The Quadratic Character Experiment

Jeffrey Stopple

CONTENTS

A fast new algorithm is used compute the zeros of 10^6 quadratic character L-functions for negative fundamental discriminants with absolute value $d > 10^{12}$. These are compared to the 1-level density, including various lower-order terms. These terms come from, on the one hand, the explicit formula, and on the other, the L-functions ratios conjecture. The latter give a much better fit to the data, providing numerical evidence for the conjecture.

1. INTRODUCTION

1.1 Predictions

Standard conjectures [Katz and Sarnak 99] predict that the low-lying zeros of quadratic Dirichlet L-functions should be distributed according to a symplectic random matrix model. To make this more precise, we shall introduce some notation. Let χ_d be a real primitive character modulo d, and suppose furthermore that $\chi_d(-1) \cdot d$ is a fundamental discriminant. Let $g(\tau)$ be a Schwartz-class test function. Then the 1-level density for the zeros $\frac{1}{2}+\gamma_d$ of $L(s, \chi_d)$ should satisfy

$$\frac{1}{X^*} \sum_{d \leq X} \sum_{\gamma_d} g\left(\gamma_d \frac{\log X}{2\pi}\right) \tag{1–1}$$
$$= \int_{-\infty}^{\infty} g(\tau)\left(1 - \frac{\sin(2\pi\tau)}{2\pi\tau}\right) d\tau + O\left(\frac{1}{\log X}\right),$$

where X^* is the cardinality of fundamental discriminants $\chi_d(-1) \cdot d$ with $d < X$. This is a theorem [Özlük and Snyder 92] if the support of the Fourier transform of g is suitably restricted.

Recently, Conrey and Snaith [Conrey and Snaith 07] made a precise prediction for the lower-order arithmetic terms in the 1-level density. Their prediction is conditional, assuming the L-functions ratios conjecture [Conrey et al. 08]. Miller [Miller 08] then proved (under typical restrictions for the test function $g(\tau)$) that these lower-order terms exist and agree with the prediction in [Conrey and Snaith 07].

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1.2 Experiments

Zeros of Dirichlet L-functions were first computed by Davies and Haselgrove, by Spira, and by Rumley. Rubinstein was the first to compute, as one portion of his thesis [Rubinstein 98], enough low-lying zeros to meaningfully test (1–1). However, the numerical methods developed in [Rubinstein 98] were optimized to compute $L\left(\frac{1}{2}+it,\chi_d\right)$ for large real t rather than large d.

1.3 This Paper

The next section develops an algorithm to compute low-lying zeros ($0 \le t < 1$) that is fast for large d. This is a modification of the idea behind [Stopple 07]. The subsequent section has a discussion of the data from the computation of the zeros of more than 10^6 quadratic character L-functions for negative fundamental discriminants $-d$ with $d > 10^{12}$. This is followed by some implementation notes, and an appendix (Section 5) on Miller's "refined" 1-level density and the L-functions ratios conjecture.

2. ALGORITHM

We are going to compute the L-function on the critical line by means of an approximate functional equation, an idea that goes back to Lavrik and was first implemented by Weinberger [Weinberger 75]. With χ a real character modulo d, let $a = (1-\chi(-1))/2$, and with $t > 0$ use s to denote $\left(\frac{1}{2}+it+a\right)/2$.[1] Define

$$Z(t,\chi) = \xi\left(\frac{1}{2}+it,\chi\right) = \sum_n \chi(n)n^a 2\,\mathrm{Re}(G(s,\pi n^2/d)), \tag{2–1}$$

where

$$G(s,x) = x^{-s}\Gamma(s,x) = \int_1^\infty \exp(-yx)y^s\frac{dy}{y}.$$

As in [Weinberger 75], the tail of the series, the sum of terms $n > N$, is bounded by $d^2\exp(-N^2\pi/d)/(\pi N)^2$, so if we want to compute to D digits of accuracy, we should have

$$\frac{d^2\exp(-N^2\pi/d)}{(\pi N)^2} < 10^{-D}. \tag{2–2}$$

Certainly

$$N \ge d^{1/2}\log(d^2 10^D)^{1/2}\pi^{-1/2} \tag{2–3}$$

would suffice; later we shall see that we can do better with any particular d.

