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Eigenvalues of the Laplacian and of the Hecke operators for $\mathrm{PSL}(2, \mathbb{Z})$

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Abstract

A new method is described to compute with high accuracy a large number of eigenvalues and eigenfunctions (Maaß wave forms) of the Laplacian and of the Hecke operators for the modular group. It relies essentially on the theory of Hecke operators. The results of the computations confirm some important conjectures from number theory, namely Ramanujan–Petersson, Sato–Tate, and the conjecture that the discrete spectrum of the Laplacian be simple. Examples of the numerical data are included as a reference. The algorithm can be generalized to other non-cocompact but cofinite arithmetic groups, like Picard group $\mathrm{PSL}(2, \mathbb{Z}[i])$ and Hecke triangle groups $\Gamma(\sqrt{2})$ and $\Gamma(\sqrt{3})$.

1 Introduction and summary

The spectrum of the hyperbolic Laplacian for the modular group $\mathrm{PSL}(2, \mathbb{Z})$ seems to be one of the most interesting in modern number theory and the formalism of the Selberg trace formula, cf. [15, 21, 35]. While the continuous part of the spectrum can be described rather explicitly in terms of the Eisenstein series, less is known about its discrete part whose existence is not even a trivial fact [9, 23, 31]. In line with the increasing power of computers, in the past some 15 years the idea of getting numerical insight into this and related (discrete) spectra attracted more and more interest, indicating as well a creeping motion of new "technical" techniques towards hard mathematics. Lately physicists got involved into this business by the discourse of quantum chaos.

The relevant references concerning the computational work in the case of the modular group are [6, 7, 8, 10, 13, 14, 16, 17, 18, 19, 20, 34, 36, 37, 42]; reviews can be found in [15, 37].

In this paper we present a numerical method for computing with high accuracy a large number of eigenvalues and eigenfunctions (Maaß wave forms) of the Laplacian and of the Hecke operators for the modular group. We compute simultaneously eigenvalues and square-summable eigenfunctions of

$$-\Delta f(z) = \lambda f(z) = \left(\frac{1}{4} + R^2\right) f(z), \quad (1)$$

$$T_p f(z) = c_p f(z), \quad p \text{ prime}, \quad (2)$$

subject to the automorphy condition

$$f(\gamma z) = f(z), \quad \gamma \in \mathrm{PSL}(2, \mathbb{Z}), \quad \mathrm{Im} z > 0. \quad (3)$$

The Laplacian is given by

$$\Delta = y^2(\partial_x^2 + \partial_y^2), \quad (4)$$

for details and the definition of the Hecke operators T_p see section 2 below. The eigenvalues c_p of the Hecke operators enter the Fourier expansion (20) of $f(z)$ as coefficients. Coefficients with non-prime index are polynomials in the c_p 's. To facilitate language we occasionally shall refer to the eigenvalues of the Laplacian simply as eigenvalues and to those of the Hecke operators as coefficients.

The algorithm takes as starting point the Fourier expansion of the eigenfunctions with the coefficients expressed as polynomials in the prime coefficients c_p . This fulfils eq. (1) and part of the invariance condition (3). The c_p 's are determined as functions of R from the nonlinear system that arises from writing

down explicitly eq. (2) for the respective p . The eigenvalues are found iff the remaining conditions (3) are fulfilled. This proceeding can also be applied to other systems for which Hecke operators with similar properties exist. This is the case for the subgroups (so-called Hecke triangle groups) $\Gamma(\sqrt{m})$, $m = 2, 3$, of the modular group [11], and for the Picard group $\text{PSL}(2, \mathbb{Z}[i])$ which corresponds to a 3-dimensional system [22]. For the latter, we have been computing the first eigenvalues recently. Results will be reported in future paper.

Most of the cited papers deal with the determination of the eigenvalues R (this is the usual parameter) as solutions of eqs. (1) and (3). The first eigenvalues have been computed by Cartier and Haas [7, 13]. Major progress is due to Hejhal [16] who was the first to go beyond $R \approx 25$ (so far only 20 correct eigenvalues have been known). More than one thousand eigenvalues were respectively found in [8, 34, 37]; the first two papers consider only odd eigenfunctions, the latter developed the present method.

The determination of eigenfunctions essentially consists in finding the appropriate Fourier coefficients. Stark was the first to recognize that equation (2) could be useful in this respect [36]. Apart from this, only Hejhal considers coefficients/eigenfunctions in two recent papers [17, 19]. Huntebrinker [20] presents finite element approximations of eigenfunctions.

Our computations cover the ranges $0 < R < 350$ and $500 < R < 510$ which include about 10000 eigenvalues (tables 4, 5 show examples). The completeness was checked by comparison of the results with a generalized Weyl's law (cf. figure 1). Additionally, a couple of large eigenvalues around $R = 1000, 2000$, and 4000 have been found, the largest of which lies above the 1.3×10^6 th eigenvalue (table 1). The spectrum is simple in the whole range, but nearly degeneracies occur frequently (in the language of quantum chaos the spectrum is Poissonian, see [4, 5]).

The Sato–Tate conjecture asserts that the c_p 's of any eigenfunction should be distributed according to Wigner's semicircle law. To get numerical hints on its validity we prepared extensive lists of c_p 's for a couple of Maass wave forms which include up to 30000 coefficients. They clearly confirm the conjecture (fig. 2). (See also [17].)

Keeping p fixed, it is seen (fig. 3) that the distribution of the Fourier coefficients c_p agree with the predictions of a theorem of Sarnak [32].

The Ramanujan–Petersson conjecture states

$$|c_p| \leq 2. \quad (5)$$

We have not found any violation of this bound among more than 300000 coefficients.

The results are also of interest in the context of quantum chaos (see e.g. [12] for general informations) where the eigenvalues of the Laplacian correspond to the energy levels of a quantum mechanical particle sliding freely on the modular domain. The classical counterpart of this system has a chaotic geodesic flow [2, 28]. Nevertheless, it turned out [3, 4, 34, 37] that the statistical properties of the spectrum look more like those of an integrable system. At reasonable high energies the spectrum shows Poissonian fluctuations, i.e. fluctuations similar to those of a sequence of equidistributed random numbers, whereas most (time-reversal invariant) chaotic systems exhibit GOE statistics as described by the random matrix theory [29]. The origin of this exceptional behaviour lies in the arithmetic structure of the modular group. For this and related systems which are based on arithmetic groups the notion of arithmetic chaos was recently introduced. For detailed informations consult [3, 4, 5, 33].

