^{(\ell)}(y) \ll C^\ell e^{-y} \quad \forall y \geq \ell + 1$.

Here, as usual, $\lambda = \frac{1}{4} + r^2$. (In (3) both C and the implied constant are absolute.)

Proof. Recall $K_{ir}(z) = \int_0^\infty e^{-z\cosh t}\cos(rt)\,dt$ for all complex z with $\mathrm{Re}\ z > 0$, and $W_{ir}(z) = \sqrt{z}K_{ir}(z)$. Using $\cosh t \geq 1 + t^2/2$ ($\forall t \in \mathbb{R}$) we get $|W_{ir}(z)| \leq \sqrt{\frac{\pi}{2}\frac{|z|}{\mathrm{Re}\ z}} \cdot e^{-\mathrm{Re}\ z}$. Keeping now $y \in \mathbb{R}$, $y \geq \varepsilon$ and applying Cauchy's formula on a circle of radius $\varepsilon/2$ about y (note that $\frac{|z|}{\mathrm{Re}\ z} < 2$ on this circle), we obtain $|W_{ir}^{(\ell)}(y)| \leq (\ell!)\left(\frac{\varepsilon}{2}\right)^{-\ell}\sqrt{\pi}e^{-y/2}$. Similarly, if $y \geq \ell + 1$ and we apply Cauchy's formula on a circle of radius $\frac{\ell+1}{2}$ about y we get $|W_{ir}^{(\ell)}(y)| \leq (\ell!)\left(\frac{\ell+1}{2}\right)^{-\ell}\sqrt{\pi}e^{\frac{\ell+1}{2}-y}$. The last two bounds lead to (1) and (3) via Stirling's formula.

For (2), note that $\frac{\partial}{\partial\lambda} = (2r)^{-1}\frac{\partial}{\partial r}$, so that $\frac{\partial}{\partial\lambda}W_{ir}(z) = -\frac{\sqrt{z}}{2}\int_0^\infty e^{-z\cosh t}t^2\mathrm{sinc}(rt)\,dt$ when $\mathrm{Re}\ z > 0$, where we use the standard notation $\mathrm{sinc}(x) = \frac{\sin(x)}{x}$ for $x \neq 0$, $\mathrm{sinc}(0) = 1$. Applying $\cosh t \geq 1 + t^2/2$ as before, together with $|\mathrm{sinc}(x)| \leq 1$, $\forall x \in \mathbb{R}$, we obtain $|\frac{\partial}{\partial\lambda}W_{ir}(z)| \leq (\pi|z|)^{\frac{1}{2}}(2\mathrm{Re}\ z)^{-\frac{3}{2}}e^{-\mathrm{Re}\ z}$. Using Cauchy's formula as before we obtain (2). □

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

$$|P(x, y; r, s, k, \ell)| \leq (d+4)!\big[1 + \max(|x|, |y|)\big]^d. \tag{58}$$

Proof. From (53), 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 of Theorem 2. 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 $|x| \leq AB^d y$.

We treat first the final term $F^{(d)}(u^*)/d!$ of (50). From (48), for each $r + s = d$ we must estimate

$$\left|\frac{\partial^{r+s}E}{\partial t^r\partial\theta^s}(t^*, \theta^*)\right| \leq \left|\frac{\partial^{r+s}f}{\partial t^r\partial\theta^s}(t^*, \theta^*)\right| + \left|\frac{\partial^{r+s}f}{\partial t^r\partial\theta^s}(-t^*, \theta^*)\right|, \tag{59}$$

where (t^*, θ^*) lies on the line segment between (t_0, θ_0) and (t_1, θ_1). These are handled, using (51), by estimates for $\frac{\partial^{k+\ell}f}{\partial x^k\partial y^\ell}(x^*, y^*)$ at points (x^*, y^*) corresponding to $(\pm t^*, \theta^*)$. We have

$$\frac{\partial^{k+\ell}f}{\partial x^k\partial y^\ell}(x^*, y^*) = \sum_{n=1}^M \frac{a_n}{\sqrt{n}}(2\pi n)^{k+\ell}W_{ir}^{(\ell)}(2\pi n y^*)\cos^{(k+\epsilon)}(2\pi n x^*). \tag{60}$$

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 (cf. footnote 1 on p. 3). Since y^* is bounded away from 0, Lemma 6 part 1 yields

$$\frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell}(x^*, y^*) \prec^d M\big[M(1+d)\big]^d. \tag{61}$$

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 (51) and (59), we get

$$\frac{\partial^{r+s} E}{\partial t^r \partial \theta^s}(t^*, \theta^*) \prec^d M\big[M(1+d)^2\big]^d. \tag{62}$$