[1] We are not actually assuming the generalized Riemann hypothesis, but we are only looking for zeros on the critical line.

Differentiating with respect to x under the integral defining $G(s,x)$, we see that

$$\frac{d}{dx}G(s,x) = -\int_1^\infty \exp(-xy)y^{s+1}\frac{dy}{y} = -G(s+1,x), \tag{2–4}$$

while integration by parts, on the other hand, gives

$$G(s+1,x) = \frac{\exp(-x)}{x} + \frac{s}{x}G(s,x). \tag{2–5}$$

Equations (2–4) and (2–5) give a nice recurrence relation for all the derivatives $G^{(k)}(s,x)$ in terms of $G(s,x)$. This, in turn, motivates a consideration of Taylor expansions.

Suppose we compute $G(s,x)$ by a Taylor series expansion (in the second variable, centered at x_0) to B terms, where B is a parameter to be determined.

Lemma 2.1. *We can bound the remainder in the Taylor expansion by a function $R_B(x,x_0)$ (defined below) that satisfies*

$$R_B(x,x_0) \le \frac{(x/x_0-1)^B}{B!}\Gamma(B,x_0) \le \frac{(x/x_0-1)^B}{B}. \tag{2–6}$$

Proof: We have

$$\left|G^{(B)}(s,x)\right| = |G(s+B,x)| \le \int_1^\infty \exp(-xy)y^B\,dy,$$

since s is in the critical strip. By the integral formula for the remainder in Taylor's theorem, we can bound that remainder by

$$R_B(x,x_0) \stackrel{\text{def}}{=} \frac{1}{B!}\int_{x_0}^x\int_1^\infty \exp(-uy)y^B dy\,(x-u)^B du.$$

Change the order of integration and let $t = x-u$ to get

$$= \frac{-1}{B!}\int_1^\infty \exp(-xy)\int_{x-x_0}^0 \exp(-ty)t^B dt\, y^B dy.$$

Now integrate by parts in the t integral to get

$$= \frac{1}{B!}\int_1^\infty \exp(-xy)(x-x_0)^B\exp((x-x_0)y)y^{B-1}dy \\ - R_{B-1}(x,x_0).$$

Or in other words,

$$\begin{aligned} R_B(x,x_0) + R_{B-1}(x,x_0) &= \frac{(x-x_0)^B}{B!}G(B,x_0) \\ &= \frac{\left(\frac{x}{x_0}-1\right)^B}{B!}\Gamma(B,x_0). \end{aligned}$$

This implies the first inequality. For the second, we observe that

$$\Gamma(B,x_0)=\int_{x_0}^{\infty}\exp(-y)y^B\frac{dy}{y}$$
$$\le\int_{0}^{\infty}\exp(-y)y^B\frac{dy}{y}=\Gamma(B)=(B-1)!,$$

which completes the proof □

The first inequality is stronger, so it is good for the actual computation. The second is weaker, but simple enough to be useful in proving the theorem.

Now we are ready to put the Taylor expansions to good use. Similar to the method of [Stopple 07], we partition the set $\{n^2 \mid 1\le n\le N\}$ into intervals

$$I_j=[F_j,F_{j+1}),$$

for $j=1,\dots,T$, where F_j is the jth Fibonacci number. We then compute the function G by a Taylor expansion in the second variable, centered at $\pi F_j/d$, and truncated to B terms:

$$2\,\mathrm{Re}(G(s,\pi n^2/d))\approx\sum_{k=0}^{B}G_{j,k}(t)(\pi/d)^k\cdot(n^2-F_j)^k,$$

where

$$G_{j,k}(t)=2\,\mathrm{Re}(G^{(k)}(s,\pi F_j/d))/k!. \qquad (2\text{–}7)$$

Theorem 2.2. *We can compute $Z(t,\chi)$ as*

$$Z(t,\chi)=\sum_{j=1}^{T}\sum_{k=0}^{B}G_{j,k}(t)(\pi/d)^k\sum_{n^2\in I_j}\chi(n)n^a(n^2-F_j)^k \qquad (2\text{–}8)$$

to D digits of accuracy, where T and B are both $O(\log(d))$, the implied constants depending on D.

