## **ON FOURIER COEFFICIENTS OF MAASS WAVEFORMS FOR** PSL(2, $\mathbb{Z}$ )

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Dedicated to the memory of D. H. Lehmer

ABSTRACT. In this paper, we use machine experiments to test the validity of the Sato-Tate conjecture for Maass waveforms on  $PSL(2, \mathbb{Z}) \setminus H$ . We also elaborate on Stark's iterative method for calculating the Fourier coefficients of such forms.

#### 1. INTRODUCTORY REMARKS

Around 20 years ago, D. H. Lehmer [19] empirically investigated the extent to which the numbers  $\xi_p \equiv \tau(p) p^{-11/2}$  obey Sato-Tate statistics as  $p \to \infty$ . Here,  $\tau(n)$  is the usual Ramanujan tau-function<sup>1</sup> and the proposed statistics assert that

(1.1) 
$$\lim_{x \to \infty} \frac{N[p \le x : \theta_p \in E]}{\pi(x)} = \frac{2}{\pi} \int_E \sin^2 \theta \, d\theta$$

for  $\xi_p = 2\cos(\theta_p)$  and any Jordan measurable  $E \subseteq [0, \pi]$ .  $[\pi(x)]$  is the usual counting function for the primes.]

The corresponding assertion for  $\xi_p$  itself will then read:

(1.2) 
$$\lim_{x \to \infty} \frac{N[p \le x : \xi_p \in E]}{\pi(x)} = \frac{1}{2\pi} \int_E \sqrt{4 - \xi^2} \, d\xi$$

for  $E \subseteq [-2, 2]$ . In this form, the proposed distribution coincides with the so-called Wigner semicircle law familiar from the study of spectra of random Hermitian matrices (cf. [1, 2, 21, 22, 29, 36] for the proper perspective).

Lehmer looked at  $\xi_p$  for p < 10000 and found fairly good agreement with (1.1)-(1.2). Such agreement is important partly because of Serre's observation that (1.1) would follow, not only for  $\Delta$ , but also for more general automorphic representations  $\pi$  on  $GL_2(\mathbb{A})$ , anytime the Langlands L-functions  $L(s, \operatorname{Sym}^k)$ of the symmetric powers of  $\pi$  have good holomorphy properties on  $\{\text{Re}(s) \geq 1\}$ (cf. [33, 37, 18] and, more recently, [4, 7, 25, 27, 28]). (Any exceptional cases should reduce to [10].)

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The first author was partially supported by NSF Grant DMS 89-10744 with computer time from the Minnesota Supercomputer Institute (CRAY2), Pittsburgh Supercomputing Center (YMP832), and Supercomputing Research Center (CRAY2). <sup>1</sup>Associated with  $\Delta(z) = e^{2\pi i z} \prod_{n=1}^{\infty} (1 - e^{2\pi i n z})^{24}$ .

An *alternative* way of suggesting that (1.2) typically holds was recently found by Sarnak [31]. His method, which is *un*conditional, rests on taking a kind of average over  $\pi$  and exploits the Selberg trace formalism for PSL(2,  $\mathbb{Z}$ ) à la [11, 12, 32]. One finds an interesting interplay between p and  $\pi$  (cf. [3] for some related ideas).

Our primary objective in this paper is to extend [19] to the case of Maass waveforms. We will do this by making an empirical test of (1.1)-(1.2) [and equation (1.5) below] in a variety of cases wherein  $\pi$  corresponds to a run-of-the-mill Maass waveform of weight zero on PSL(2,  $\mathbb{Z}$ )\H. (The observation of Serre will thus apply.)

In classical terms, we propose to study functions

(1.3) 
$$\varphi(z) = \sum_{n=1}^{\infty} c_n y^{1/2} K_{iR}(2\pi n y) \left\{ \frac{\cos(2\pi n x)}{\sin(2\pi n x)} \right\}$$

on  $PSL(2, \mathbb{Z}) \setminus H$  such that [12, 20, 34]

(1.4<sub>a</sub>) 
$$\varphi(Tz) = \varphi(z)$$
 for  $T \in PSL(2, \mathbb{Z})$ ,

(1.4<sub>b</sub>) 
$$y^2(\varphi_{xx} + \varphi_{yy}) + (\frac{1}{4} + R^2)\varphi = 0$$
 for  $z \in H$ ,

(1.4<sub>c</sub>) 
$$\sum_{n=1}^{\infty} \frac{c_n}{n^s} = \prod_p \frac{1}{1 - c_p p^{-s} + p^{-2s}} \quad \text{for } s \gg 1,$$

and shall seek to prepare extensive lists of  $c_p$ -values, whose statistics we shall then proceed to analyze directly.

For  $\varphi$  of this type, the analog of the Ramanujan-Petersson conjecture asserts that

$$(1.5) |c_p| \le 2$$

This estimate remains unproved. The best (unconditional) estimate presently available (1991) says that

$$(1.6) |c_p| \le p^{1/5} + p^{-1/5}$$

(cf. [4, 7, 24, 26]). (See [27, Theorem 4] and [25, pp. 436-438, 433 (Theorem 4)] for several improvements of a probabilistic nature.)

Before continuing, it should be stressed that implementation of the proposed empirical test of (1.5) and (1.1) is by no means trivial.

In fact, until fairly recently, there were *major* difficulties associated with computing the eigenvalues  $\frac{1}{4} + R_k^2$  themselves, particularly when  $R_k$  exceeded 25 or so. Even in smaller cases, computing  $c_p$  for p > 7 (!) seemed very problematic.

Part of these difficulties were successfully addressed in [14, 15]. Indeed, it is now possible to reliably determine<sup>2</sup> not only the eigenvalue, but also the first few Fourier coefficients  $c_n$  in (1.3) for *R*-values ranging out to 500 or so. The number of "good" coefficients scales something like  $2 + \frac{1}{4}R$ . (See [12, Appendix C] for a glimpse of the situation prior to [14, 15].)

Having reached this stage, the next step is obviously one of "refining things" so as to allow the systematic computation of significantly larger numbers of  $c_p$ -values (for each  $R_k$ ).

246

<sup>&</sup>lt;sup>2</sup>To 5 or more places.

Currently, the only published work in this direction is that of Stark [35]. Though very suggestive, Stark's technique suffers from three drawbacks:

(A) the method was tested only for relatively small *R*-values (compare [12, p. 729]);

(B) Stark's subroutine for  $K_{iR}(X)$  needs to be applied outside its demonstrated region of validity [35, p. 266, paragraph 3];

(C) the method does not seem to include sufficient internal checks on the accuracy of the computed  $c_p$ -values, particularly for larger p (cf. [35, pp. 266 (bottom), 268 (middle)]).

In order to develop a "firmer"  $c_p$ -algorithm, we therefore decided to make our own investigation of Stark's main idea (focussing, in particular, on any subtleties that occurred).

Sections 4 and 5 will contain a brief report on the outcome of our experiments —plus a general description of the (production) algorithm that we ultimately implemented.

Prior to that time, we will simply proceed as if there were no major problems expanding Stark's original idea into *some* type of algorithm capable of computing both  $R_k$  and the first  $\pi(10^4)$   $c_p$ 's out to 9–10 places. This possibility was alluded to in [35, pp. 268 (middle), 266 (top)].

Incidentally: to help get the main iteration started, it is understood that one may need to use the data in [14] or [15, Chapter 2] as an 0-order approximation (for each  $R_k$  that we consider). Compare [35, p. 266 (lines 5–8)].