Finally, from (48) and the bounds $t_1, \theta_1 - \theta_0 \ll N^{-1}$, we have

$$\frac{F^{(d)}(u^*)}{d!} \prec^d M\big[N^{-1}M(1+d)\big]^d. \tag{63}$$

Next we estimate the terms of (50) 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 (49). 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 (57), Lemma 6 parts 1 and 2, and the mean value theorem, we have, for (x_0, y_0) a point on the arc $\big\{z \in \mathbb{H} : |z| = 1, |\mathrm{Re}\ z| \le \frac{1}{2}\big\}$,

$$\begin{aligned} &\frac{a_n}{\sqrt{n}} W_{ir}^{(\ell)}(2\pi n y_0) - \frac{\tilde{a}_n}{\sqrt{n}} W_{i\tilde{r}}^{(\ell)}(2\pi n y_0) \\ &\qquad = \left(\frac{a_n}{\sqrt{n}} - \frac{\tilde{a}_n}{\sqrt{n}}\right) W_{ir}^{(\ell)}(2\pi n y_0) + \frac{\tilde{a}_n}{\sqrt{n}} \Big(W_{ir}^{(\ell)}(2\pi n y_0) - W_{i\tilde{r}}^{(\ell)}(2\pi n y_0)\Big) \\ &\qquad \prec^\ell 10^{-D}(1+\ell)^\ell. \end{aligned} \tag{64}$$

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

$$\prec^i 10^{-D} M\big[N^{-1}M(1+i)\big]^i. \tag{65}$$

For the terms $n > M$, we assume that $2\pi y_0 M \ge k + \ell + 1$. Lemma 6 part 3 then gives

$$\sum_{n>M} \frac{\tilde{a}_n}{\sqrt{n}} (2\pi n)^{k+\ell} W_{i\tilde{r}}^{(\ell)}(2\pi n y_0) \cos^{(k+\epsilon)}(2\pi n x_0) \prec^{k+\ell} \sum_{n>M} n^{k+\ell} e^{-2\pi n y_0} \ll M^{k+\ell+1} e^{-2\pi M y_0}. \tag{66}$$

Since $y_0 \ge \sqrt{3}/2$ the right hand side is $\le M^{k+\ell+1} e^{-\pi\sqrt{3}M}$. We deduce in the same manner as the foregoing computations that the contribution of the terms $n > M$ to $F^{(i)}(0)/i!$ is $\prec^i M\big[N^{-1}M\big]^i e^{-\pi\sqrt{3}M}$.

Combining the estimates (63), (65) and (66), we have finally

(67)
$$E(t_1,\theta_1) \ll M\big[C_1N^{-1}M(1{+}d)\big]^d{+}10^{-D}M\sum_{i=0}^{d-1}\big[C_2N^{-1}M(1{+}i)\big]^i{+}e^{-\pi\sqrt{3}M}M\sum_{i=0}^{d-1}\big[C_3N^{-1}M\big]^i,$$

for appropriate constants C_1, C_2 and C_3. We now make the choice of parameters $d = D$, $M = \lceil \frac{\log 10}{\pi\sqrt{3}} D \rceil$, and $N = \lceil C_4 D^2 \rceil$ for a sufficiently large, absolute constant C_4. (Note that the inequality $2\pi y_0 M \geq k + \ell + 1$, which was needed for (66), is then satisfied, since $y_0 \geq \sqrt{3}/2$ and $k + \ell \leq i < d$.) Thus, altogether we have $E(t_1, \theta_1) \ll 10^{-D} D$.

Finally, we combine this bound with Proposition 1. Our choice of δ on p. 16 means that δ is of size N^{-1}; thus $\delta^{-3/2} \ll D^3$. From the K-Bessel asymptotic [2] one deduces that for $y \geq c\sqrt{\lambda}$ for any fixed $c > 1$, $W_{ir}(y) \gg_c e^{-\frac{\pi}{2}y}$. Thus, for δ sufficiently small we have

$$\begin{aligned}\int_{pe^\delta}^\infty W_{ir}(2\pi y)^2 \frac{dy}{y^2} &\gg \max\big(pe^\delta, \sqrt{\lambda}\big)^{-2} \exp\big(-2\pi^2 \max\big(pe^\delta, \sqrt{\lambda}\big)\big) \\ &\gg \exp\big(-20 \max\big(p, \sqrt{\lambda}\big)\big).\end{aligned} \tag{68}$$

Hence by Proposition 1, applied with $p = 1$ or an arbitrary prime, there is a cusp form of eigenvalue $\tilde{\lambda}'$ such that

$$\big|\lambda - \tilde{\lambda}'\big| \ll D^4 10^{-D} e^{10\max(p,\sqrt{\lambda})} C_{f,p}, \tag{69}$$

where the implied constant is absolute.

To conclude, we need to show that for even forms f we may always find a prime 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. Recall that f^* is a true Hecke-Maass cusp form with Laplacian eigenvalue $\tilde{\lambda}$ and Hecke eigenvalues $\tilde{a}_n$ (thus $\tilde{a}_1 = 1$). Hence an argument similar to that of [26] for holomorphic forms implies that there exists a $p \ll_\nu \tilde{\lambda}^{1/2+\nu}$ such that $|p^{i\tilde{r}} + p^{-i\tilde{r}} - \tilde{a}_p| \gg_\nu \tilde{\lambda}^{-\nu}$ (where $\nu > 0$ is arbitrarily small). In fact, [26] shows a corresponding result but without the restriction "p prime"; however, it is easy to see that one can restrict from general integers to primes at the cost of a factor $\tilde{\lambda}^\nu$.