2 Preliminaries

In this section we shortly collect well-known basic notions and facts which are necessary to construct the algorithm in the following section. A more detailed presentation and many references to the original literature can be found e.g. in Terras' book [39].

Let

$$\mathcal{H} = \{z = x + iy \in \mathbb{C} \mid x \in \mathbb{R}, y > 0\} \quad (6)$$

be the Poincaré upper half plane which is equipped with the Riemannian metric

$$ds^2 = y^{-2} (dx^2 + dy^2). \quad (7)$$

The (hyperbolic) Laplace operator and the volume element associated with ds^2 are

$$\Delta = y^2 (\partial_x^2 + \partial_y^2), \quad (8)$$

$$dz = y^{-2} dx dy. \quad (9)$$

\mathcal{H} has constant negative Gaussian curvature $K = -1$ and is a model for hyperbolic geometry in two dimensions. Geodesics are semicircles and straight lines orthogonal to the real axis.

The group of orientation preserving isometries is

$$G = \text{PSL}(2, \mathbb{R}) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathbb{R}^{2 \times 2} \mid ad - bc = 1 \right\} / \{\pm I\} \quad (10)$$

acting on \mathcal{H} by (fractional) linear transformations

$$gz = \frac{az + b}{cz + d}, \quad g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in G. \quad (11)$$

Both the volume element and the Laplacian are invariant under the action of G .

The modular group

$$\Gamma = \text{PSL}(2, \mathbb{Z}) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathbb{Z}^{2 \times 2} \mid ad - bc = 1 \right\} / \{\pm I\} \quad (12)$$

is one of the simplest discrete subgroups of G . Its standard fundamental domain, which is together with appropriate boundary conditions a realisation of the quotient $\Gamma \backslash \mathcal{H}$, is the modular domain

$$\mathcal{F} = \{z \in \mathcal{H} \mid |z| \geq 1, |x| \leq 1/2\}. \quad (13)$$

Γ is generated by the translation $z \mapsto z+1$ and the inversion $z \mapsto -1/z$ identifying opposite sides of $\partial\mathcal{F}$. Γ is co-finite since $\text{vol}(\Gamma \backslash \mathcal{H}) = \int_{\mathcal{F}} dz = \pi/3 < \infty$, but not co-compact since \mathcal{F} has a cusp at $i\infty$. Functions on $\Gamma \backslash \mathcal{H}$ can be considered as automorphic functions on \mathcal{H} which have to satisfy $f(\gamma z) = f(z)$ for all $\gamma \in \Gamma$ and $z \in \mathcal{H}$.

Let $L^2(\Gamma \backslash \mathcal{H})$ be the Hilbert space of square summable automorphic functions $(f, f) = \int_{\mathcal{F}} f(z) \overline{g(z)} dz < \infty$. Δ is essentially self-adjoint on $L^2(\Gamma \backslash \mathcal{H})$ and therefore has a unique self-adjoint extension [9]. We will not distinguish between both of them in the following. The spectrum of Δ splits $L^2(\Gamma \backslash \mathcal{H})$ into the orthogonal sum [23, 31]

$$L^2(\Gamma \backslash \mathcal{H}) = \text{Eisenstein} \oplus \text{Constant} \oplus \text{Cusp} \quad (14)$$

Eisenstein is spanned by the Eisenstein series and contains the continuous spectrum of Δ which extends from $\frac{1}{4}$ to ∞ . Functions in *Eisenstein* are even functions in x .

Constant contains the constant eigenfunctions associated with the trivial eigenvalue $\lambda_0 = 0$ which exists since \mathcal{F} has finite hyperbolic area.

We are concerned with the third part *Cusp* of the spectral decomposition. It contains the discrete spectrum of Δ which is embedded in the continuous spectrum, and which is supposed but not proven to be simple.

Let the Hecke operators T_n , $n \in \mathbb{N}$, be defined as [25, 26]

$$T_n f(z) = \frac{1}{\sqrt{n}} \sum_{\substack{ad=n, d>0 \\ b \bmod d}} f\left(\frac{az+b}{d}\right) \quad (15)$$

and let the parity operator be

$$Pf(z) = f(-\bar{z}). \quad (16)$$

Then,

$$\{\Delta, T_n, P\}_{n \in \mathbb{N}} \quad (17)$$

forms a commutative family of self-adjoint operators on $L^2(\Gamma \backslash \mathcal{H})$. Let $(f_j)_{j \in \mathbb{N}}$ be a orthogonal basis of *Cusp* consisting of simultaneous eigenfunctions of this family. The f_j 's are called Maaß wave forms or cusp forms. We describe in the following the properties of these functions which could be deduced by the application of the different operators. Occasionally we will drop the indices of individual cusp forms and related quantities.

The cusp forms fall into two parity classes containing even and odd functions with respect to P and satisfying Neumann ($\frac{\partial f}{\partial n} = 0$) and Dirichlet ($f = 0$) boundary conditions on $\partial\mathcal{F} \cup \{x = 0\}$, respectively. Accordingly, we will speak about even and odd eigenvalues. The fulfilment of the boundary conditions is equivalent to automorphy in each parity class.

By definition cusp forms are eigenfunctions of the Laplacian,

$$\Delta f_j + \lambda_j f_j = \Delta f_j + \left(\frac{1}{4} + R_j^2\right) f_j = 0, \quad (18)$$

and we may order the f_j 's by the size of their eigenvalues

$$\frac{1}{4} < \frac{3\pi^2}{2} < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \quad (19)$$

with $\lambda_j \rightarrow \infty$ as $j \rightarrow \infty$. The lower bound $3\pi^2/2$ [30] allows to write $\lambda_j = \frac{1}{4} + R_j^2$ with positive R_j which henceforth will be called eigenvalue as well.

Formal solutions of (18) can be obtained by a separation ansatz and the employment of periodicity in x . This leads to the Fourier expansion

$$f_j(z) = \sum_{n=1}^{\infty} c_n^j \sqrt{y} K_{iR_j}(2\pi n y) \cos(2\pi n x) \quad (20)$$

for even cusp forms while in the odd case sines replace the cosines. It can be shown that the first Fourier coefficient never vanishes. Otherwise one would deduce from

relations like (25) that all other coefficients have to vanish, too. The rest of the paper will be dealing with so-called normalized cusp forms whose first coefficient is fixed to be

$$c_1 = 1. \quad (21)$$

We remark that normalized cusp forms do not have an L^2 -norm of one.