## 2. Concerning Hecke operators

Recall that  $\varphi$  satisfies  $(1.4_a)-(1.4_c)$ . Condition (c) is just another way of saying that

(2.1) 
$$T_n[\varphi] = c_n \varphi,$$

where  $T_n$  is the familiar Hecke operator

(2.2) 
$$T_n[f] \equiv \frac{1}{\sqrt{n}} \sum_{\substack{ad=n \\ d>0}} \sum_{0 \le b < d} f\left(\frac{az+b}{d}\right) \text{ on } \mathrm{PSL}(2, \mathbb{Z}) \setminus H$$

(cf. [34] or [23] modulo a slight change in normalization). This fact is largely a reflection of the basic multiplicative property of  $T_n$ ; i.e.,

(2.3) 
$$T_n T_m = \sum_{d \mid (m, n)} T_{nm/d^2}.$$

In particular, one checks that

(2.4) 
$$c_n c_m = \sum_{d \mid (m, n)} c_{nm/d^2}$$

The identities implicit in (2.4) are very important and need to be constantly kept in mind in what follows. Note, for instance, that

$$c(mn) = c(m)c(n) \text{ for } (m, n) = 1,$$
  

$$c(p^2) = c(p)^2 - 1,$$
  

$$c(p^3) = c(p)^3 - 2c(p),$$
  

$$c(p^4) = c(p)^4 - 3c(p)^2 + 1,$$
  

$$c(p^5) = c(p)^5 - 4c(p)^3 + 3c(p).$$

When one is "sitting" exactly on  $\varphi$ , equation (2.4) holds perfectly. In numerical work, however, there are always errors in R and  $c_n$  to contend with.

To pave the way for our later discussion in  $\S$  4–5, it is helpful to use a simple (but loose) example to illustrate how the relations embodied in (2.4) can be turned around to help one "zero in" on the correct data for  $\varphi$ .

To start with, we assume that R is known at least approximately (say from [14]). In the Fourier expansion (1.3), we suppose that the "harmonics" with n > N contribute terms of (relative) order  $10^{-14}$  at most, at least for  $y \ge \frac{1}{2}\sqrt{3}$ .

[As usual in this business, it is helpful to renormalize any  $K_{iR}(X)$  terms by multiplying through by  $\exp(\frac{\pi}{2}R)$ . We tacitly assume this has been done. We also let  $\mathscr{F}$  represent the standard fundamental polygon for  $PSL(2, \mathbb{Z})\setminus H$ .]

Fundamental to Stark's method is a certain nonlinear system of equations in  $\{c_2, c_3, \ldots, c_N\}^3$ , which one seeks to solve by iteration. (This is where an approximate knowledge of  $c_2, c_3, \ldots, c_N$  comes in handy.) The system  $(\mathscr{S})$  has R as an input parameter and is (essentially) obtained from (2.1) by neglecting those terms in (1.3) deemed to have order less than  $10^{-14}$  on  $\mathscr{F}$ (cf. [35, pp. 265 (line 22), 266 (lines 5-8)]).

To the extent there are errors in R, there will be corresponding uncertainties in  $c_2, c_3, \ldots, c_N$ .

For the sake of argument, suppose that  $17 \le N \le 32$  (say).

Our method for "zeroing in" on the correct  $\varphi$ -data basically consists of little more than minimizing some functional like

(2.5) 
$$\max[|c(33) - c(3)c(11)|, |c(34) - c(2)c(17)|, |c(35) - c(5)c(7)|]$$

with respect to R. Here, since N < 33, one needs to explain precisely what is meant by c(33), c(34), c(35). These numbers are simply auxiliary functions of the solution data  $\{c_2, c_3, \ldots, c_N\}$ , which are obtained by *rewriting* (2.1) as

(2.6) 
$$c_n = \frac{T_n[\varphi](z_0)}{T_1[\varphi](z_0)}$$

and then substituting a suitable value for  $z_0$ . In each case,  $\varphi$  is understood to be truncated after n = N, and the relevant points in (2.2) "tossed back over" to within  $\mathscr{F}$ .

To the extent that (2.5) can be "brought down" to something like  $10^{-14}$ , one is inclined to suspect that  $R_{\text{critical}}$  must be very close to the true eigenvalue (i.e.,  $R_k$ ). [At a random R, there is simply no a priori reason for c(33) to be exactly  $c(3) \cdot c(11)$ . Accidents do occur, but a simultaneous accident at 33, 34, 35 is well nigh impossible!]

Once a successful "minimization" has been achieved, the  $c_p$ -values for p > N are then determined by repeating the procedure used for c(33), c(34), c(35).

This is the story in a nutshell.

As N and R grow, one naturally needs to employ different composite n's in (2.5). It is in the use of *such* n that our approach differs (most significantly) from that of Stark [35].

Incidentally: in (2.6), note that varying  $z_0$  furnishes an additional check on any proposed  $\varphi$ -data.

<sup>3</sup>Call it  $(\mathcal{S})$ .

For later use, we remark that

(2.7) 
$$L(s) = \sum_{n=1}^{\infty} \frac{c_n}{n^s} = \prod_p \frac{1}{1 - c_p p^{-s} + p^{-2s}}$$

is actually an entire function satisfying

(2.8) 
$$G(s)L(s) = \eta G(1-s)L(1-s),$$

where

$$\begin{cases} \eta = +1, \ G(s) = \pi^{-s} \Gamma\left(\frac{s+iR}{2}\right) \Gamma\left(\frac{s-iR}{2}\right) & \text{for even } \varphi, \\ \eta = -1, \ G(s) = \pi^{-s} \Gamma\left(\frac{s+1+iR}{2}\right) \Gamma\left(\frac{s+1-iR}{2}\right) & \text{for odd } \varphi. \end{cases}$$

The proof is a standard application of Mellin transforms to (1.3) and (1.4). One exploits [38, p. 388(8)] along the way.

## 3. STATEMENT OF RESULTS

Our primary goal was to study the first five even and odd Maass waveforms on  $PSL(2, \mathbb{Z}) \setminus H$ , as accurately as possible, for p ranging out to 10000.

Since the K-Bessel routine in [14] has an intrinsic accuracy of about 11-12 places (for  $R \leq 100$ ), one would naively expect problems to occur if we tried to obtain *more* than this number of places in R and  $c_p$ . In fact, since  $c_p$  is determined using (2.6), it is clear that the accuracy must gradually begin to taper off as p grows (due to the increasing amount of roundoff error in the numerator). In line with this, we made a very slight change in the procedure outlined in §2; viz., we replaced  $10^{-14}$  by  $10^{-12}$ .

In addition to testing the first five even and odd  $R_k$ 's, we thought it would be interesting to see if our method could still be applied successfully in a couple of cases with somewhat larger R. For this purpose, we chose two *even* values; one near R = 50, the other near 125.

The total number of production runs was thus 12.

In this connection, however, it should be stressed that the production stage is reached only *after*  $c_2, c_3, \ldots, c_N$ , R are computed to sufficient accuracy. Achieving this, basically requires a *number* of test runs, each aimed at trying to "successfully" minimize (2.5) through a sequence of steps reminiscent of regula falsi. [Ultimately achieving the desired accuracy is not a foregone conclusion, since system ( $\mathscr{S}$ ) tends to become rather sensitive as R increases. Suffice it to say, though, that the only place a little persistence was really needed was with the two larger R. Further details can be found in §4.]

The *R*-values we used to get the whole process started were taken from [14] and read as in Table 1 (next page). To speed things up in solving  $(\mathcal{S})$ , we did not hesitate to use the approximate values of the first few  $c_n$  found in [14] or [12, Appendix C]. We mentioned this point earlier in §1.

For the production runs, we then used Table 2 (next page).

In each case, our tests with the analog of (2.5) suggested that the indicated

249

TABLE 1						
A	13.779751	Η	9.533695			
B	17.738563	Ι	12.173008			
C	19.423481	J	14.358509			
D	21.315796	K	16.138073			
E	22.785909	L	16.644259			
F	47.926558					
G	125.313840					
even			odd			

TABLE 2

case	R	N	p < x	$\pi(X)$
A	13.7797513518907	9	p < 10000	1229
B	17.7385633810580	9	p < 10000	1229
С	19.423481470828	10	p < 10000	1229
D	21.3157959402041	10	p < 10000	1229
E	22.785908494190	10	<i>p</i> < 10000	1229
F	47.926558330595	20	p < 10000	1229
G	125.3138401770	32	<i>p</i> < 5000	669
Н	9.5336952613536	9	<i>p</i> < 10000	1229
Ι	12.1730083246801	9	p < 10000	1229
J	14.358509518259	9	p < 10000	1229
K	16.138073171521	9	p < 10000	1229
L	16.6442592018999	9	p < 10000	1229

*R*-value should be accurate to within

 $\begin{cases} 3 \times 10^{-13}, & \text{if 13 places are shown,} \\ 2 \times 10^{-12}, & \text{if 12 places are shown and } R < 23, \\ 3 \times 10^{-12}, & \text{in case F}, \\ 2 \times 10^{-10}, & \text{in case G}. \end{cases}$ 

Tables of  $c_p$ -values were then prepared. Our spot checks (using both composite *n* and variation of  $z_0$ ) suggest that the accuracy we obtained is quite good: 9-10 places initially, dropping off to 8-9 for *p* around *X*. (Incidentally: there was generally 9-10 place agreement between [35, Table 1] and case A.)