Hence, as long as $D \gg \lambda^{1/2+\eta}$ for fixed $\eta > 0$, choosing $0 < \nu < \eta$ and using (57) we get $|p^{ir} + p^{-ir} - a_p| \gg_\nu \lambda^{-\nu}$ and $\max(p, \lambda) = o(D)$. Thus, by (69) and (19),

$$\big|\lambda - \tilde{\lambda}'\big| < 10^{-(1-\varepsilon)D}, \tag{70}$$

for all sufficiently large D, as required.

3.5. **Running time analysis.** 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 (51) for each r and s and each sample point from the tabulated data. That amounts to about Nd^5 arithmetic operations.

To conclude, we need a bound on the precision needed in the computations. For this we assume that the computations are done using fixed point precision, i.e. all numbers are internally represented as $a \cdot 10^{-D_1}$ ($a \in \mathbb{Z}$), where D_1 some large fixed integer (although in practice it seems to be more efficient to use floating point precision and interval arithmetic, cf. Section 3.2). By carrying out an error analysis in the computations described in Section 3.2 (with d, M and N as chosen in Section 3.4) one shows that there are choices of $D_1 \ll D \log D$ such that the the numerically computed value for the $E(t_1, \theta_1)$-bound will provably be within distance $10^{-D}D$ from the *exact* bound given by our formulas, and we see from Section 3.4 that this suffices for our needs. We omit the details of the proof. One also shows that all numbers $a \cdot 10^{-D_1}$ ($a \in \mathbb{Z}$) appearing in these computations will need $\ll D \log D$ digits in a. In view of these observations, we may assume that each arithmetic operation takes time $O_\varepsilon(D^{1+\varepsilon})$.

The proof in Section 3.4 above shows that it suffices to take $d, M \asymp D$ and $N \asymp D^2$. With these choices, we see that the total running time of the algorithm is $O_\varepsilon(D^{8+\varepsilon})$. This completes the proof of Theorem 2.

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 $\frac{1}{4} + \frac{\pi^2 k^2}{R^2}$, 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 ([21, 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 (holomorphic or Maass) newform on $\mathbb{H}$ for some group $\Gamma_0(N)$, with Nebentypus $\chi_f : (\mathbb{Z}/N\mathbb{Z})^\times \to \mathbb{C}$. We allow for the possibility that f is an Eisenstein series. Let $t \in \mathbb{R} \cup i\mathbb{R}$ be so that the Casimir eigenvalue of 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 or Eisenstein series 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

$$\lambda_p(f) = \zeta\alpha^t + \zeta'\alpha^{-t}? \tag{71}$$

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 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 (71) follows from the existence of the associated Galois representation. Indeed, by [9], 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, (71) 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 (71).

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 (71) 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

$$\lambda_p(f) = \chi(\omega_1) + \chi(\omega_2). \tag{72}$$

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

$$(x, y) \mapsto (x/|x|)^{\epsilon_1}(y/|y|)^{\epsilon_2}|x|^{ir}|y|^{-ir}, \tag{73}$$

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 (71) 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

$$r = \frac{2\pi q}{\log \sigma_1(\eta^2)}, \qquad \text{for some } \; q \in \frac{1}{M}\mathbb{Z} + \frac{1}{2}\mathbb{Z} \subset \mathbb{Q}. \tag{74}$$

(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 (71), 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 (71) 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, (71) 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 [7, 2.6.3 and 2.7.2].

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

$$m_d\alpha^d + m_{d-1}\alpha^{d-1} + \ldots + m_0 = 0, \tag{75}$$

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 2. *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 $|q|\le 10$ and denominator $d(q)\le 30$. (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 (74) above.)

4.3. **Algebraic relations between coefficients–numerical results.** Furthermore, we searched for *joint relations* of the form (71) 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

$$\lambda_p(f)=e^{i(2\pi q+r\log\alpha)}+e^{-i(2\pi q+r\log\alpha)} \tag{76}$$

with $p\in\{2,3,5\}$, $\alpha>0$, $\left|2\pi q+r\log\alpha\right|\le\pi$, 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	$\lvert q\rvert\le 30$	$d(q)\le 100$
α $[10,10^{66}]$-algebraic	$\lvert q\rvert\le 30$	$d(q)\le 10$
α $[30,10^{22}]$-algebraic	$\lvert q\rvert\le 4$	$d(q)\le 10$
α $[50,10^{12}]$-algebraic	$\lvert q\rvert\le 4$	$d(q)\le 10$

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 (71) 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 [6] 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 his or her own tests using the numbers from [6]!

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