$K_{iR}(x)$ denotes the modified Bessel function of the third kind [1, 41] which is real for real x and R . For fixed R , $K_{iR}(x)$ oscillates about 0 in the interval $x \in (0, R)$ with a period approximately proportional to x and an amplitude of order $\sqrt{2\pi/R} \exp(-\pi R/2)$. The last extremum is positive and the following turning point lies slightly below $x = R$. For $x > R$, $K_{iR}(x)$ remains positive and dies off roughly exponentially as $x \rightarrow \infty$. Consequently, for numerical purposes one can find a value $x_{\max} = x_{\max}(R, \epsilon) > R$ and take $K_{iR}(x) = 0$ for $x > x_{\max}$ with an error being smaller than any desired $\epsilon > 0$.

Series (20) is absolutely convergent on \mathcal{H} due to the exponential decrease of the Bessel function and the estimate [40]

$$|c_n| \leq d(n)n^{1/4}, \quad (22)$$

where $d(n)$ counts the number of divisors of n .

Letting the Hecke operators act on normalized cusp forms given by the Fourier expansion (20), their eigenvalues turn out to be the Fourier coefficients,

$$T_n f(z) = c_n f(z) \quad \forall n \in \mathbb{N}. \quad (23)$$

Since T_n is self-adjoint $c_n \in \mathbb{R}$ for all $n \in \mathbb{N}$ causing normalized cusp forms to be real functions. More explicitly, equation (23) with the definition (15) reads for $n = p$ prime

$$c_p f(z) = \frac{1}{\sqrt{p}} \left(\sum_{j=0}^{p-1} f\left(\frac{z+j}{p}\right) + f(pz) \right). \quad (24)$$

The coefficients are not all independent but obey the Hecke relations

$$c_m c_n = \sum_{d|(m,n)} c_{mn/d^2}. \quad (25)$$

E.g., for $n \in \mathbb{N}$, p prime, one has

$$c_{np} = c_n c_p - c_{n/p} \quad (26)$$

where $c_{n/p}$ has to be taken as zero if p is not a divisor of n . It follows that the coefficients c_n are polynomials in the c_p 's with $p \leq n$.

3 The algorithm

Consider the Fourier expansion (20). Let $R > 0$ and

$$\vec{c}_p = (c_2, c_3, c_5, \dots) \quad (27)$$

be any real vector whose components fulfil (22). Using (26) \vec{c}_p determines the vector

$$\vec{c} = (1, c_2, c_3, c_4, \dots) = \vec{c}(\vec{c}_p) \quad (28)$$

of "fake" coefficients that could be inserted into the Fourier expansion. The resulting function $f(z) = f(z; \vec{c}_p, R)$ is square summable over \mathcal{F} and an eigenfunction of the Laplacian on \mathcal{H} . But generally it is not an eigenfunction of Δ on $\Gamma \backslash \mathcal{H}$, i.e. not a cusp form, since it is not necessarily Γ -invariant.

Γ is generated by the translation $T(z) = z+1$ and the reflection $S(z) = -1/z$. The Fourier expansion automatically assures translation invariance $f(z) = f(z+1)$. Hence the only remaining condition for f to be a cusp form is

$$f(z) = f\left(-\frac{1}{z}\right) \quad \text{for all } z \in \mathcal{H}. \quad (29)$$

An equivalent requirement would be the imposition of the correct (Dirichlet or Neumann) boundary conditions on the lower part $|z| = 1$ of $\partial\mathcal{F}$.

The basic idea is the following. Let $z_0 \in \mathcal{F}$ be fixed and

$$\Phi_z(R) = f(z; \vec{c}_p, R) - f(-1/z; \vec{c}_p, R). \quad (30)$$

Then by scanning the R -axis we are looking for zeroes \tilde{R} of $\Phi_{z_0}(R)$ which are candidates for eigenvalues. The correct eigenvalues are picked up by testing $\Phi_z(\tilde{R})$ to vanish (numerically) as a function of $z \in \mathcal{H}$. The corresponding f will be a cusp form.

The main question in this approach is how to determine \vec{c}_p for the actual R . We do this with the help of the eigenvalue equations of the Hecke operators (24) which hold for any $z \in \mathcal{H}$ and any cusp form. Fixing $z = \hat{z} \in \mathcal{F}$ we interpret (24) for any $R > 0$ as an equation for the unknown c_p . Since f shall be Γ -invariant one is allowed to write

$$c_p f(\hat{z}) = \frac{1}{\sqrt{p}} \left(\sum_{j=0}^{p-1} f(z_j^p) + f(z_p^p) \right). \quad (31)$$

where $z_p^p = p\hat{z}$ and $z_j^p \in \mathcal{F}$ denotes the point in the modular domain which is Γ -equivalent to $(\hat{z}+j)/p$. The point z_j^p is easily found by translations into the strip

$|\operatorname{Re} z| \leq 1/2$ and reflections by $z \mapsto -1/z$ in turn. This choice minimizes the number of terms needed to compute the Fourier series to a prescribed accuracy. Since the Bessel function $K_{iR}(x)$ is a monotonically decreasing function of x above $x = R$, the convergence of (20) is better the larger y is. The modular domain and its translates just contain the points with largest imaginary part of all Γ -equivalent points.

Truncating the Fourier series and exchanging summations yields the polynomial, i.e. nonlinear, system of equations for the prime coefficients

$$0 = \sum_{n=1}^N c_n(\tilde{c}_p) \left[c_p SKC(1, n) - SKC(p, n) \right], \quad (32)$$

$$p = 2, 3, 5, \dots, P, \quad \pi(N) = \pi(P)$$

where the constants

$$SKC(1, n) = \sqrt{y} K_{iR}(2\pi n \hat{y}) \cos(2\pi n \hat{x}),$$

$$SKC(p, n) = \frac{1}{\sqrt{p}} \sum_{j=0}^p \sqrt{y_j^p} K_{iR}(2\pi n y_j^p) \cos(2\pi n x_j^p) \quad (33)$$

contain numerical data.