In no instance were any counterexamples to Ramanujan-Petersson detected.

Readers interested in scanning the actual  $c_p$ -values should refer to the Supplemental Listing available directly from the authors.

On the matter of "extreme" values, Table 3 holds. These values should be compared with the numbers found by D. H. Lehmer for  $\tau(p)$ :

$$\max_{p \le 10^4} |\xi_p| = 1.961, \qquad \min_{p \le 10^4} |\xi_p| = .00062.$$

Finally, to check (1.1) and (1.2), we made some histograms [using the values contained in the Supplemental Listing]. These are included as Figures 1-6 in the Supplement section at the end of the issue. We are grateful to Andrew Odlyzko for his assistance with this.

Α	c(8317) = 1.984	c(9539) = .000540	
	c(7687) = -1.987	c(97) =003257	
В	c(4217) = 1.984	c(7583) = .000637	
	c(7451) = -1.962	c(8329) =000357	
C	c(2699) = 1.969	c(4703) = .000576	
	c(8543) = -1.980	c(6277) =004243	
D	c(1201) = 1.973	c(1741) = .001437	
	c(8233) = -1.951	c(9539) =000048	
E	c(6599) = 1.997	c(6043) = .005829	
	c(7451) = -1.978	c(727) =002484	
F	c(8629) = 1.990	c(2903) = .002581	
	c(4217) = -1.991	c(2953) =001902	
0	a( 121) 1044	(1201) 001100	5000 1
G	c(131) = 1.944	c(1381) = .001109	p < 5000 only
G	$\begin{array}{c} c(131) = 1.944 \\ c(3347) = -1.958 \end{array}$	c(1381) = .001109 $c(1451) =006469$	p < 5000 only
H	$\begin{array}{l} c(131) = 1.944 \\ c(3347) = -1.958 \\ c(3457) = 1.998 \end{array}$	$\begin{array}{l} c(1381) = .001109\\ c(1451) =006469\\ c(5953) = .003227 \end{array}$	<i>p</i> < 5000 only
H	$\begin{array}{c} c(131) = 1.944 \\ c(3347) = -1.958 \\ c(3457) = 1.998 \\ c(1277) = -1.987 \end{array}$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615	<i>p</i> < 5000 only
H I	$\begin{array}{l} c(131) = 1.944 \\ c(3347) = -1.958 \\ c(3457) = 1.998 \\ c(1277) = -1.987 \\ c(7517) = 1.993 \end{array}$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142	<i>p</i> < 5000 only
H I	c(131) = 1.944 $c(3347) = -1.958$ $c(3457) = 1.998$ $c(1277) = -1.987$ $c(7517) = 1.993$ $c(5501) = -1.988$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142 c(601) =000066	<i>p</i> < 5000 only
H I J	$\begin{array}{l} c(131) = 1.944\\ c(3347) = -1.958\\ c(3457) = 1.998\\ c(1277) = -1.987\\ c(7517) = 1.993\\ c(5501) = -1.988\\ c(7309) = 1.963 \end{array}$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142 c(601) =000066 c(5009) = .006958	<i>p</i> < 5000 only
H I J	c(131) = 1.944 $c(3347) = -1.958$ $c(3457) = 1.998$ $c(1277) = -1.987$ $c(7517) = 1.993$ $c(5501) = -1.988$ $c(7309) = 1.963$ $c(4561) = -1.945$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142 c(601) =000066 c(5009) = .006958 c(7411) =000487	<i>p</i> < 5000 only
H I J K	$\begin{array}{l} c(131) = 1.944\\ c(3347) = -1.958\\ c(3457) = 1.998\\ c(1277) = -1.987\\ c(7517) = 1.993\\ c(5501) = -1.988\\ c(7309) = 1.963\\ c(4561) = -1.945\\ c(8837) = 1.993 \end{array}$	c(1381) = .001109 $c(1451) =006469$ $c(5953) = .003227$ $c(3121) =000615$ $c(709) = .001142$ $c(601) =000066$ $c(5009) = .006958$ $c(7411) =000487$ $c(2311) = .002891$	<i>p</i> < 5000 only
H I J K	c(131) = 1.944 $c(3347) = -1.958$ $c(3457) = 1.998$ $c(1277) = -1.987$ $c(7517) = 1.993$ $c(5501) = -1.988$ $c(7309) = 1.963$ $c(4561) = -1.945$ $c(8837) = 1.993$ $c(9539) = -1.914$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142 c(601) =000066 c(5009) = .006958 c(7411) =000487 c(2311) = .002891 c(7583) =002180	<i>p</i> < 5000 only
H I J K L	c(131) = 1.944 $c(3347) = -1.958$ $c(3457) = 1.998$ $c(1277) = -1.987$ $c(7517) = 1.993$ $c(5501) = -1.988$ $c(7309) = 1.963$ $c(4561) = -1.945$ $c(8837) = 1.993$ $c(9539) = -1.914$ $c(1259) = 1.977$	c(1381) = .001109 c(1451) =006469 c(5953) = .003227 c(3121) =000615 c(709) = .001142 c(601) =000066 c(5009) = .006958 c(7411) =000487 c(2311) = .002891 c(7583) =002180 c(8933) = .000010	<i>p</i> < 5000 only

TABLE 3

The agreement with (1.1), (1.2) certainly seems reasonable.

Out of curiosity, we also tested the *individual* R-values (but on somewhat coarser scales). This gave the results illustrated in Figures 7–18 of the Supplement.

In all cases, the agreement (still) seems fairly good.

The obvious question now is why can't we do  $p < 10^5$ , or maybe even  $p < 10^6$ ?

To address this point, we need to first look at the CPU times for our production runs (Table 4 on next page). Since these jobs typically included spot checks at about a half a dozen composite n as well,<sup>4</sup> the *actual* time (for obtaining just the  $c_p$ ) will be about 10%–15% less.

CPU times in the range of  $1\frac{1}{2}-6\frac{1}{2}$  hours are, of course, nontrivial.

The key issue then is how things scale with respect to X (and R).

The asymptotics of  $\exp(\frac{\pi}{2}R)K_{iR}(v)$  are known from [5], say. These asymptotics and the shape of  $\mathscr{F}$  make it clear that N must scale something like (constant)R. In determining  $c_p$  by means of (2.6), approximately N(p+1) [independent] K-Bessel calls will be needed. To tabulate  $c_p$  for all  $p \leq X$  will

<sup>&</sup>lt;sup>4</sup>The form of these *n* being either 5p or 13p.

0000	machine	time (in secs)	V
Lase	machine	time (in secs.)	
A	Cray2	10103	10000
В	YMP	8151	10000
C	Cray2	12631	10000
D	Cray2	13454	10000
Е	Cray2	14039	10000
F	YMP	25718	10000
G	YMP	11791	5000
Η	YMP	5812	10000
Ι	YMP	6861	10000
J	YMP	7441	10000
K	YMP	7820	10000
L	YMP	7887	10000

TABLE 4

therefore require about

$$N\sum_{p \le X} (p+1) \approx \frac{N}{2} \frac{X^2}{\log X} \approx (\text{constant}) R \frac{X^2}{\log X}$$

calls.<sup>5</sup> The essential point is the occurrence of  $X^2/(\log X)$ . Unless the K-Bessel calls can somehow be speeded up, raising X by a factor of 10 is going to cause the CPU time to go up by something closer to 100. (Expressed differently: two hours of CRAY time is one thing, 200 is another!)

It is here, with the K-Bessel calls, that some major improvement (or restructuring) seems essential for further progress.