The expression

$$C_{jk}\overset{\text{def}}{=}\sum_{n^2\in I_j}\chi(n)n^a(n^2-F_j)^k \qquad (2\text{–}9)$$

is a precomputation independent of s in *integers* that is $O(N\cdot B)=O(d^{1/2}\log(d)^2)$. Subsequently, individual evaluations of $Z(t,\chi)$ cost only $O(T\cdot B)=O(\log(d)^2)$.

Proof: Of course, the outermost sum on $j\le T$ and the innermost sum on n^2 in I_j combine to give the squares of all $n\le N$, the middle sum giving the needed Taylor expansions. We need N^2 to be in the last interval I_T, so

$$N^2<F_{T+1}\approx\frac{\Phi^{T+1}}{\sqrt{5}},\quad\text{where}\quad\Phi=\frac{1+\sqrt{5}}{2},$$

with $N\ll d^{1/2+\epsilon}$ by (2–3). This implies that $T\ll\log(d)$ suffices.

This is all well and good, but we need to show that using Taylor expansions at points spaced in what is essentially a geometric progression does not require an unreasonable number of terms B in each expansion in order to compute accurately. Use $|\chi(n)|\le 1$, $n^a\le n$, and the rough estimate $d^{1/2}$ for the L-series truncation parameter N. Assuming that the errors we make in computing each $G(s,\pi n^2/d)$ are independent with standard deviation ϵ, then the standard error in the sum (2–1) is bounded by [Dahlquist 74]

$$\Big(\sum_{n=1}^{d^{1/2}}(n\epsilon)^2\Big)^{1/2}\ll\epsilon\cdot d^{3/4},$$

where we have approximated a sum by an integral. We want $\epsilon\cdot d^{3/4}<10^{-D}$, or

$$\epsilon<10^{-D}d^{-3/4},$$

which will determine how many terms B we need in each Taylor expansion. We shall use the weaker inequality in the lemma with

$$x_0=\pi F_j/d,\quad x<\pi F_{j+1}/d,$$

which makes the error satisfy

$$\epsilon<\frac{(F_{j+1}/F_j-1)^B}{B}<(\Phi-1)^B.$$

Thus we want

$$(\Phi-1)^B<10^{-D}d^{-3/4},$$

or

$$10^D d^{3/4}<(\Phi-1)^{-B}=\left(\frac{\sqrt{5}-1}{2}\right)^B,$$

and so $B=O(\log(d))$ suffices. □

For a single function evaluation (for example, determining whether $Z(0,\chi)>0$), this algorithm is no improvement over [Weinberger 75]; summing the series requires $O(d\log(d))^{1/2}$ terms by (2–3). If one wants to do an arbitrarily large number of function evaluations, the improvement is spectacular, from exponential down to polynomial (in terms of the number of digits of d, which is approximately $\log(d)$). This is deceptive, though, because what one really wants to do is find the all zeros with, say, $0\le t<1$. (Larger t intervals requires computing $G(s,x)$ via the methods of [Rubinstein 98], which