This system is solved with Newton's method. Since one does not know in advance where to find its solutions it turns out to be effective to generate starting values for the Newton iteration randomly. In more detail a typical step of the calculations looks like follows. System (32) is nonlinear and therefore one generally has a couple of solutions \tilde{c}_p^{old} for a given $R = R^{\text{old}}$. Going to the next $R = R^{\text{new}} = R^{\text{old}} + \Delta R$ one takes each \tilde{c}_p^{old} as a starting value for a Newton iteration. Each time the iteration converges one tests if

$$\Phi_{z_0}(R^{\text{old}}) \Phi_{z_0}(R^{\text{new}}) \leq 0 \quad (34)$$

holds. In this case one expects a zero of Φ_{z_0} in the interval $[R^{\text{old}}, R^{\text{new}}]$ which we detect by a modified secant method or a modified Regula Falsi. If such a zero R_0 is found one has to check with different points $z \neq z_0$ whether $\Phi_z(R_0) = 0$ or not. In the former case one has hunted up an eigenvalue, and the corresponding cusp form is given by its Fourier expansion.

However, since it is impossible to know if the list of solutions of (32) is complete for the actual R^{new} , the next step is very important as well as for getting the whole procedure started. We try to find new solutions by choosing randomly starting

values for the iteration, i.e. typically $c_p \in [-2p^{1/4}, 2p^{1/4}]$ or $c_p \in [-2, 2]$ due to (22) and Ramanujan-Petersson conjecture (5), respectively.

With a single run one does usually not find all eigenvalues in a given interval. To circumvent this problem there is still the freedom of choosing the parameter $\hat{z} \in \mathcal{F}$ in eqs. (32) and (33). Since \hat{z} carries no a priori information about the eigenvalues one can hope for the statistical independence of the solutions found with distinct \hat{z} . For "macroscopically" different \hat{z} this seems to be true, and by doing several runs with different values of \hat{z} we were able to complete the list of eigenvalues.

Some technical remarks

From Weyl's law (cf. (40,41)) one expects a mean distance between successive even or odd eigenvalues of about $12/R$. The grid on which one searches for sign changes of $f(z) - f(-1/z)$ should therefore have a (nonconstant) width of $\Delta R = \pm \frac{1}{F} (\frac{12}{R})$ with $F > 1$. Good values of F turn out to be typically $10 < F < 30$.

The number N of random \tilde{c}_p 's at each step of the computations was mostly held between 10 and 30. Both quantities, F and N , have to be coordinated since small values worsen the number of found eigenvalues in a single run and large values can increase the running time without an appropriate gain in the output of eigenvalues.

As an example we mention in more detail three of our runs in the interval $R \in [100, 250]$, the parity was odd. We took $\hat{z} = 0.2 + i1.1$, $0.2 + i1.15$, and $0.3 + i1.25$. The R -grid was of width $\frac{1}{15} (\frac{12}{R})$, the number of random \tilde{c}_p was 30 and each $c_p \in [-2.2, 2.2]$. To yield an accuracy of 13 digits demands about 11 prime coefficients at $R = 100$ and 19 at $R = 250$. The maximum number of simultaneously found solutions of (32) increases from about 20 to nearly 40. Each run found about 70 – 80% of the eigenvalues and all three together between 95% and 100%. The portion of found eigenvalues in a single run is slightly decreasing with R . At $R \approx 500$ we got typically about 50%.

For the evaluation of the Bessel functions we have been using either a routine of Hejhal and Bombieri [16], or our own routine which is based on asymptotic formulae, as proposed in [8], combined with a Miller algorithm [38] for certain arguments. The latter one is faster without loss of accuracy, but in any case the Bessel function calls are the most time consuming part of the algorithm besides the linear algebra associated with Newton's method. For this reason it was nec-

essary to reduce drastically the Bessel function calls by interpolation techniques. For small and moderate indices ($R < 250$, say) a Lagrange interpolation in R for each argument $2\pi n y_j^p$ works well. For (fixed) large R a Newton interpolation relative to the argument is to be preferred.

Most of the computations were carried out on IBM RS/6000 workstations.

4 Discussion of the algorithm

The idea to use Hecke operators in connection with computations concerning Maass wave forms is mentioned by Stark [36]. He proposed to compute Fourier coefficients by a direct iteration of equation (24) or slight rearrangements of it, e.g.

$$c_n^{k+1} f^k(z) = T_n f^k(z) \quad (35)$$

where $f^k(z)$ is given by the k -th iterate $\{c_n^k\}_{n \in \mathbb{N}}$. Although he was able to detect the first even eigenvalue, this method generally does not work since one cannot assure contraction of (35). It is easy to find examples in which, even if starting close to a correct eigenvalue and the corresponding \tilde{c} , the iteration is not converging to this solution. Examples of this effect can be found in [17].

The first method to find a larger number of eigenvalues stems from Hejhal [16]; it makes use of the Hecke relations, too. The basic idea is to write down explicitly the equation $f(z) - f(-1/z) = 0$ for different points $z \in \mathcal{H}$ where f is given by its Fourier expansion (20) and to deduce a system of linear equations which is solved for the unknown (not only prime) coefficients. The eigenvalues are found by varying R and by the requirement that the Hecke relations be fulfilled. The main drawback of this method is its lack of stability which is sufficient to find the eigenvalues but not sufficient to get out correctly all the coefficients involved. The reason of this behaviour is the ill-conditioning of the established matrix. (To avoid this problem Hejhal & Arno [17] went back to the ideas of Stark's iterative method to compute the coefficients of certain cusp forms from given approximations. In spite of some tricky improvements their method has still a kind of experimental stage. It deserves some supervision and is not well suited for detecting unknown solutions.)

Our method does not have these problems with stability and convergence. At first sight the introduction of the nonlinear system (32) might seem to increase the problems at hand, but this is not true. The problem of convergence is simply

solved by application of Newton's method which assures locally quadratic convergence. Its use is made easier by the fact that the solutions one is looking for are contained in a finite box of dimension (see (22))

$$[-2 \cdot 2^{1/4}, 2 \cdot 2^{1/4}] \times [-2 \cdot 3^{1/4}, 2 \cdot 3^{1/4}] \times [-2 \cdot 5^{1/4}, 2 \cdot 5^{1/4}] \times \dots \quad (36)$$

The Newton method also reduces the nonlinear problem to solving linear equations. But in this case the relevant matrix of the derivative is much better conditioned, at least partly since differentiating (32) with respect to \tilde{c}_p produces a term $f(\tilde{z})$ in each element of the diagonal which dominates (as long as it stays away from zero) the much smaller off-diagonal elements of the last columns.