The routine that we used was simply that of [14, 15]. (We wanted to use something well tested!) Though highly stable, this routine requires Gaussian quadrature and a deformation of path. [Typical CPU time: .00012 secs.]

Iterative techniques, or asymptotic expansions, may offer some better possibilities (at least in certain ranges). Another idea worth exploring would be interpolation.

## 4. The basic algorithm in greater detail

Let  $g(t) = \sqrt{t^2 - 1} + \arcsin(1/t)$  for  $t \ge 1$ . In line with [5], one knows that  $\exp(\frac{\pi}{2}R)K_{iR}(v)$  behaves something like  $e^{-R[g(v/R) - \pi/2]}$  for v > R. It is therefore possible to determine relatively easily how big v must be in order to guarantee that  $\exp(\frac{\pi}{2}R)K_{iR}(v)$  will be less than  $10^{-14}$  (say). When  $v = 2\pi ny$ , as in (1.3), this typically translates into a condition on n of the form

$$n>\frac{R+\mu R^{1/3}}{2\pi v}\,,$$

where  $\mu$  is some modest constant. [For large *R*, the constant  $\mu$  is about 12.] If *y* is known to be at least  $\frac{1}{2}\sqrt{3}$ , taking

(4.1) 
$$n > \frac{R + \mu R^{1/3}}{\pi \sqrt{3}}$$

<sup>&</sup>lt;sup>5</sup>To be completely correct, these calls should be subdivided into cases  $v \ll R$ ,  $v \approx R$ ,  $v \gg R$ . For fixed R, the relative proportion of each type remains relatively constant as  $X \to \infty$ . (Calls with  $v \ll R$  take the most time...)

will then accomplish exactly what was asked for in §2 with regard to N. (Similarly for  $10^{-12}$ , as used in §3.)

As a temporary notation, let  $\hat{z}$  denote the point in  $\mathscr{F}$  which is equivalent to z under the action of PSL(2,  $\mathbb{Z}$ ).<sup>6</sup>

In our earlier discussion, system  $(\mathscr{S})$  was intentionally kept a bit vague. This was done partly to avoid mentioning that several variants are, in fact, possible.

To see this, suppose for a moment that  $R = R_k$  is known.

One way of getting a system of equations for  $\{c_2, c_3, \ldots, c_N\}$  is obvious. Simply rewrite (2.1) as (2.6) and then insist that, in forming  $T_l[\varphi](z_0)$  according to (2.2), the points  $(az_0 + b)/d$  are all given hats. Follow this by replacing  $\varphi$  with its truncation after N terms. The resulting system will then make sense for any R (and will clearly depend on both R and  $z_0$ ). We will refer to  $z_0$  as the test point.

To the extent that the denominator remains bounded away from 0, one would expect to see (at  $R = R_k$ ) a final accuracy roughly commensurate with the choice of N (cf. (1.5) and (1.6)). Letting the denominator go to 0, however, tends to reduce this accuracy by causing *catastrophic* cancellation in the numerator. [Bear in mind here that the early K-Bessel terms are roughly O(1) in size and only accurate to about 11–12 places.]<sup>7</sup> For this reason, some care in the choice of  $z_0$  is definitely necessary.

An alternative system can be obtained by using (2.4) to re-express any  $c_l$  with composite  $l \leq N$  as a polynomial in the  $c_p$ 's (with  $p \leq N$ ). One then considers (2.6) for prime  $n \ (\leq N)$  only. This is basically what Stark does (cf. [35, p. 266 (paragraph 1)]).<sup>8</sup>

This "smaller" system seems especially appropriate on  $PSL(2, \mathbb{Z}) \setminus H$ .

In either case, the final format of our system will be

$$\mathbf{c} = T(\mathbf{c}),$$

where **c** is a point in  $\mathbb{R}^M$ ,

(4.3) 
$$M = \left\{ \frac{N-1}{\pi(N)} \right\},$$

and the component functions  $T_i$  of T are all rational.

Anytime one tries to solve a nonlinear equation like (4.2) by iteration, strange things can happen. One need only examine some of the recent literature on dynamical systems to be convinced of this.

In the absence of any kind of "hard" information about T, one simply has to expect that:

- (a) there may be multiple solutions;
- (b) the limiting behavior of  $T^n(\mathbf{c}_0)$  as  $n \to \infty$  may depend strongly on the choice of (initial point)  $\mathbf{c}_0$ ;
- (c) to get convergence, one may have to take c<sub>0</sub> rather close to the proposed fixed point;

<sup>&</sup>lt;sup>6</sup>The algorithm for finding  $\hat{z}$  is familiar: one simply does the obvious flip-flop between translation and inversion. Cf. [30, p. 51 (lines 19–27)].

<sup>&</sup>lt;sup>7</sup>Readers unfamiliar with catastrophic cancellation may wish to quickly consult §5, Example 5.

<sup>&</sup>lt;sup>8</sup>In Stark's approach, the denominator  $T_1[\varphi](z_0)$  is left as  $\varphi(z_0)$  and is not replaced by  $\varphi(\hat{z}_0)$ . This is important only if  $z_0 \notin \mathscr{F}$ . Since the (modular) correspondence  $T_l\{z\}$  "lives" on PSL(2,  $\mathbb{Z}$ )\H, our version has the effect of requiring that  $z_0 \in \mathscr{F}$ .

(d) the limiting behavior of  $T^n(\mathbf{c}_0)$  may be significantly affected by small perturbations in T (e.g., movement in  $z_0$ ).

Though the "bigger" system is not without interest, we decided to follow Stark [35] and concentrate solely on the case of  $\pi(N)$ -variables (cf. (4.3)).

One of the advantages to using the CRAY was that its speed allowed us to plot the "trajectories"  $\{T^n(\mathbf{c}_0): n \ge 1\}$  virtually instantaneously.

In the next section, we will present several examples which illustrate points (a)-(d).

The upshot will be that the global situation is not nearly so simple as was suggested in [35].

In cases where  $T^n(\mathbf{c}_0)$  converges, we like to think of the point as having made its way into some type of "attracting basin". The problem is, that as the dimension M grows, it becomes easier for  $T^n(\mathbf{c}_0)$  to get "lost".

In a certain sense: one wants to "help"  $T^n(\mathbf{c}_0)$  find its way (particularly when  $R \approx R_k$ ).

Before explaining how we do this, it should be noted that, in defining the "smaller" system, declaring n = prime at the very last step was a bit arbitrary. Indeed, one can legitimately maintain that

(4.4)  

$$c_{2} = \frac{T_{2}[\varphi](z_{0})}{T_{1}[\varphi](z_{0})}, \qquad c_{2} = \frac{T_{6}[\varphi](z_{0})}{c_{3}T_{1}[\varphi](z_{0})}$$

$$c_{2} = \frac{T_{10}[\varphi](z_{0})}{c_{5}T_{1}[\varphi](z_{0})}, \qquad c_{2} = \frac{T_{14}[\varphi](z_{0})}{c_{7}T_{1}[\varphi](z_{0})}, \text{ etc.}$$

should all be considered on an equal footing.

This adds still another variant to  $(\mathcal{S})$ , and simultaneously supplies us with an important hint.

The point is this. In numerous cases, one knows (from [14]!) the first few  $c_p$ -values for  $\varphi(z)$  out to, say, six decimal places. [We will temporarily refer to these approximate values as  $\hat{c}_2, \hat{c}_3, \ldots, \hat{c}_q$ .] Philosophically speaking, one is inclined to believe that there simply *must* be *some* way of exploiting this knowledge to help keep  $T^n(\mathbf{c}_0)$ 's "nose" pointed in the right direction. (One seeks to impose a kind of potential field.)

In this context, one naturally assumes that any  $c_0$  we start with will have components at least as good as  $\hat{c}_2, \hat{c}_3, \ldots, \hat{c}_q$ . With this in mind, one way of introducing a kind of "restraining force" [to prevent divergence] would be to replace

$$c_2 = \frac{T_2[\varphi](z_0)}{T_1[\varphi](z_0)}$$

in (2.6) by

 $c_2$  = that quotient in (4.4) which lies *closest* to  $\hat{c}_2$ .

