ZEROS OF DIRICHLET L-FUNCTIONS NEAR THE REAL AXIS AND CHEBYSHEV'S BIAS

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Abstract. We examine the connections between small zeros of quadratic L-functions, Chebyshev's bias, and class numbers of imaginary quadratic fields.

1. Introduction and Summary.

Let $\Delta_{q,a,b}(x) = \pi_{q,a}(x) - \pi_{q,b}(x)$, where $\pi_{q,r}(x)$ denotes the number of primes $p \leqslant x$ with $p \equiv r \pmod q$. Rubinstein and Sarnak [33] have recently shown that on the generalized Riemann hypothesis (GRH) and grand simplicity hypothesis (GSH) one can compute logarithmic densities for the set of x giving $\Delta_{q,a,b}(x) > 0$ for $q \geqslant 3, (a,q) = (b,q) = 1$. The GRH asserts that all non-trivial zeros of all Dirichlet L-functions have real part equal to $\frac{1}{2}$, and the GSH asserts that for each q, the collection of non-trivial zeros of the L-functions modulo q are linearly independent over the rational numbers. The logarithmic density of a set S of real numbers is defined as

$$\delta(S) = \lim_{X\to\infty} \frac{1}{\log X} \int_{t \in S \cap [1,X]} \frac{dt}{t},$$

if the above limit exists. For $q \geqslant 3$, let $c(q)$ be the ratio of the number of quadratic nonresidues to the number of quadratic residues, and define the scaled counting function

$$P_{q,N,R}(x) = \frac{\log x}{\sqrt{x}} \left(\sum_b \pi_{q,b}(x) - c(q) \sum_a \pi_{q,a}(x) \right), \tag{1.1}$$

where a runs over the quadratic residues modulo q, and b runs over the quadratic non-residues. If q has a primitive root ($q = 2,\ 4,\ p^m,\ 2p^m$ for prime p), then $c(q) = 1$. On the GRH and GSH, Rubinstein and Sarnak [33, p. 188] compute logarithmic densities of $\{x : P_{q,N,R}(x) > 0\}$ for $q = 3, 4, 5, 7, 11, 13$ and they prove that this density is greater than $\frac{1}{2}$ for all primes q. They show, for example, that $P_{4,N,R}(x) > 0$, on a logarithmic scale, for 99.59% of all x. These computations provide a very precise determination of the "sense" in which we may interpret Chebyshev's [9] remark that there are many more primes of form $4n+3$ than of form $4n+1$. We shall refer to these densities as the "bias for q".

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Values of x with $P_{q,N,R}(x) < 0$ occur infrequently on a logarithmic scale if Chebyshev's bias is high, and values of x with $\pi_{4,3}(x) < \pi_{4,1}(x)$ or $\pi_{3,2}(x) < \pi_{3,1}(x)$ occur so rarely that the regions are of special interest (see [3], [4]).

There are several natural questions arising from Rubinstein and Sarnak's paper which are treated here. Throughout this paper all densities and biases referred to are on a logarithmic scale, since Rubinstein and Sarnak [33] and Kaczorowski [19] have made it clear that natural densities cannot be expected to exist for any q.

1. Is there an easier way to compute Chebyshev's bias? We give an affirmative answer to this, although our method is non-rigorous. The method depends only on knowledge of small zeros of the appropriate L-functions, and the numbers agree very well with more complicated (and more rigorous) computations made in [33]. This makes it possible to quickly approximate the bias for any modulus q for which zeros have been computed [33], including q lacking primitive roots such as $q = 8$ and $q = 24$, where, as Shanks [35] first noted, the bias is quite high; see also [21, p. 302].

2. Although the bias approaches $\frac{1}{2}$ as $q \to \infty$ ([33], Theorem 1.6) the convergence is far from monotone. For example, the bias is much higher for $q = 409$ than for $q = 43, 67$, or 163. As will be described more fully in section 2, when q has a primitive root the bias depends heavily on the location of the first few zeros (closest to the real axis) of $L(s, \chi_q)$, χ_q being the real nonprincipal character mod q. In particular, the bias is heavily influenced by the size of the first zero (see Tables III–VII). Several authors ([28], [30], [40]) have noted a connection between small values of $h(-q)$, Chebyshev's bias, and small first zeros of $L(s, \chi_q)$. Making use of the Chowla-Selberg formula, we show that if $\mathbb{Q}(\sqrt{-q})$ is an imaginary quadratic number field with class number 1, we can expect that $L(s, \chi_q)$ has a relatively low first zero. This is especially true for $L(s, \chi_{163})$ with its smallest zero near $\frac{1}{2} + 0.2029i$. Our Tables VII–VII in §3 further illustrate the connection between low-lying zeros and small class numbers (see also [28],[30]). We observe that if moduli are arranged according to class number, the smallest zero of $L(s, \chi_q)$ is nearly monotonic in q when the class number is small (see Tables VI, VII).