The reduced matrix dimensions of $\pi(N) \times \pi(N)$, in the nonlinear case, instead of $(N-1) \times (N-1)$, in the linear case, compensates for the effort of computing multiple solutions. Recall the expense of a Gauss elimination is roughly proportional to the third power of the matrix dimension. In the extreme case of $R \approx 4000$ where $N \approx 825$ and $\pi(N) \approx 145$ this leads to a factor of $(825/145)^3 \approx 184$.

The ambiguity of the non-linear system allows to find more than a single eigenvalue in one mesh of the R -grid. This is good for two reasons. First it makes it possible to detect without complications degenerated eigenvalues, if existing. However, this possibility has not yet occurred. Secondly, the R -grid has not to be finer than the distance between successive eigenvalues. This is important in view of the fact that the eigenvalues tend to prefer small distances, level clustering in the parlance of quantum chaos, as was shown in [4, 34]. Table 3 clearly demonstrates the effect of nearly degenerate eigenvalues in the most extreme cases. It is visible even at small R : until recently [16] the two odd eigenvalues 23.20^+ and 23.26^+ were not known correctly. They are missing in [7, 18], and [10] displays somehow diplomatically the mean 23.23 . Generally, the separation of such close lying solutions is difficult for any algorithm based on linear equations, whereas the presented method is not affected by this behaviour.

To explore the limits of the algorithm we have done a couple of test runs at $R = 1000, 2000$, and 4000 . In either case eigenvalues were found although the running time is increasing enormously. The results are presented in the tables 1 and 2.

even	odd	$n \approx$
1000.02199511676	1000.27230927167	39155 (even)
1000.06366726075	1000.28599362215	40561 (odd)
1000.11061578997	1000.29288170050	
1000.11952236414	1000.36237116994	
1000.14318460208	1000.37009864881	
1000.17315583652	1000.39238529136	
1000.19228308221	1000.39691060345	
1000.25974630314		
2000.03261184360	2000.01919434933	160982 (even)
2000.05158832762	2000.04473789000	164235 (odd)
2000.06353658232	2000.05785938212	
2000.12752840208	2000.08253608295	
2000.14541255499		
4000.01102588972	4000.05723539020	653973 (even)
4000.01746322179	4000.05981212797	661361 (odd)
	4000.06807822332	
	4000.10329568733	

Table 1: Large eigenvalues R_n for the modular group (not complete). The third column exhibits the approximate value of n . Displayed are the respective values of $N_{\text{mean}}^{\pm}(1/4 + R^2)$, for $R = 1000, 2000$, and 4000 , cf. eqs(40),(41).

$R = 4000.01102588972$ (even)					
p	c_p	p	c_p	p	c_p
2	+1.86152900987	229	+0.40240262889	523	-0.79130478848
3	-0.92703892921	233	-0.91005983320	541	-0.81280846921
5	-1.49515928669	239	+1.45447815199	547	-0.29048332219
7	+1.41609304830	241	+1.84183990712	557	-0.07804495400
11	+0.59083640633	251	+1.77696920305	563	+0.13778840313
13	-1.10371440498	257	+1.22804101784	569	+0.07778930576
17	-1.81591719288	263	-1.38486170210	571	+0.83186815755
19	-0.00059943179	269	+0.79760601225	577	+0.25429506830
23	-1.15691899782	271	+1.44260220951	587	-0.18669290000
29	-1.93030329169	277	-1.35250477123	593	+0.68261695040
31	-1.09508769312	281	-0.89566315809	599	-0.52751449102
37	-0.63275087480	283	+1.15067558493	601	-0.21482133252
41	+0.24155719241	293	-0.73790889097	607	+0.05605604815
43	+0.13153011095	307	+0.82646033248	613	-0.14807826405
47	+0.98917826888	311	-1.10717669769	617	+1.58718124320
53	+0.23986793193	313	-0.76681186015	619	+1.08120349554
59	+0.79542391321	317	-1.81745120782	631	+0.20040709253
61	+1.02319296879	331	+0.07898804822	641	-1.09300402439
67	+0.61248808946	337	-0.14490104335	643	+0.59335255754
71	-0.22374550490	347	-1.20233805528	647	+1.53232568969
73	-0.24139477345	349	+0.79698998800	653	+0.62721920109
79	-0.19410698510	353	-1.06738973040	659	-0.24096680598
83	-0.39407408315	359	-1.49803981313	661	-1.37369501480
89	-1.20504335370	367	+0.86493750133	673	-0.09724230159
97	+1.76194709700	373	+0.21241186162	677	+0.51406521141
101	+0.62445217323	379	+0.20422929697	683	+0.39332271020
103	+1.61285055953	383	+0.04775783212	691	-0.06666354459
107	-1.09753341225	389	+0.50992150601	701	+1.37975283234
109	-1.50818375918	397	-1.50877637775	709	-0.25867275495
113	-0.69043125185	401	-1.08194363005	719	-0.68643969888
127	-0.14430197494	409	-0.69953202889	727	-1.78283036350
131	+0.17148692012	419	-0.00160379742	733	+0.97904688103
137	-0.37454999405	421	+1.68814255660	739	+0.63799172079
139	-1.01094537096	431	+0.48269642557	743	-0.62877041130
149	+1.31945062199	433	-1.01139767455	751	+0.14043116498
151	+1.42546578251	439	+0.73170342766	757	+0.25119631130
157	-0.97276137210	443	-0.13530325375	761	+0.63129565363
163	-0.63386438223	449	+0.11891073872	769	-1.44770863042
167	+1.55524394856	457	+0.29680219504	773	+1.39689981865
173	-1.92304601702	461	+1.71162158491	787	-0.39594362338
179	-0.69946345685	463	-1.67320503010	797	-1.75571847264
181	-0.75181511422	467	-1.28404594592	809	-0.94014648438
191	+1.13777924414	479	+0.20388074569	811	+0.57098050887
193	-0.82577940186	487	+1.24343585378	821	-1.57416488537
197	-1.71902309526	491	+1.57921023359	823	-1.49389838667
199	-1.44573363611	499	-0.25964442752	827	+0.77284508214
211	+0.48218884999	503	+1.86280891281	829	-1.68885757885
223	-0.21103202962	509	-0.97220977121		
227	+1.45212225278	521	-1.36012101331		

Table 2: Fourier coefficients of a normalized even cusp form ($c_1 = 1$).