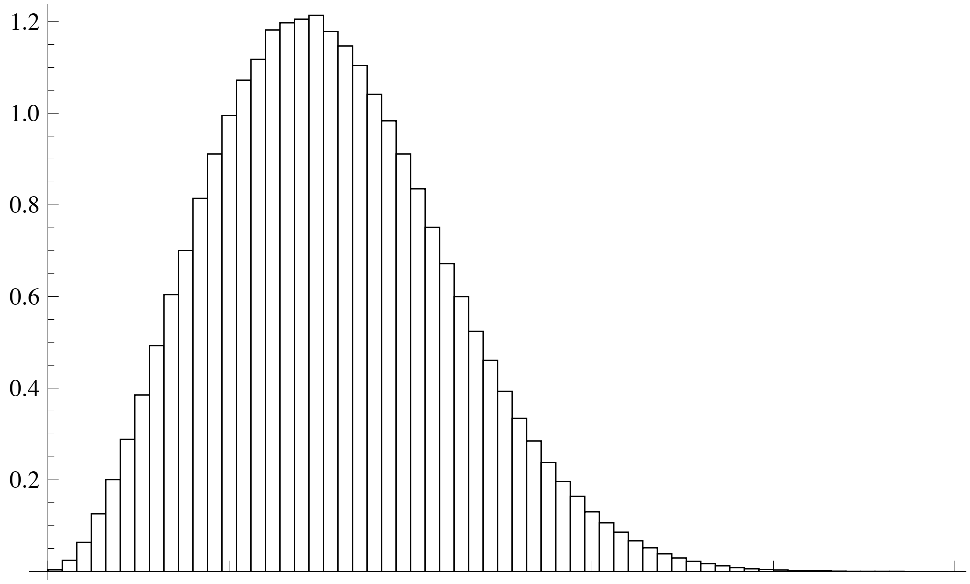

FIGURE 1. Histogram of the lowest zero.

in turn necessitates redoing the precomputation.) Since there are $O(\log(d))$ such zeros and each can be found with $O(1)$ evaluations, the precomputation still dominates as a theoretical result. But as Jan L. A. van de Snepscheut[2] wrote, "In theory, there is no difference between theory and practice. But in practice, there is."

3. DATA

Zeros with $t < 1$ were computed for 1,003,089 negative fundamental discriminants $-d$ in the range $10^{12} \leq d \leq 10^{12} + 3.3 \cdot 10^6$, a total of 4,027,115 zeros. Figure 1 shows a histogram for the imaginary part of the lowest-lying zero, rescaled by $\log(10^{12})/(2\pi)$. The lowest zero found was at $t = 0.00242936$, corresponding to the discriminant $-1{,}000{,}000{,}030{,}163$.

Figure 2 shows the histogram of imaginary parts of all the zeros, again rescaled by $\log(10^{12})/(2\pi) \approx 4.39761$. The upper curve (dashed) is the main term $1 - \sin(2\pi\tau)/(2\pi\tau)$ for the symplectic random matrix model for the 1-level density. The lower curve (dotted) also includes terms from (5–2) that are $O(1/\log(X))$. (In the notation of the appendix, $X = 10^{12}$ and $\Delta X = 3.3 \cdot 10^6$.) This version is derived from the explicit formula. The fit is visibly poor for these values of X and ΔX.

[2]Not Yogi Berra.

As usual, we assumed in (1–1) that $\operatorname{supp}(\hat{g}) \subset (-\sigma, \sigma) \subset (-1, 1)$, so that

$$\int_{-\infty}^{\infty} g(\tau) \left(-\frac{\sin(2\pi\tau)}{2\pi\tau} \right) d\tau = -\frac{g(0)}{2}.$$

It is really the $-g(0)/2$ term that appears in the proof via the explicit formula. Miller [Miller 08] derives a version of the 1-level density in which the term $-g(0)/2$ is replaced by a more complicated expression; see (5–3). This version is graphed as a solid line in Figure 2. The fit appears to be very good. Since (5–3) was first derived in [Conrey and Snaith 07] from the L-functions ratios conjecture, the data seem to provide good numerical evidence for the conjecture. This also seems to indicate that there is great deal of structure in the $O(1/\log(X))$ error in (1–1), and the L-functions ratios conjecture captures that structure. The data are available at http://www.math.ucsb.edu/~stopple/quadratic.experiment.