This choice suffers, however, from the defect of wanting to pull  $c_2$  too much in the direction of  $\hat{c}_2$  (which is, after all, *not* the exact answer). To rectify this, it seems better to "sit on the particle itself" and go with:

(4.5) 
$$c_2 =$$
 that quotient in (4.4) which lies *closest* to  $c_2$ .

Note that the right-hand side is, in fact, a legitimate function of c. (This requires a moment's thought!)

254

To prevent "runaways", one can erect a kind of "fence" by taking

(4.6)  $c_2 = \begin{cases} \text{RHS of } (4.5), & \text{if that lies within } \delta \text{ units of } \hat{c}_2, \\ \hat{c}_2, & \text{otherwise.} \end{cases}$ 

Similarly for the other  $c_p$  (with  $p \leq q$ ).

To avoid confusion in what follows, we will let  $(\mathcal{S})$  denote the *original* "smaller" system. The variants associated with (4.5) and (4.6) are then denoted by  $(\mathcal{S}^*)$  and  $(\mathcal{S}^{**})$ .

Once a system has been decided upon, the basic procedure is essentially that outlined in  $\S 2$ .

In practice, one minor irritation with both  $(\mathscr{S}^*)$  and  $(\mathscr{S}^{**})$  is that T is no longer real-analytic [especially with respect to R]. This allows the limiting trajectory to exhibit occasional *non*smooth behavior, which, in turn, can adversely affect the minimization procedure being used in connection with (2.5) (cf. §3, paragraph 5). The problem is basically one of trying to get  $\mathbf{c}_0$  as close as possible to the true coefficient vector (cf. point (c)).

Even when the "pump is primed" with data from [14], the process of computing  $\{R_k, c_2, c_3, \ldots, c_N\}$  to sufficient accuracy can be time-consuming. As R and M grew, it was found to be increasingly difficult to get by with just  $(\mathscr{S})$ . [One would typically try many  $z_0$  and have almost no luck finding the right attracting basin!] To a lesser extent, the same thing happened with  $(\mathscr{S}^*)$ . In order to treat R = 47.926558 and 125.313840, passing to  $(\mathscr{S}^{**})$  seems to be the key.

Even then, depending on the quality of the initial data, great sensitivity with respect to  $z_0$  can still occur. At R = 125.313840, one needed to try something like 20 different test points (before finally achieving success).

To accelerate the process of determining  $\{R_k, c_2, c_3, \ldots, c_N\}$ , we made a slight modification in the approach outlined in §2. Namely: once an approximation better than  $c_0$  became available (from one of our runs), we did not hesitate to use it as the "new"  $c_0$ . These updates were then repeated, as necessary. (We also found it helpful to run a variety of test points simultaneously.)

At some point, it might be useful to implement these ideas in a separate code. For purposes of §3, however, we were content to do everything "by hand".

For simplicity, we decided to use  $\mathscr{S}^{**}$  throughout.

Prior to making the final production run at  $R = R_k$ , we generally liked to run two or three mini-versions (out to p = 103 or so) using significantly different test points. These runs always included six composite n (à la footnote 4) plus a direct calculation of  $T(\mathbf{c}) - \mathbf{c}$ . The case displaying the "best" behavior on these two items was the one we then chose for our full-scale run.

[The mini-runs also provided a further form of "insurance" in that it was always very satisfying to be able to watch the  $c_p$ -values (for p > N) consistently agree to 9–10 places, no matter how disparate the  $z_0$  were!]

#### 5. Some subtleties in the iteration

The task of setting up the production runs for §3 was very instructive. By working interactively through the various steps, one was able to gain important insight into the (dynamical) behavior of  $\mathcal{S}$ ,  $\mathcal{S}^*$ ,  $\mathcal{S}^{**}$ .

In several cases, prompted by what was seen, it was natural to push things a bit further just for their own sake.

Our aim in this section will be to report on *some* of the more interesting things we found (see [16] for a fuller list).

Before doing this, however, we need to preface things with a number of preliminary remarks.

First and foremost: we have not really sought to make any kind of rigorous, all-inclusive analysis of  $\mathcal{S}$ ,  $\mathcal{S}^*$ ,  $\mathcal{S}^{**}$ . Our use of these systems has basically been only as a means to an end. On the matter of rigor, it is the usual story; the computer may suggest (to 12 decimal places!) that T has a fixed point at  $\mathbf{p}$ , but that does not constitute a proof. Accordingly, any phenomena depicted in our examples must<sup>9</sup> technically be regarded as conjectural. We hasten to add, however, that T is basically rational with respect to  $\mathbf{c}$  (cf. (4.3) and (4.4)). This fact, combined with the existence of a variety of very similar examples, leads us to believe (in each instance) that the properties highlighted are, in fact, quite rigorous.

Secondly: it has been more or less implicit in our earlier discussion that, when  $R = R_k$ , the transformation T for case  $(\mathcal{S})$  does have an actual fixed point someplace very close to the  $c_p$ -vector for  $\varphi_k(z)$ . In what follows, we will simply assume that this is so.

[In practice, the only cases which give one pause are those where the prevailing flow pattern seems to be repellent. Here, however, a little numerical differentiation with respect to c will (in all likelihood) suffice to settle the matter. The problem is essentially one of computing the Jacobian matrix of  $T(\mathbf{x}) - \mathbf{x}$ .]

For convenience, we will generally engage in a slight abuse of language and make no distinction between the fixed point and the actual  $\varphi$ -data.

Our third point concerns  $\mathscr{S}^*$  and  $\mathscr{S}^{**}$ . The physical analogies used earlier were intended mainly as motivation. To a large extent, the expressions in (4.5) and (4.6) can only be regarded as ad hoc. The thing to keep in mind, though, at (say)  $R \approx 125$  is that the problem confronting us was basically one of "cautiously groping through the fog" so as to be able to successively improve the accuracy in our  $c_p$ -values (after starting with the partial result found in [14]). We thus tend to see  $\mathscr{S}^{**}$  more as a kind of *device* than anything else [a device which is applied only near  $\varphi_k$  !].

Though successful at R = 125.313840, it was not a case of running it once and then, presto, there was the answer. What was needed was a willingness to test a variety of  $z_0$  and to make updates in  $c_0$  as one moved along. In this connection we often found it helpful to have the machine display the results of the *best* iteration [as measured by (2.5)] and not simply those of the last. (If  $\mathscr{S}^*$  had been used instead, similar remarks would still apply.)

The fourth, and final preliminary, is simply a reminder that the nature of a fixed point **p** is, to a large extent, characterized by the eigenvalues of the Jacobian matrix  $J_T(\mathbf{p})$ . For good convergence, one wants these eigenvalues to have modulus less than 1.

[In specific cases, if worst comes to worst, one can of course seek to calculate  $J_T(\mathbf{c})$  numerically. This is not unreasonable when T is rational.]

To avoid ambiguities below, let  $T_0$  be the *T*-transformation associated with system  $(\mathscr{S})$ .<sup>10</sup>

<sup>&</sup>lt;sup>9</sup>At least for now.

<sup>&</sup>lt;sup>10</sup>Note too that any  $T_0$ -fixed point is automatically one for  $\mathscr{S}^*$  (but not conversely)!

**Example 1.** The following data came from a job of type  $(\mathscr{S}^{**})$  with parameters as shown. The vector  $(c_0(p))$  is accurate to about eight places. On the next level, the *first* c(p)-vector is the answer after 400 iterations (of T). The middle column shows what one then gets after an application of  $T_0$ . The final column lists the difference between the two. (The *largest* difference, i.e., 1.7E-10, will be called the  $T_0$ -indicator.) Incidentally: in this example, the size of the analog of (2.5) was about 4.2E-11.