	R	dR		R	dR
even	242.6673326133	1	odd	231.7806243370	1
	242.6673535416	2668		231.7806342045	5543
	271.7958204649	6.47		348.8593978542	6.43
	272.1148275386			349.0893379077	

Table 3: Successive eigenvalues $R \in (0, 350)$ with the most extreme relative distances dR . dR is measured in units of the mean expected distance given by Weyl's law, eqs. (40),(41).

+	0	450	2141	9325
1	13.7797513518907389	123.8331309255	250.0142918545	500.0388246192
2	17.7385633810573779	123.8727236673	250.1570226403	500.0480426360
3	19.4234814708282552	124.1395466897	250.1715412434	500.0664609711
4	21.3157959402037188	124.2126870734	250.1998488441	500.0759968907
5	22.7859084941898736	124.3508437282	250.2205188129	500.1139410029
6	24.1123527298408640	124.4979173823	250.2941562035	500.1380623518
7	25.8262437127091584	124.5181798749	250.3230632640	500.1417069147
8	26.1520854492213488	124.5823857987	250.3600047846	500.1519712977
9	27.3327080831494099	124.7999715417	250.5126017731	500.2147562702
10	28.5307476929183202	124.8986908677	250.5215749611	500.2322981577
11	28.8633943539222970	124.9944384466	250.6110083423	500.2712342591
12	30.4106788046542568	125.0368588880	250.6264347412	500.2835512456
13	31.5265821967902692	125.3138401770	250.6309088536	500.3275946928
14	31.5662754117538871	125.3475585710	250.7200641698	500.3528235961
15	32.5081177599090003	125.5239875728	250.7482615783	500.3595282663
16	32.8911702135103197	125.6736019295	250.8287516940	500.3944749497
17	34.0278842001002688	125.8964729376	250.8494850031	500.4081702583
18	34.4562715330310283	126.0187785113	251.0096635387	500.4304849651
19	35.5023497713694011	126.0663817855	251.0206514583	500.4854369799
20	35.8416764325828391	126.1139945203	251.0595380115	500.5042750580
21	36.6775529931452006	126.2504058608	251.0926894563	500.5387670349
22	36.8563494959215496	126.3135693958	251.1131940447	500.5551887337
23	37.8250722905930271	126.3211487082	251.2710099800	500.5729304251
24	38.3032761524950115	126.3797686713	251.2884826640	500.5887269688
25	39.1680849679279492	126.6407541406	251.3219346949	500.6672979560

Table 4: Even eigenvalues R_n of the Laplacian for $\text{PSL}(2, \mathbb{Z})$. The index n indicates the n -th even eigenvalue, and is the sum of the numbers at the very top and the very left of the respective eigenvalue.

—	0	1500	3500	10000
1	9.53369526135355756	200.2518741643	301.0302010452	501.9847360659
2	12.1730083246796778	200.2580950447	301.0402448107	502.0222609522
3	14.3585095182598128	200.3958010057	301.1187593097	502.0391021629
4	16.1380731715210306	200.4227411463	301.1736468811	502.1150314774
5	16.6442592018998199	200.5245258224	301.2186015631	502.1177585828
6	18.1809178345307039	200.5997034279	301.2236844511	502.1273121331
7	19.4847138547410134	200.6198039845	301.2591944152	502.1332352300
8	20.1066946825523129	200.6499781469	301.2888877222	502.1534067708
9	21.4790575447485450	200.6550046228	301.2941914205	502.1711402021
10	22.1946739775723304	200.8146803730	301.3496957296	502.1946528131
11	23.2013961812270875	200.9185589240	301.4655904599	502.1980076715
12	23.2637115379396382	200.9444508522	301.5452135943	502.2593584926
13	24.4197154423254233	200.9995646841	301.5764451197	502.2920024737
14	25.0508548507616351	201.0851848471	301.5768016298	502.2924299865
15	26.0569177606664270	201.1369300987	301.5878738659	502.3506265321
16	26.4469964180468775	201.2018927851	301.5909436571	502.4040281720
17	27.2843840116822503	201.2694635188	301.6298575970	502.4645005738
18	27.7759207017968351	201.2995037852	301.7093530841	502.4766515547
19	28.5102777031464807	201.3653199545	301.7205684940	502.5094637752
20	29.1375875578395346	201.4125363106	301.8205764778	502.5108813650
21	29.5463881241460127	201.4210768703	301.8497937810	502.5135527742
22	30.2790484991474997	201.4707419985	301.9332581402	502.5310764428
23	30.4043270540436687	201.5938041875	302.0021004356	502.5370504927
24	31.0565339621067000	201.7198256463	302.0078365485	502.5566016515
25	31.9161824709196205	201.7836083392	302.0507893299	502.5634889499

Table 5: Odd eigenvalues R_n of the Laplacian for $\text{PSL}(2, \mathbb{Z})$. The index n is determined as in table 4.

5 Eigenvalues of the Laplacian

We have been computing all eigenvalues up to $R = 350$ (4401 even and 4776 odd) and between 500 and 510 (395 even and 410 odd). We have not found any degeneracies and the values are in agreement with the results of other authors we know (the references are given in the introduction). As mentioned before we computed additionally eigenvalues up to $R \approx 4000$, a region that lies above the 1.3×10^6 th eigenvalue.

The precision that could be obtained is mainly restricted by the accuracy of the available Bessel function routine. Most of our runs were done with an accuracy of 13 to 15 digits. For the smaller R values of tables 4 and 5 we have enhanced the accuracy to 18 digits using the 10 bytes extended arithmetic of a PC.

We exhibit a couple of examples of our eigenvalues in the tables 4, 5, 1. They are chosen so as to contain the regions of former results, especially those of Hejhal [16].