4. IMPLEMENTATION NOTES

4.1 Error Estimates

With $D = 15$ digits of accuracy and d near 10^{12}, the crude estimate (2–3) requires $N = 5.4 \cdot 10^6$ terms in the series. We can actually do a little better. Using this as a starting estimate, Mathematica's `FindRoot` uses a variant of the secant method to determine that $N = 4.3 \cdot 10^6$ satisfies (2–2), for a savings of better than 20%.

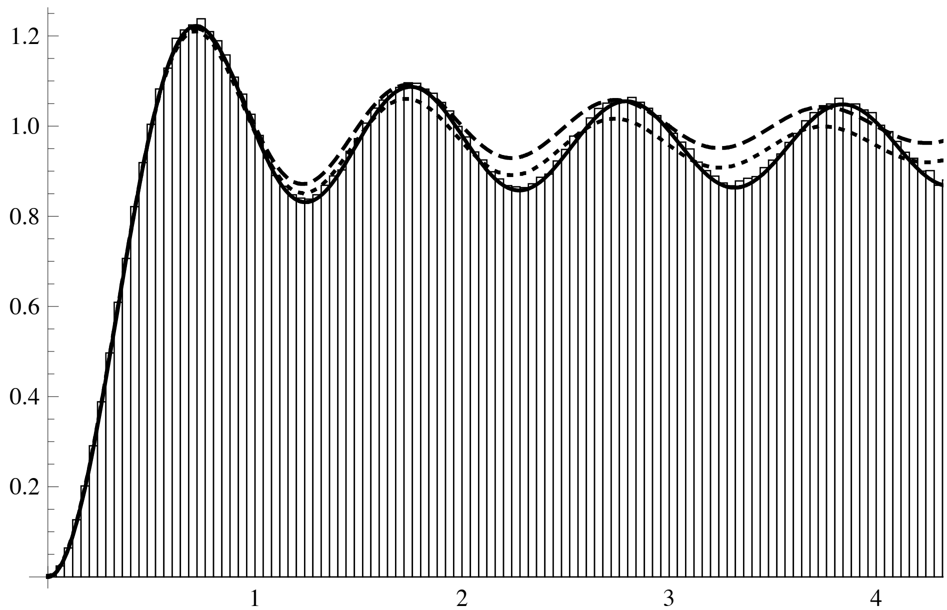

FIGURE 2. Histogram of all zeros.

The stronger inequality in the lemma determines good values for the Taylor series truncation parameter B in computing $G(s,\pi n^2/d)$. Consider the case $a=1$, i.e., a negative discriminant. Assuming that the errors (2–6) in the terms are independent, and using $|\chi(n)|\le 1$, $n^a=n$, the standard error in the sum over all n^2 in I_j is bounded by [Dahlquist 74]

$$\frac{\Gamma(B,\pi F_j/d)}{B!}\Big(\sum_{F_j\le n^2<F_{j+1}} n^2(n^2/F_j-1)^{2B}\Big)^{1/2}.$$

We can estimate the sum by an integral:

$$\int_{\sqrt{F_j}}^{\sqrt{F_{j+1}}} t^2(t^2/F_j-1)^{2B}dt \approx F_j^{3/2}\int_1^{\Phi^{1/2}} u^2(u^2-1)^{2B}du.$$

So the error from the sum over n^2 in I_j is about

$$\frac{\Gamma(B,\pi F_j/d)}{B!}F_j^{3/4}\Big(\int_1^{\Phi^{1/2}} u^2(u^2-1)^{2B}du\Big)^{1/2}. \qquad (4\text{–}1)$$

For d near 10^{12}, we need $T=65$ intervals, and it is easy to compute (4–1) in Mathematica for various B. We see that $B=B(j)$ should increase linearly from 84 at $j=31$ to 107 at $j=65$, in order that the total of all errors be only about 10^{-15}. (For $j<31$, the intervals I_j contain not many more than $B(j)$ squares n^2, so the contribution of these n, namely $1\le n\le 1160$, is computed directly.)