		Parameters	s for $(4.3)$ and $(4.6)$	
		$N=32,\ M=\pi(N$	$\delta (\delta) = 11, \ \delta = 10^{-4}, \ q = 13$	
R= FOR and CO( CO( CO( CO( CO( CO( CO( CO( CO( CO(	125.3 X= initi 1)= 2)= 3)= 5)= 7)= 11)= 13)= 17)= 19)= 23)= 29)= 31)=	13840177000 ICOU 0.0570000000 Y= al values: 1.000000000000 -0.332695680000 1.056573770000 -0.946096480000 0.324132110000 0.40097140000 0.479453980000 1.254988810000 0.893140170000 1.605561140000 0.856710520000 -0.250878130000	NT: 400 MAX: 400 0.9230000000	
C( CC( CC( CC( CC( CC( CC( CC(	1) = 2) = 3) = 5) = 7) = 11) = 13) = 17) = 19) = 23) = 29) = 31) =	1.0000000000 -0.332695683096 1.056573773111 -0.946096480439 0.324132112930 0.040097144250 0.479453986303 1.254988815396 0.893140180104 1.605561152662 0.856710527884 -0.250878136751	1.00000000000 -0.332695683078 -0 1.056573773281 -0 -0.946096480532 0 0.324132112918 0 0.040097144250 0 0.479453986287 0 1.254988815396 0 0.893140180104 0 1.605561152662 0 0.856710527884 0 -0.250878136751 -0	).0000E+00 ).1845E-10 ).1700E-09 ).9242E-10 ).1231E-10 ).2220E-15 ).1646E-10 ).1421E-13 ).4974E-13 ).7105E-14 ).4619E-13 ).3197E-13

the (2.6) denominator was: .6331E00

With  $(c_0(p))$  accurate to 8 places, one might think that the same job run with  $(\mathscr{S})$  would converge. This did not happen, however. The fact is, after n = 24 or so, the point  $T_0^n(\mathbf{c}_0)$  basically became "lost" (and began to wander aimlessly).

Switching to 11-place  $c_0$ -data made very little difference; 24 just became 29. This shows how sensitive things can be (and provides some indication of the utility of  $\mathscr{S}^{**}$ ).

In both  $\mathscr{S}$ -jobs, there was a steady growth in the size of  $(2.5)^{11}$  prior to things getting completely lost. We are inclined to speculate that the vector

<sup>11</sup>And in the  $T_0$ -indicator.

ITER.	$T_0$ -indicator	(2.5) analog	$T_0$ -indicator	(2.5) analog
100	9.8E-8	7.7E-8	3.7E-3	4.6E-3
400	1.7E-10	4.2E-11	2.1E-10	2.3E-10
800	1.7E-10	4.1E-11	2.1E-10	2.3E-10
	system	S**	system	n <i>S</i> *
	with eight-place $c_0(p)$			

TABLE 5

TABLE	6
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R = 125.313840
$c_{00}(2) = -0.332696$
$c_{00}(3) = 1.056574$
$c_{00}(5) = -0.946097$
$c_{00}(7) = 0.324132$
$c_{00}(11) = 0.040097$
$c_{00}(13) = 0.479454$
$c_{00}(17) = 1.254990$
$c_{00}(19) = 0.893140$
$c_{00}(23) = 1.605562$
$c_{00}(29) = 0.85671$
$c_{00}(31) = -0.25088$

(c(p)) must simply represent some type of *repellent* fixed point for  $T_0$ . [We did not compute  $J_{T_0}(\mathbf{c})$ , however.]

For the original (eight-place)  $c_0(p)$ , system ( $\mathscr{S}^*$ ) yields results very similar to those of ( $\mathscr{S}^{**}$ ), but with less accuracy.

In this connection, Table 5 tells an interesting story.

To give some indication of how much additional accuracy  $(\mathcal{S}^{**})$  ultimately provided, we remark that the *original* data taken from [14] was simply Table 6. [The eight-place vector  $(c_0(p))$  used in Table 5 is update #2.]

Finally, let:

$$\mathscr{A} = \{z_0 \in H : T_0 \text{ has an attractive fixed point} \\ \text{at the } \varphi \text{-data for } R = R_k = 125.3138401770\}$$

Since none of the many  $\mathscr{S}$ -jobs that we ran with  $(c_{00}(p))$ , or with 8–11 place  $(c_0(p))$ , ever managed to converge properly,<sup>12</sup> we suspect that  $\mathscr{A}$  is rather sparse. (It should also be borne in mind here that for 19 earlier choices of  $z_0$ ,  $\mathscr{S}^{**}$  failed to converge properly as well.)

One might also ask, for given  $z_0$  (and, say, R = 125.3138401770), how big a set

$$\mathcal{N}_{z_0} \equiv \left\{ \mathbf{p} \in \mathbb{R}^m \colon \lim_{n \to \infty} T_0^n(\mathbf{p}) \text{ does not exist} \right\}$$

is (cf. our earlier remarks about wandering aimlessly for  $n \ge 24, 29$ ).

<sup>&</sup>lt;sup>12</sup>I.e., to the correct  $\varphi$ -data.

**Example 2.** Passing to  $(\mathcal{S}^*)$  or  $(\mathcal{S}^{**})$  does *not* always yield improved dynamics.

Тур	pe $(\mathscr{S})$	N=20	0, M = 7	$\pi(N) =$	8	
۷=	17.9265583 0 1280000	30590 000 Y=	ICOUNT:	265	MAX:	400
initi	al values	:	0.713			
1)=	1.00000	0000000				
2)=	0.51105	8000000				
3)=	1.70068	1000000	r		ſ	
5)=	-1.35858	3000000	crude	e data		
7)=	0.02892	6000000	from	[14]		
11)=	-0.29554	3000000	h			
13)=	-0.08748	0000000				
17)=	0.00000	0000000				
19)=	0.00000	0000000				
	Typ X= inition 1)= 2)= 3)= 5)= 7)= 11)= 13)= 17)= 19)=	Type (S) 47.9265583 X= 0.1280000 initial values 1)= 1.00000 2)= 0.51105 3)= 1.70068 5)= -1.35858 7)= 0.02892 11)= -0.29554 13)= -0.08748 17)= 0.00000 19)= 0.00000	Type ( $\mathscr{S}$ ) $N = 20$ 47.926558330590X= 0.1280000000 Y=initial values:1)= 1.00000000000002)= 0.5110580000003)= 1.7006810000005)= -1.3585830000007)= 0.02892600000011)= -0.29554300000013)= -0.08748000000017)= 0.00000000000000000000000000000000000	Type ( $\mathscr{S}$ ) $N = 20, M = 7$ 47.926558330590ICOUNT:X=0.1280000000Y=0.719initial values:0.7191)=1.000000000002)=0.5110580000003)=1.7006810000005)=-1.3585830000007)=0.02892600000011)=-0.0874800000013)=-0.0874800000017)=0.00000000000	Type ( $\mathscr{S}$ ) $N = 20, M = \pi(N) =$ 47.926558330590ICOUNT: 265X= 0.1280000000Y= 0.719500000initial values:0.7195000001)= 1.0000000000000.5110580000003)= 1.7006810000000.0289260000005)= -1.358583000000crude data7)= 0.028926000000from [14]11)= -0.0874800000017)= 0.000000000000019)= 0.00000000000000000000000000000000000	Type ( $\mathscr{S}$ ) $N = 20, M = \pi(N) = 8$ 47.926558330590 ICOUNT: 265 MAX: X= 0.1280000000 Y= 0.7195000000 initial values: 1)= 1.00000000000 2)= 0.511058000000 3)= 1.700681000000 5)= -1.358583000000 7)= 0.028926000000 11)= -0.295543000000 13)= -0.087480000000 17)= 0.00000000000000

# (with *attractive* behavior throughout as measured by the successive differences)

$\alpha$	1 \	1 00000000000	1 000000000000	
C (	1)=	T.000000000000	T.00000000000000	0.0000E+00
С(	2)=	0.511058433834	0.511058433833	0.1208E-12
С(	3)=	1.700681262519	1.700681262519	0.7816E-13
С(	5)=	-1.358582751399	-1.358582751399	0.6537E-12
С (	7)=	0.028925945761	0.028925945761	-0.2591E-12
С(	11)=	-0.295544126038	-0.295544126039	0.5276E-12
С(	13)=	-0.087366865379	-0.087366865379	0.3979E-12
С(	17)=	0.937817000442	0.937817000442	0.2878E-12
С(	19)=	1.795503232584	1.795503232584	0.2061E-12

(2.6) denominator was: -.4314E00final value of the (2.5) analog: 5.6E-11  $T_0$ -indicator: 6.5E-13

Even when the iteration count was only about 100, one was finding  $T_0$ -indicators and (2.5) values of about  $10^{-8}$ . There is little doubt that, for this test point, the  $\varphi$ -data is  $T_0$ -attractive.