The completeness was checked by comparison with a generalized Weyl's law which describes the asymptotic behaviour of the spectral staircase ($\lambda = \frac{1}{4} + R^2$)

$$N(\lambda) = \#\{\lambda_j \leq \lambda\}. \quad (37)$$

$N(\lambda)$ can be written as a sum

$$N(\lambda) = N_{\text{mean}}(\lambda) + N_{\text{fluct}}(\lambda) \quad (38)$$

where $N_{\text{mean}}(\lambda)$ is a smooth function which describes a mean value of the number of eigenvalues below λ , and the fluctuating part $N_{\text{fluct}}(\lambda)$ is given by a function that oscillates about zero

$$\lim_{\lambda \rightarrow \infty} \frac{1}{\lambda} \int_0^\lambda N_{\text{fluct}}(s) ds = 0. \quad (39)$$

From Selberg's trace formula one can deduce [24, 27] the Weyl formulae ($\lambda \rightarrow \infty$)

$$N_{\text{mean}}^+(\lambda) = \frac{\lambda}{24} - \frac{3}{4\pi} \sqrt{\lambda} \ln \lambda + \frac{6 + 4 \ln \pi - \ln 2}{4\pi} \sqrt{\lambda} - \frac{13}{144} + \frac{3}{32\pi} \frac{\ln \lambda}{\lambda} + O\left(\frac{1}{\lambda}\right) \quad (40)$$

$$N_{\text{mean}}^-(\lambda) = \frac{\lambda}{24} - \frac{1}{4\pi} \sqrt{\lambda} \ln \lambda - \frac{3 \ln 2 - 2}{4\pi} \sqrt{\lambda} + \frac{23}{144} + \frac{1}{32\pi} \frac{\ln \lambda}{\lambda} + O\left(\frac{1}{\lambda}\right) \quad (41)$$

where the upper indices indicate the parity. Figure 1 shows the numerical analogue to N_{fluct} ,

$$\delta_n = N_{\text{mean}}(\lambda_n) - [N(\lambda_n) - 1/2], \quad (42)$$

indicating the oscillatory behaviour about 0. As an example we took the first 1000 eigenvalues of even parity. The bracket in (42) is equal to $n - 1/2$ which is the middle of the step at the n -th eigenvalue (if the spectrum is simple). If an eigenvalue λ_N is missing, all subsequent $n \geq N$ are underestimated by 1. Accordingly, δ_n is shifted by 1 for all $n \geq N$. By searching eigenvalues around such jumps we have completed our list. It should be noted that $N_{\text{mean}}(\lambda)$ describes the mean very well from the very beginning, in spite of its asymptotic character.

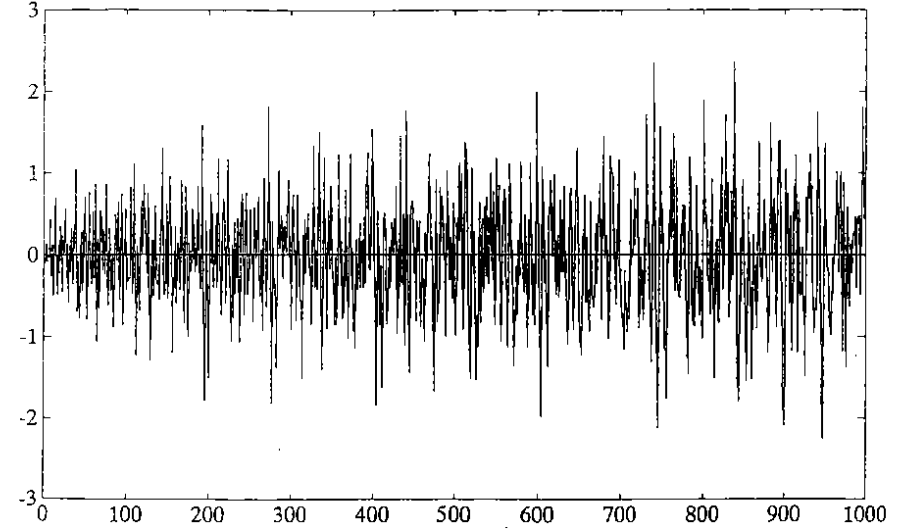


Figure 1: Difference δ_n of the spectral staircase $N(\lambda)$ to Weyl's law for the first 1000 even eigenvalues λ_n as a function of n .

6 Eigenvalues of the Hecke operators

It is known that the eigenvalues of the Hecke operators, i.e. the Fourier coefficients of the normalized cusp forms, obey the bounds [32, 40]

$$|c_p| \leq 2(p^{1/5} + p^{-1/5}), \quad (43)$$

$$|c_p| \leq 2p^{1/4}, \quad (44)$$

a fact we have been exploiting in the algorithm. From a number theoretical point of view the first estimate is the better one because of the smaller exponent but the second one delivers smaller numerical bounds for moderate p . The Ramanujan-Petersson conjecture asserts an improvement to

$$|c_p| \leq 2. \quad (45)$$

All about 320000 prime coefficients we know agree with this conjecture, being so far the most extensive (numerical) test.

Table 2 exhibits as a reference eigenvalues of the Hecke operators for a large even R . This is equivalent to the numerical knowledge of the corresponding eigenfunction.

We turn now to statistical properties of the c_p 's. A result of Sarnak [32] shows that not too much coefficients can violate the Ramanujan–Petersson conjecture: Consider the sequence $(c_p^j)_{j \in \mathbb{N}}$, p prime, of coefficients with fixed index and ordered by increasing corresponding eigenvalues. Then they are equidistributed with respect to

$$d\mu_p(x) = \begin{cases} \frac{(p+1)\sqrt{4-x^2}dx}{2\pi[(p^{1/2}+p^{-1/2})^2-x^2]}, & |x| < 2 \\ 0, & \text{otherwise.} \end{cases} \quad (46)$$

Equidistribution of a sequence $(x_j)_{j \in \mathbb{N}} \subset \mathbb{R}$ with respect to $d\lambda$ means

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n f(x_j) = \int_{\mathbb{R}} f(x) d\lambda(x) \quad \text{for all } f \in C_c(\mathbb{R}). \quad (47)$$

The densities $d\mu_p(x)$ are by no means trivial and show a strong dependence upon p for small values of p . This delivers an additional overall test of the correctness of our results. Figure 3 compares the distribution of the numerically given coefficients with the prediction for a couple of p 's. One recognizes a good agreement.