The case $a=0$, i.e., positive discriminant, is treated similarly. It turns out that one needs $B(j)$ to increase linearly from 70 at $j=31$ to 78 at $j=65$.

4.2 Algorithms

To find fundamental discriminants, I check the congruence condition and test for divisibility by the squares of the first 200 primes. (The 94 examples divisible by the square of a prime larger than the 200th prime were easily identified with Mathematica and removed from the data by hand.)

To compute $\Gamma(s)$ I use the Lanczos algorithm as in [Press et al. 92]. Precomputed values of $\Gamma(s)$ allow efficient computation of incomplete gamma functions $\Gamma(s,x)$ for various x by the methods of [Press et al. 92]: series expansion for $x<6$ and continued fractions for $x\ge 6$. These algorithms compare well with those implemented in Mathematica, giving both absolute and relative error no worse than 10^{-18} for the relevant range of x and $|\operatorname{Im}(s)|<1$.

To find zeros of $Z(t,\chi)$, the computation is stepped through values in increments of t of size $2\pi/\log(10^{12}/(2\pi))/50$, i.e., 1/50th the mean gap between zeros. When a sign change was observed, Ridder's method [Press et al. 92] was used to find the root. No effort was made to verify the generalized Riemann hypothesis, or that all zeros of $Z(t,\chi)$ with $t<1$ were located. (However, the obvious check that $Z(0,\chi)>0$ was made.)

4.3 Hardware

Computations were done on a 3.0-GHz 8-core Mac Pro. Both the integer arithmetic and the recursion for the derivatives $G^{(k)}(s,x)$ were done with GMP 4.2.1 (ported to the Intel Core 2 Duo 64-bit processor by Jason Worth Martin). For the rest of the floating-point computations, the C types `long double`, `long double complex` sufficed.

4.4 Parallelization

Most of the computation consists in computing the values $(n^2-F_j)^k$ in (2–9). Since this is independent of d, there is a gain in efficiency by computing the quantities C_{jk} in (2–9) for eight discriminants at a time. Parallelism is easily implemented using Pthreads. The contribution of the intervals I_j is computed in T separate threads for eight discriminants at a time. Once all the precomputation is done, the zeros of $Z(t,\chi)$ for each of the eight characters χ are computed in eight separate threads.

4.5 Testing

Accuracy of computed zeros was tested three ways: first, by recomputing well-known examples [Watkins 00, Watkins 03, Weinberger 75] of moderate-sized discriminants such as −115,147 and −175,990,483. Second, I also implemented the method of [Weinberger 75] directly in Mathematica and compared a few examples for discriminants with absolute value greater than 10^{12}, with agreement to 15 digits. Third, I compared with the unpublished data from Rubinstein's thesis [Rubinstein 98]. This includes 3601 prime discriminants $-d$ with $10^{12}\le d\le 10^{12}+2\cdot 10^5$. The data were in agreement with his to the ten digits of accuracy he computed.

5. APPENDIX: REFINED 1-LEVEL DENSITY

This appendix closely follows [Miller 08] to determine the 1-level density, including lower-order terms, for the family of quadratic Dirichlet L-functions. Instead of considering the set of all fundamental $d<X$, I adapted the proof for

$$\mathcal{F}(X)=\{X<|d|<X+\Delta X\}.$$

Where Miller treats the case that χ_d is an even function, i.e., $d>0$, I instead considered χ_d an odd function, $-d<0$. Throughout, I assumed about ΔX that

$$X^{1/2}\log(X)=o(\Delta X)\quad\text{and}\quad \Delta X=o(X). \tag{5–1}$$

Theorem 5.1. (Miller.) *Let g be an even Schwartz test function such that $\operatorname{supp}(\hat g)\subset(-\sigma,\sigma)$, where $\hat g$ denotes the Fourier transform of g. Let*