3. Can Chebyshev's bias be approximated well using actual prime counts? We computed $P_{q,N,R}(x)$ up to $x = 10^{12}$ for various q, and this interval appears insufficient to approximate the bias well (see Table I). In particular, $P_{163,N,R}(x)$ is negative (on a standard scale) for over 93% of the integers less than 10^{10}, in contrast to all other moduli < 500. This seemingly aberrant behavior (since $P_{163,N,R}(x)$ must have a logarithmic density greater than $\frac{1}{2}$ on the GRH and GSH) can be explained by the low first zero of $L(s, \chi_q)$ together with an explicit formula for $P_{q,N,R}(x)$ in terms of the zeros of $L(s, \chi_q)$. The analog of the Riemann-von Mangoldt formula for nonprincipal Dirichlet characters [23, §138] gives

$$\pi_{q,a}(x) = \frac{\mathrm{li}(x)}{\phi(q)} - \frac{1}{2} \sum_{\substack{p \leqslant x^{1/2} \\ p^2 \equiv a \pmod q}} 1 - \frac{1}{\phi(q)} \sum_{\chi \bmod q} \bar{\chi}(a) \sum_{|\rho| \leqslant x} \mathrm{li}(x^\rho) + O(x^{1/3}), \tag{1.2}$$

where ρ runs over the non-trivial zeros of $L(s, \chi)$ and for non-real z,

$$\mathrm{li}(e^z) = e^z \int_0^\infty \frac{e^{-t}}{z - t}\, dt.$$

Suppose now that q has a primitive root ($c(q) = 1$). Then we obtain the relatively simple formula

$$(1.3) \qquad P_{q,N,R}(x) = \frac{\log x}{\sqrt{x}} \left(\frac{\pi(x^{1/2})}{2} + \sum_{\substack{|\rho| \leqslant x \\ L(\rho,\chi_q)=0}} \operatorname{li}(x^\rho) \right) + O(x^{-1/6} \log x).$$

If $\rho = 1/2 + i\gamma$, we also have the approximation

$$(1.4) \qquad \frac{\operatorname{li}(x^\rho) + \operatorname{li}(x^{\overline{\rho}})}{x^{1/2}/\log x} \approx \left(\frac{x^{i\gamma}}{\frac{1}{2} + i\gamma} + \frac{x^{-i\gamma}}{\frac{1}{2} - i\gamma} \right) = \frac{2\sin(\gamma \log x + \omega_\gamma)}{\sqrt{1/4 + \gamma^2}},$$

where $\omega_\gamma = \cot^{-1}(2\gamma)$. Let γ_0 be the imaginary part of the first zero of $L(s, \chi_q)$ above the real axis. When γ_0 is small, the terms in the sum on ρ in (1.3) corresponding to $\rho = 1/2 + i\gamma_0$ and its conjugate contribute a large amount and empirical observations show it often dominating the other terms of the sum. As the right side of (1.4) is periodic in $\log x$ with period $2\pi/\gamma$, we shall refer to $p = 2\pi/\gamma_0$ as the *quasi-period* for $P_{q,N,R}$. This will be described in §2. For $q = 163$ we have $p \approx 2\pi/0.2029 \approx 30.967$ so to obtain a complete period with actual prime counts, one has to compute out to about 2.810×10^{13}. Only when computers are capable of carrying actual prime counts out beyond several of these enormous quasi-periods will such counts begin to approximate the bias of 59% which we obtain using the method described in section 2 (see Figure 6 and Tables VI and VII).

In §2 we describe our method of computing Chebyshev's bias, and Figures 1–6 show plots of $P_{q,N,R}(x)$ for all q with $h(-q) = 1$. In §3 we describe how the Chowla-Selberg formula can be used to show that moduli q such that $\mathbb{Q}(\sqrt{-q})$ has relatively small class number can be expected to have a small first zero and, consequently, a longer quasi-period and lower bias; see Tables III–VIII following §3. In §4, we use a tool which has recently been developed by the second author, which will be treated in detail elsewhere, to locate sign changes of $\pi_{q,a}(x) - \pi_{q,b}(x)$ for values of x as large as 10^{19}. For example, when $x = 1.9282 \times 10^{14}$, we have $\pi_{8,1}(x) > \pi_{8,7}(x)$, a computation which takes about 10 minutes. We also examine Chebyshev's bias for $q = 8$, which does not have a primitive root.