As $p \rightarrow \infty$, $d\mu_p(x)$ converges to the so-called semicircle distribution

$$d\mu(x) = \begin{cases} \frac{1}{2\pi} \sqrt{4-x^2} dx, & |x| < 2 \\ 0, & \text{otherwise.} \end{cases} \quad (48)$$

The question arises if one is allowed to reverse the limits $j \rightarrow \infty$ and $p \rightarrow \infty$ in considering $(c_p^j)_{j \in \mathbb{N}, p \in \mathbb{P}}$. If this were the case the so-called Sato–Tate conjecture would be true which states that the prime coefficients of a single cusp form $(c_p^j)_{p \in \mathbb{P}}$ are equidistributed with respect to $d\mu$. Since this conjecture is unproved it is interesting to get some numerical hints on its validity. First studies in this direction were done in [17] where the respective first five even and odd cusp forms and two even ones of larger eigenvalue ($R = 47.9^+$, $R = 125.31^+$) are considered. With the exception of the last one, all corresponding c_p 's with $p < 10000$ have been computed whose number is 1229. To improve the statistical significance we have done similar computations including more coefficients and larger R . The examples are listed in table 6. Figure 2 shows the numerical data together with

	R	parity	# c_p	$p \leq$
a.	9.533695261354	odd	30000	350377
b.	13.77975135189	even	"	"
c.	99.86259201648	even	"	"
d.	249.9355630821	even	"	"
e.	502.0222609522	odd	10000	104729
f.	aggregation of a. to e.		130000	

Table 6: Eigenvalues for which the Sato–Tate conjecture is checked in figure 2.

the semicircle law. The agreement is very good and a clear confirmation of the Sato–Tate conjecture.

The method at hand is to take (24) as an explicit equation for c_p whenever p exceeds the truncation index N of the Fourier series (20), as proposed in [36]. The crucial point is the increasing computing time as R and p get large since each c_p requires an effort of about $\frac{1}{2}Np$ Bessel function evaluations. Here, a factor of $\frac{1}{2}$ is introduced due to the fact that one can restrict the evaluations to those arguments for which $2\pi ny_j^p < x_{\max}$. The points y_j^p are assumed to be randomly distributed over the modular domain with respect to dz as $p \rightarrow \infty$ [36], and for that reason $n = N$ is only needed for the lowest lying points in \mathcal{F} . To save cpu time it is best first to tabulate the Bessel function in the whole needed range of its argument and then to compute it by means of a simple interpolation.

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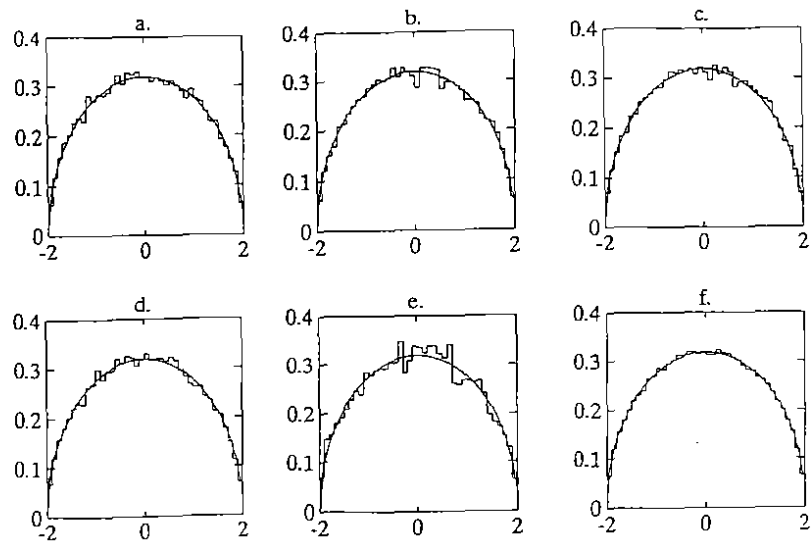


Figure 2: Distribution of prime coefficients (Hecke eigenvalues) of certain cusp forms in comparison to the semicircle law as predicted by the Sato-Tate conjecture. The small letters correspond to table 6.

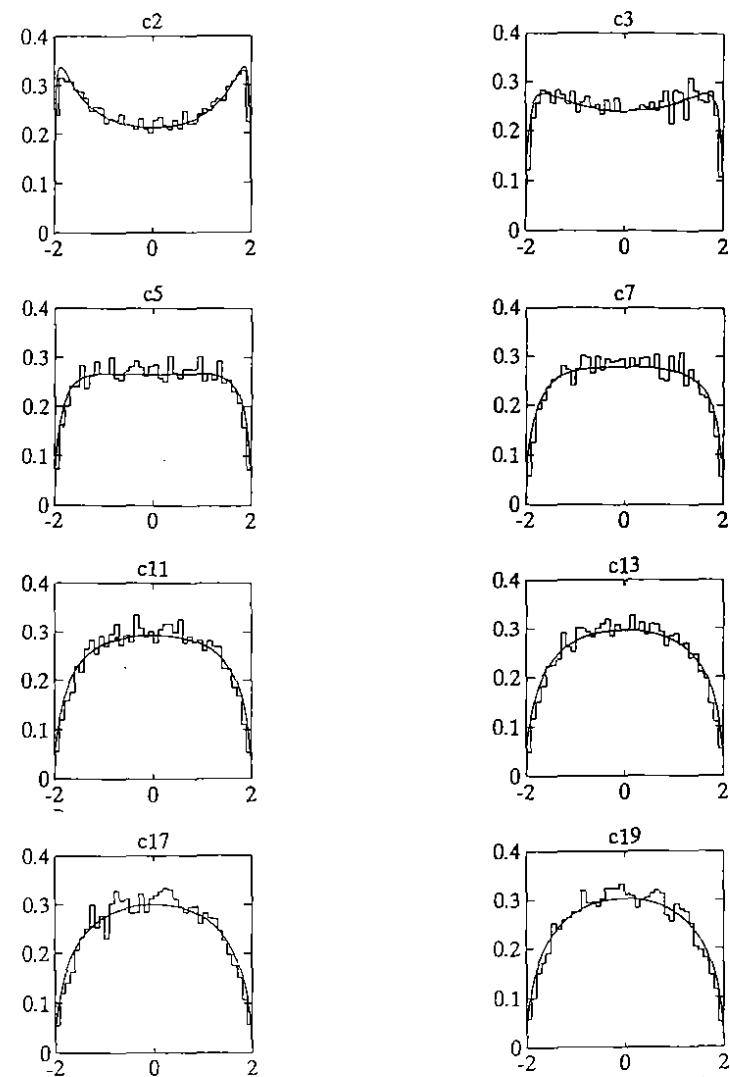


Figure 3: Collected c_p 's of cusp forms with $R < 350$ in comparison with the asymptotic distributions (46).

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