$$A'(r)=\sum_p \frac{\log p}{(p+1)(p^{1+2r}-1)}.$$

Then

$$\begin{aligned}
&\frac{1}{\sharp\mathcal{F}(X)}\sum_{d\in\mathcal{F}(X)}\sum_{\gamma_d} g\left(\gamma_d\frac{\log X}{2\pi}\right) \qquad\qquad (5\text{–}2)\\
&\quad=\int_{-\infty}^{\infty} g(\tau)\left(1-\frac{\sin(2\pi\tau)}{2\pi\tau}\right)d\tau\\
&\qquad+\frac{1}{\log X}\int_{-\infty}^{\infty} g(\tau)\Bigg[-\log(\pi)+\operatorname{Re}\frac{\Gamma'}{\Gamma}\left(\frac34+\frac{i\pi\tau}{\log X}\right)\\
&\qquad\qquad+2\operatorname{Re}\frac{\zeta'}{\zeta}\left(1+\frac{4\pi i\tau}{\log X}\right)+2\operatorname{Re}A'\left(\frac{2\pi i\tau}{\log X}\right)\Bigg]d\tau\\
&\qquad+o\left(\frac{1}{\log X}\right)+O\left(\frac{X^{\sigma/2}\log^6 X}{\Delta X^{1/2}}\right).
\end{aligned}$$

Of course, to get the $O(X^{\sigma/2}\log^6 X/\Delta X^{1/2})$ error to be $o(1/\log X)$, we would need to restrict the support of $\hat g$ to be a subset of $\left(-\frac12,\frac12\right)$.

Figure 3 shows each of the three nonconstant terms that are absorbed in the $O(1/\log(X))$ error in (1–1), all on the same scale $2\pi\tau/\log(X)=t$. The Γ'/Γ term (dotted) is slowly increasing and very smooth, while A' (dashed) is small and wobbly. Observe that when $\zeta\left(\frac12+i\gamma\right)=0$, the contribution at $t=\gamma/2$ of $\zeta'/\zeta(1+2it)$ (solid) is positive and large. This follows from [Titchmarsh 86, Theorem 9.6(A)], which says that

$$\frac{\zeta'(s)}{\zeta(s)}=\sum_{|t-\gamma|\le 1}\frac{1}{s-\rho}+O(\log(t)),$$

so up to a small error, the logarithmic derivative is determined by the nearby zeros ρ. This "resurgence" of the zeros of $\zeta(s)$ does not play much of a role in the data ($t<1$) presented here.

Since the fit of the data to even the "refined" 1-level density is poor, we turn instead to the prediction inspired by the L-functions ratios conjecture. The term

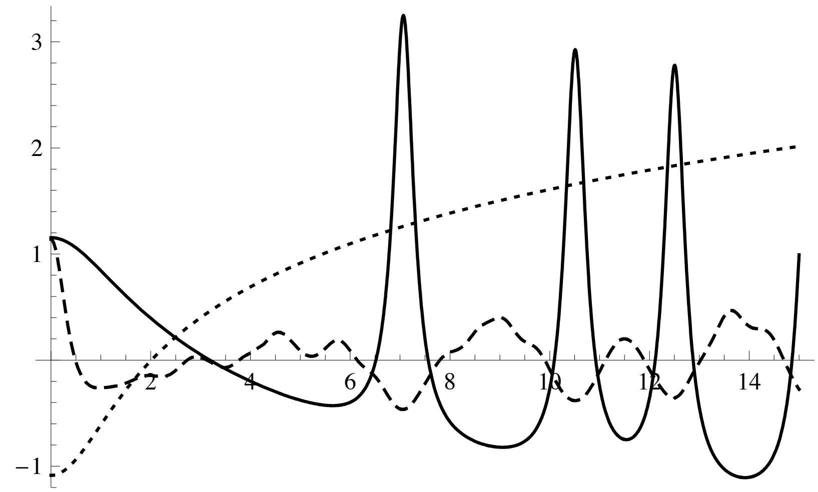

FIGURE 3. All three nonconstant $O(1/\log(X))$ terms. The ζ'/ζ term is the solid line, the Γ'/Γ term is dotted, and the A' term is dashed.