2. Approximating Chebyshev's bias

We confine ourselves in this section to moduli q having a primitive root. The first term on the right side of (1.3) accounts for Chebyshev's bias (see [13], [15] for a combinatorial derivation of this term). By (1.4), each pair of conjugate zeros ρ, $\overline{\rho}$ produces an oscillatory term with amplitude about $2/\gamma$ and period $2\pi/\gamma$ in $\log x$. When γ is large, the right side of (1.4) is approximated well by $(2/\gamma)\sin(\gamma \log x)$. However, for small zeros this is poor and the right side of (1.4) is far superior.

As an approximation, we truncate the sum in (1.3), including only zeros with $|\gamma| \leqslant T$, and use the approximation (1.4). Specifically, we work with the scaled function

$$(2.1) \qquad P^*_{q,N,R}(x; T) = 1 + \sum_{\substack{\rho \\ 0 < \gamma \leqslant T}} \frac{2\sin(\gamma \log x + \omega_\gamma)}{\sqrt{1/4 + \gamma^2}}.$$

We also define

$$\delta(S;x,y) := \frac{1}{\log(y/x)} \int_{[x,y]\cap S} \frac{dt}{t},$$

which we call the density (or bias) of S over $[x,y]$. We compute values of $P^*_{q,N,R}(x;T)$ for logarithmically equally spaced points x with $x_0 \leqslant x \leqslant x_1$, using sample points $x = x_0 e^{\Delta k}$, $k = 0,1,2,\dots$. With $x_0 = 10^{10}$, $x_1 = 10^{300}$ and $\Delta = 0.001$ this gives 667750 data points. The bias is computed by dividing the number of points above and on the zero line by the total number of points. These produce numbers, denoted $b(q,T;x_0,x_1,\Delta)$, which are approximations of $\delta(P^*_{q,N,R}(x;T) > 0; x_0, x_1)$. Robert Rumely [34] has generously provided us with the zeros from his extensive computations, and this includes zeros to height $T = 10000$ which are accurate to within 10^{-12} for most small moduli.

It is easy to show ([33], §2) that the bias for q is equal to

$$\lim_{T\to\infty} \delta\{x \geqslant 1 : P^*_{q,N,R}(x;T) > 0\}.$$

Suppose there are M zeros $\rho = \frac{1}{2} + i\gamma_j$ $(0 \leqslant j \leqslant M-1)$ with imaginary part in $(0,T]$. If the γ_j are linearly independent and $\frac{2\pi}{\Delta}$ is not a rational linear combination of the set of the γ_j, then the numbers $1, \frac{\gamma_0\Delta}{2\pi}, \dots, \frac{\gamma_{M-1}\Delta}{2\pi}$ are linearly independent over $\mathbb{Q}$. Hence, by the Kronecker-Weyl Theorem, the vectors

$$\left(\frac{\gamma_0(\log x_0 + \Delta k) + \omega_{\gamma_0}}{2\pi}, \dots, \frac{\gamma_{M-1}(\log x_0 + \Delta k) + \omega_{\gamma_{M-1}}}{2\pi} \right)$$

are uniformly distributed modulo 1 in $[0,1]^M$. Hence (see [33, Lemma 2.3]),

$$\delta\{x : P^*_{q,N,R}(x;T) > 0\} = \lim_{y\to\infty} b(q,T;x_0,y,\Delta).$$

Therefore, with enough zeros and enough data points we can approximate the bias to any number of digits. However, the values of T, y and Δ required to obtain the bias to a given accuracy cannot be determined without more knowledge of the distribution of the zeros. The method in [33] does not lend itself immediately to a measure of how rapidly the logarithmic density of $\{1 \leqslant x \leqslant Y : P_{q,N,R}(x) > 0\}$ approaches the bias as $Y \to \infty$. This requires some quantitative bounds on linear combinations of the zeros. It does appear that moduli for which $L(s,\chi_q)$ has a small first zero require more data points to obtain the same accuracy of the bias. This will be discussed further below.

All of our computed biases using (2.1) agree well with the values given in [33]. As an example, when $q = 11$, we compute that $b(11, 10000; 10^{10}, 10^{300}, 0.001) = 0.917039\cdots$ and $b(11, 10000; e^1, e^{60000}, .05) = 0.916884\dots$. Assuming the GRH and GSH, Rubinstein and Sarnak compute a bias of $.916795\dots$. Table I gives various values of $b(q,T;x_0,x_1,\Delta)$, truncated in the last decimal place (columns B_1, B_2), plus values of the actual bias over the intervals $[1, 10^{12}]$ and $[10^4, 10^{12}]$ (columns B_3, B_4). Also shown are values of Chebyshev's bias computed by Rubinstein and Sarnak (these values were only given to 4 decimal places in [33], and were not computed for $q > 13$).