Surely, then, running  $(\mathscr{S}^*)$  should produce the same answer. Not so!

# Type $(\mathscr{S}^*)$

R=		17.92655833	0590	ICOUNT	: 800	MAX:	800
FOR	X=	0.12800000	00 Y=	= 0.71	1950000	00	
and	init	ial values:					
C0(	1)=	1.000000	000000	)			
C0 (	2)=	0.511058	000000	)			
C0 (	3)=	1.700681	000000	)			
C0(	5)=	-1.358583	000000	)			
C0 (	7)=	0.028926	000000	)			
C0(	11)=	-0.295543	000000	)			
C0(	13)=	-0.087480	000000	)			
C0(	17)=	0.00000	000000	)			
C0 (	19)=	0.00000	000000	)			

#### D. A. HEJHAL AND S. ARNO

## (with repellent behavior before $I \approx 50$ and attractive behavior after $I \approx 120$ as measured by the successive differences)

С (	1)=	1.00000000000	1.000000000000	.000E+00
С(	2)=	0.376415454703	0.885343665274	.533E-14
С (	3)=	1.188036394793	1.337190554675	.000E+00
С(	5)=	-0.820559895739	-1.797243672303	.355E-14
С(	7)=	0.215736965622	0.215736965622	.799E-14
С (	11)=	-1.168200588376	-1.168200588376	.711E-14
С (	13)=	-0.360588849565	-0.360588849565	.355E-14
С (	17)=	0.994237766499	0.994237766499	.142E-13
С (	19)=	1.247090592260	1.247090592260	.711E-14

(2.6) denominator was: -.3023E00largest successive difference: about  $10^{-7}$  at I = 200about  $10^{-12}$  at I = 300

In this batch, we have changed the format so that the third column displays the absolute value of the last *successive* difference. The middle column continues to be the  $T_0$ -image of the first. As the numbers show, things have clearly stabilized (with respect to T) but *not* at a  $T_0$ -fixed point.

So how did  $\mathscr{S}^*$  escape from  $\varphi$ ? The answer would seem to be that, for at least one choice among the various quotients in (4.4), etc., the  $\varphi$ -data is a *repellent* fixed point of rather strong intensity.

Going over to  $\mathscr{S}^{**}$  [with q = 13 and  $\delta = 10^{-3}$ ] did not help. This yielded only a random wandering within a small neighborhood of the true  $\varphi$ -data; hence a divergence. (Note, too, the relevance of the *third* preliminary remark.)

We should also mention that, once  $c_0(p)$  started to differ appreciably from the true  $\varphi$ -data for at least one small p, we were *un*able to come up with a single instance of  $T_0$ -convergence (after  $10^4$  iterations) in over 50 test cases. This illustrates point (c) in §4.<sup>13</sup>

By switching over to X = .234, Y = .7195 and modifying the vector  $(c_0(p))$  with appropriate  $\pm$  signs, it is possible to produce at least two fixed points for  $T_0$  in addition to the fixed point at the  $\varphi$ -data (cf. [16]). The former are presumably attractive; the latter repellent.

In one of the attractive cases, Ramanujan-Petersson is clearly violated. (The behavior reported in [35, pp. 266 (bottom), 268] thus seems to be *atypical*.)

**Example 3.** The following S-data came from some jobs we ran to investigate Stark's assertion [35, p. 266 (lines 9–11)] that, for small R, it is possible to start literally from nothing.

<sup>&</sup>lt;sup>13</sup>Each test run took about 28 seconds on the CRAY-2.

FOURIER COEFFICIENTS OF MAASS WAVEFORMS FOR  $PSL(2, \mathbb{Z})$ 

$$N = 20, M = \pi(N) = 8$$

R=	1	3.77975135189	07	ICOUNT:	11	MAX:	100
FOR	X=	0.1000000000	Y=	1.00500	00000	0	
and	initi	al values:					
C0 (	1)=	1.000000000	000				
C0 (	2)=	0.000000000	000				
C0 (	3)=	0.000000000	000				
C0 (	5)=	0.00000000	000				
C0 (	7) =	0.000000000	000				
C0 (	11)=	0.000000000	000				
C0 (	13)=	0.000000000	000				
C0 (	17)=	0.00000000	000				
C0(	19)=	0.00000000	000				

# (with rapidly attractive behavior throughout)

С(	1)=	1.000000000000	1.00000000000	0.0000E+00
С(	2)=	1.549304477941	1.549304477941	0.0000E+00
С(	3)=	0.246899772454	0.246899772454	0.0000E+00
С(	5)=	0.737060385348	0.737060385348	0.0000E+00
С(	7) =	-0.261420075765	-0.261420075765	0.0000E+00
С(	11)=	-0.953564652617	-0.953564652617	0.0000E+00
С(	13)=	0.278827029162	0.278827029162	0.0000E+00
С(	17)=	1.307341714533	1.307341714533	0.0000E+00
С(	19)=	0.092558582508	0.092558582508	0.0000E+00

# (2.6) denominator was: .9699E00 final value of the (2.5) analog: 0

R=		13.779751	35189	07	ICOUNT:	9	MAX:	100
FOR	X=	0.150000	0000	Y=	1.0050	000000	C	
and	init	ial value	s:					
C0 (	1)=	1.0000	00000	000				
C0 (	2)=	0.0000	00000	000				
C0 (	3)=	0.0000	00000	000				
C0 (	5)=	0.0000	00000	000				
C0(	7)=	0.0000	00000	000				
C0 (	11)=	0.0000	00000	000				
C0 (	13)=	0.0000	00000	000				
C0 (	17)=	0.0000	00000	000				
C0 (	19)=	0.0000	00000	000				

# (with rapidly attractive behavior throughout)

C(	1)=	1.00000000000	1.000000000000	0.0000E+00
Č(	2) =	-1.122947942450	-1.122947942450	0.0000E+00
C(	3) =	-0.389949016161	-0.389949016161	0.0000E+00
C(	5) =	-0.523189739313	-0.523189739313	0.0000E+00
Ċ	7) =	0.507684269216	0.507684269216	0.0000E+00
Ċ	11) =	0.609969290410	0.609969290410	0.0000E+00
C (	13)=	0.044620901213	0.044620901213	0.0000E+00
C(	17)=	-0.049027146897	-0.049027146897	0.0000E+00
C (	19)=	0.637093574481	0.637093574481	0.0000E+00

# (2.6) denominator was: .7151E00

261

13.7797513518907 ICOUNT: 800 MAX: R= 800 FOR X= 0.120000000 Y= 0.600000000 and initial values: CO(2)= 0.000000000000 CO( 3)= 0.00000000000 CO( 5)= 0.000000000000 CO( 7)= 0.000000000000 CO(11) =0.000000000000 CO(17) = 0.00000000000

# (with repellent behavior before $I \approx 20$ ) then steadily attractive afterwards

С(	1)=	1.000000000000	1.00000000000	0.0000E+00
С(	2)=	-35.836533862512	-35.836533862514	0.1819E-11
С(	3)=	-36.625899101444	-36.625899101446	0.2046E-11
С(	5)=	-73.310502980020	-73.310502980024	0.4093E-11
С(	7)=	-31.181855497617	-31.181855497619	0.1705E-11
С(	11)=	-1.099116370964	-1.099116370963	-0.2629E-12
С(	13)=	-42.913663228011	-42.913663228013	0.2728E-11
С(	17)=	77.526863693281	77.526863693285	-0.4547E-11
С(	19)=	18.904232881022	18.904232881023	-0.9095E-12

## (2.6) denominator was: .1690E00

R=		13.77975135189	07	ICOUNT:	800	MAX:	800
FOR	X=	0.1250000000	Y=	0.6000	00000	0	
and	init	ial values:					
C0(	1)=	1.00000000	000				
C0 (	2)=	0.00000000	000				
C0 (	3)=	0.00000000	000				
C0 (	5)=	0.00000000	000				
C0(	7)=	0.00000000	000				
C0 (	11)=	0.00000000	000				
C0(	13)=	0.00000000	000				
C0(	17)=	0.00000000	000				
C0 (	19)=	0.00000000	000				