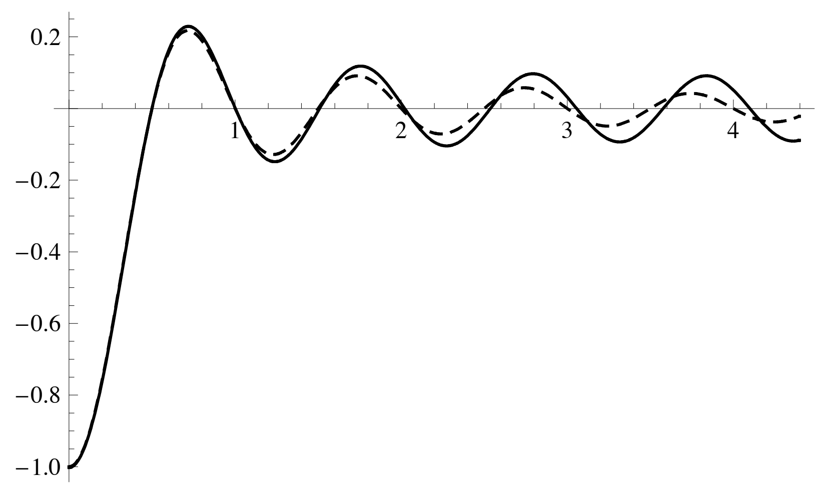

FIGURE 4. $-\sin(2\pi\tau)/(2\pi\tau)$ (dashed) v. $R_{\text{est}}(\tau, X)$ (solid)

$-\sin(2\pi\tau)/(2\pi\tau)$ is replaced by the real part of

$$R(\tau, X) = \frac{-2}{\sharp\mathcal{F}(X)\log X} \sum_{d\in\mathcal{F}(X)} \exp\left(-2\pi i\tau\frac{\log(d/\pi)}{\log X}\right) \times \frac{\Gamma\left(\frac{3}{4} - \frac{\pi i\tau}{\log X}\right)}{\Gamma\left(\frac{3}{4} + \frac{\pi i\tau}{\log X}\right)} \frac{\zeta(2)\zeta\left(1 - \frac{4\pi i\tau}{\log X}\right)}{\zeta\left(-2 - \frac{4\pi i\tau}{\log X}\right)}. \tag{5–3}$$

(We have simplified the notation from [Miller 08, (1.6)]; see also Miller's Lemma 2.4.) Miller shows [Miller 08, Lemma 2.1] that on the Riemann hypothesis,

$$\int_{-\infty}^{\infty} g(\tau)R(\tau, X)d\tau = -g(0)/2 + O(X^{-3/4(1-\sigma)+\epsilon}),$$

and unconditionally with a larger error. Here, as usual, $\operatorname{supp}(\hat{g}) \subset (-\sigma, \sigma)$.

In order that the prediction not depend on the specific discriminants in $\mathcal{F}(X)$, we use summation by parts [Miller 08, Remark 2.3] to estimate

$$\sum_{d<X} \exp\left(-2\pi i\tau\frac{\log(d/\pi)}{\log X}\right) = \frac{3X}{\pi^2}\left(\frac{X}{\pi}\right)^{\frac{-2\pi i\tau}{\log(X)}} \frac{1}{1 - 2\pi i\tau/\log(X)} + O(X^{1/2}),$$

and similarly with the sum over $d < X + \Delta X$. The difference of these divided by $\sharp\mathcal{F}(X) = 3\Delta X/\pi^2 + O(X +$

$\Delta X)^{1/2}$ is used in an estimate of (5–3) and denoted by $R_{\text{est}}(\tau, X)$. Figure 4 shows how $R_{\text{est}}(\tau, X)$ (solid) compares to $-\sin(2\pi\tau)/(2\pi\tau)$ (dashed).

The solid graph in Figure 2 has $-\sin(2\pi\tau)/(2\pi\tau)$ replaced by $R_{\text{est}}(X)$, and also includes the other $O(1/\log(X))$ terms.

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