## (with attractive behavior throughout)

C(	1)=	1.000000000000	1.00000000000	0.0000E+00
Ċ(	2) =	1.549304477941	1.549304477941	-0.6963E-12
C(	3)=	0.246899772454	0.246899772455	-0.9255E-12
C(	5)=	0.737060385349	0.737060385351	-0.1577E-11
C(	7) =	-0.261420075764	-0.261420075763	-0.8278E-12
C(	11) =	-0.953564652617	-0.953564652617	0.2132E-13
С(	13) =	0.278827029166	0.278827029167	-0.9592E-12
C (	17) =	1.307341714536	1.307341714534	0.1734E-11
С(	19)=	0.092558582508	0.092558582508	0.4245E-12

(2.6) denominator was: -.1467E00 final value of the (2.5) analog: 4E-12

In batches 3 and 4, note that the test points are rather close together. Taking X = .124 gave something which, after 800 iterations, was trying to converge to the  $\varphi$ -data but was still off by up to 5E-2. [Not surprisingly perhaps, the convergence in batch 4 was a bit on the slow side: the (2.5) analog had values 4.8E-2 and 6.8E-8 at I = 100, 400. Something like E-11 was achieved only around I = 600.]

To get a better handle on this type of situation, it is tempting to make a series of further runs (with, say, ICOUNT = 25000) at a large number of intermediate X.

Let case 1 refer to Y = .6000 and case 2 to Y = 1.005. In *both* cases, one easily checks that  $\varphi(x + iY)$  has constant sign on the given x-interval. This is important because it shows that whatever subtleties are present are not merely caused by passing through a zero of  $\varphi$ .

By running jobs with a variety of input vectors, one quickly confirms that the  $\varphi$ -data goes from being  $T_0$ -repellent at one endpoint to  $T_0$ -attractive at the other.

The transition points occur at about .1238 and .12877, respectively.

The iterative behavior near these X should prove interesting (if only for the fact that one of the eigenvalues of  $J_{T_0}(\varphi)$  now has modulus very close to 1).

Taking X = .1238 and  $c_0(p) \equiv 0$  in case 1 produces output which shows no sign of convergence even after 500000 iterations. Yet, in taking X = .1238 + (.0001)n,  $n \neq 0$ , we find output which is already quite stable at I = 25000. The resulting limit vectors continue to display the same lopsided behavior seen in batches 3 and 4. Given the size of the "gap", there is little doubt that *some*place near X = .1238, a point of true divergence must occur (for this choice of  $c_0(p)$ ).

The dynamics in case 2 were significantly different. As X approached .12877, the matrix  $J_{T_0}(\varphi) - I$  seemed to become singular, or else very nearly so (in marked contrast to case 1). In line with some standard structure theorems in several complex variables, the *zero-set* of  $T_0(\mathbf{c}) - \mathbf{c}$  must (therefore) be expected to exhibit a kind of branching behavior as X passes through .12877. Our experiments with I = 25000 tended to confirm this—in that, what was found, was a kind of *criss-cross* in the attractive and repellent fixed points (as opposed to an actual jump).

**Example 4.** Another job of type  $(\mathcal{S})$ . In this case, R is (obviously) not an eigenvalue.

$$N = 20, M = \pi(N) = 8$$

R=		5.00000000000 ICOUNT: 19 MAX:	400
FOR	X=	0.1890000000 Y= 0.865000000	
and	inıtı	nal values:	
C0(	1)=	1.00000000000	
C0(	2)=	0.0000000000	
C0(	3)=	0.0000000000	
C0(	5)=	0.0000000000	
C0(	7) =	0.0000000000	
C0(	11)=	0.0000000000	
C0(	13)=	0.0000000000	
C0(	17)=	0.0000000000	
COL	19) =	0 0000000000	

#### (with rapidly attractive behavior throughout)

C (	1)=	1.000000000000	1.00000000000	0.0000E+00
С (	2)=	3.980104536067	3.980104536067	0.0000E+00
С (	3)=	-4.353479845878	-4.353479845878	0.0000E+00
С (	5)=	3.747186760026	3.747186760026	0.0000E+00
С(	7)=	-2.495431559510	-2.495431559510	0.0000E+00
С (	11)=	0.424977267960	0.424977267960	0.0000E+00
С (	13)=	3.269324551156	3.269324551156	0.0000E+00
С (	17)=	-4.379743415131	-4.379743415131	0.0000E+00
С (	19)=	-8.749979373183	-8.749979373183	0.0000E+00

the (2.6) denominator was: .1060E-1

**Example 5** [illustrating catastrophic cancellation]. In the following  $\mathcal{S}$ -job, the 4th column displays the effect of placing *absolute value* signs on all the various harmonics [from (1.3)] which enter into the (2.6) numerator.

The input data is shown in column 1; the result of *one* iteration of (2.6) in column 2; the difference 1-2 in column 3. Note that the input data is accurate to about 12 places.

$$N=9\,,\ M=\pi(N)=4$$

R=	13.7797	7513518907 I	COUNT: 1		
FOR	X= 0.0	Y=	0.200000000		
C (	1)=	1.000000000000	1.000000000000	0.0000E+00	
C (	2)=	1.549304477942	1.549304494482	-0.1654E-07	0.5010E+00
С(	3)=	0.246899772454	0.246899868708	-0.9625E-07	0.7784E+00
C (	5)=	0.737060385348	0.737061249696	-0.8643E-06	0.2914E+01
С(	7)=	-0.261420075765	-0.261419800439	-0.2753E-06	0.1692E+01
С(	11)=		-0.953563663742		0.2037E+01
С(	13)=		0.278826741784		0.1941E+01
C (	17)=		1.307341713868		0.1805E+01
С(	19)=		0.092558532888		0.1778E+01
С(	23)=		1.138070636669		0.1629E+01
C (	29)=		0.752113320290		0.1859E+01

(2.6) denominator was: .1385E-5 typical  $c_p$ -accuracy in output: about  $10^{-6}$ 

The reason for the (accuracy) degradation lies in the size of the denominator. In terms of floating-point arithmetic in (2.6), the earliest [i.e., "lowest"] harmonics have magnitude about O(1) and a precison of (say) 11 digits. When the denominator is about  $10^{-6}$  (as here), in order for  $c_p$  to be sensibly bounded, this makes the *numerator* in (2.6) have to have value like  $O(1)10^{-6}$ . But, then, the first *five* digits in the earliest harmonics must cancel out exactly (under addition). The number of significant figures in  $c_p$  should therefore be about 11 - 5 = 6. This of course agrees with what we found.

Taking  $z_0 = i(.125)$  produces a denominator of 2.8E-14, and essentially *no* significant figures in  $c_p$ . Similar behavior would ensue anytime  $z_0$  were accidentally positioned along a nodal line of  $\varphi$ .

## 6. CONCLUDING REMARKS

Any number of worthwhile problems have been raised (either directly or indirectly) in the preceding sections.

Before closing, we only want to draw attention to one idea which may have already occurred to some readers.

Namely, recall (2.7)–(2.8). One would very much like to know where the zeros of G(s)L(s) lie; in particular, are they all located along  $\operatorname{Re}(s) = \frac{1}{2}$ ? In this connection, it would also be nice to know their spacing distribution (cf. [13]).

Having the ability to calculate many  $c_p$ -values is an important prerequisite to being able to explore problems of this kind experimentally. (Indeed, to being able to simply compute L(s)!)

In matters of this type, cases with large Im(s) will typically be most important. To reach the necessary heights, one definitely needs to know many  $c_p$ [probably out to  $p \approx (\text{constant})Im(s)$ ] and know them to good accuracy.

From this standpoint, then, the problem raised at the end of  $\S3$  takes on a new significance.

Whether it will ultimately prove to be possible to obtain enough  $c_p$  to study L(s) at heights like  $10^6$  is by no means clear. [Similar remarks apply to the more general functions  $L(s, \text{Sym}^k)$  mentioned in §1 (and to an even greater degree!).] See [6, 8, 9, 13, 17] for the proper perspective.

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