Figures 1–6 include logarithmic-scale plots of $P_{q,N,R}(x)$ for $q = 3,4,5,7,11,13,19,$ $43, 67$, and 163, as well as plots of some functions $P^*_{q,N,R}(x;T)$. Both functions tend

q	B_1	B_2	B_3	B_4	B_5
3	0.999167	0.999094	0.999981	0.999971	0.999063
4	0.995965	0.995944	0.998304	0.997456	0.995928
5	0.995558	0.995423	0.999815	0.999723	0.995422
7	0.977266	0.978452	0.979145	0.990730	0.978258
11	0.917039	0.916884	0.951735	0.948224	0.916795
13	0.946274	0.944532	0.985219	0.978192	0.944319
19	0.804196	0.804913	0.849136	0.843958	
43	0.678487	0.677984	0.700533	0.685422	
67	0.638892	0.637973	0.667905	0.684773	
163	0.601844	0.590658	0.548728	0.323093	

TABLE I. Approximations to Chebyshev's bias: $B_1 = b(q,T;10^{10},10^{300},.001)$; $B_2 = b(q,T;e^1,e^{60000},.05)$ ($T = 10000$ for $q < 17$, $T = 2500$ for $q > 17$); B_3 is the actual bias over $[1,10^{12}]$; B_4 is the bias over $[10^4,10^{12}]$; B_5 is the theoretical bias from [33] (the bias was not computed for $q > 13$).

q	T	x_0	x_1	Δ	$b(q,T;x_0,x_1,\Delta)$
19	10000	10^{10}	10^{300}	0.001	0.804196
19	1000	10^{10}	10^{300}	0.001	0.804277
19	100	10^{10}	10^{300}	0.001	0.804843
19	20	10^{10}	10^{300}	0.001	0.809789
163	2500	e^{16}	$e^{9000000}$	$\frac{2\pi}{\gamma_0}$	0.001173
163	2500	$e^{31.48}$	$e^{8980000}$	$\frac{2\pi}{\gamma_0}$	1.000000
163	2500	e^{31}	$e^{3200000}$	$\frac{2\pi}{\gamma_1-2\gamma_0}$	0.632740

TABLE II. Approximations to Chebyshev's bias, $q = 19$, different T-values; $q = 163$, different Δ-values.

to oscillate about the line $y = 1$, and for small q they rarely cross the $y = 0$ line. Graphs of $P^*_{q,N,R}(x;T)$ are produced by plotting 460 logarithmically equally spaced points between successive powers of ten. The plots of $P_{q,N,R}(x)$ are produced by dividing each power of 10 into roughly 300 logarithmically equally spaced intervals, and plotting a vertical line segment from the minimum to the maximum of the function in that interval.

Of course, computations of actual prime counts give less accurate biases. For larger q they are averaged over few quasi-periods, and for some smaller q (e.g. 3,4,5) they include very few negative regions. Also, the few primes < 100 account for $1/6$ of the integers up to 10^{12} on a logarithmic scale, and they exert great influence on bias values. This is especially evident for $q = 163$. Although the logarithmic density of the set of x giving $P_{q,N,R}(x) = 0$ is zero (on the GRH, see [33]), the subset of $[1,10^{12}]$ where $P_{q,N,R}(x) = 0$ has substantial logarithmic density. For example, $P_{4,N,R}(x) = 0$ in the intervals $[1,3)$ and $[5,7)$, and these two intervals account for 5.19% of $[1,10^{12}]$ on a logarithmic scale. Hence, whether or not these x-values are included in the computations has a large effect on the bias numbers in column B_3 of Table I. The effect of zero values of $P_{q,N,R}(x)$ is removed somewhat in column B_4, where the bias over $[10^4,10^{12}]$ is given. However, the essentially linear running time of the program using zeros of $L(s,\chi_q)$ makes it possible to estimate the bias over thousands of quasi-periods using (2.1) in a relatively short time. Whether or not zero values of $P_{q,N,R}(x)$ are included or excluded has negligible effect on the values computed in columns B_1 and B_2.

Clearly, with fixed Δ and x_0, larger values of x_1 will give more accurate bias numbers. The effect of different choices of Δ is made clear in the case of $q = 163$ (Table II). Notice that the choice $\Delta = \frac{2\pi}{\gamma_0}$ makes the first term in the sum in (2.1) constant for all sample points. The choice $\Delta = \frac{2\pi}{\gamma_1 - 2\gamma_0}$ also gives an erroneous value of the bias, since 1, $\frac{\gamma_0\Delta}{2\pi}$, $\frac{\gamma_1\Delta}{2\pi}$ are linearly independent, but the error is less in this case. Increasing T also improves the accuracy of the computed biases. However, for $q = 19$ we obtained with just 10 zeros ($T = 20$) a bias value which differs by less than 1% from the bias value using the 3184 zeros to height $T = 10000$. In Figs. 4–7, $\log_{10} x$ is written as $\log 10(x)$.

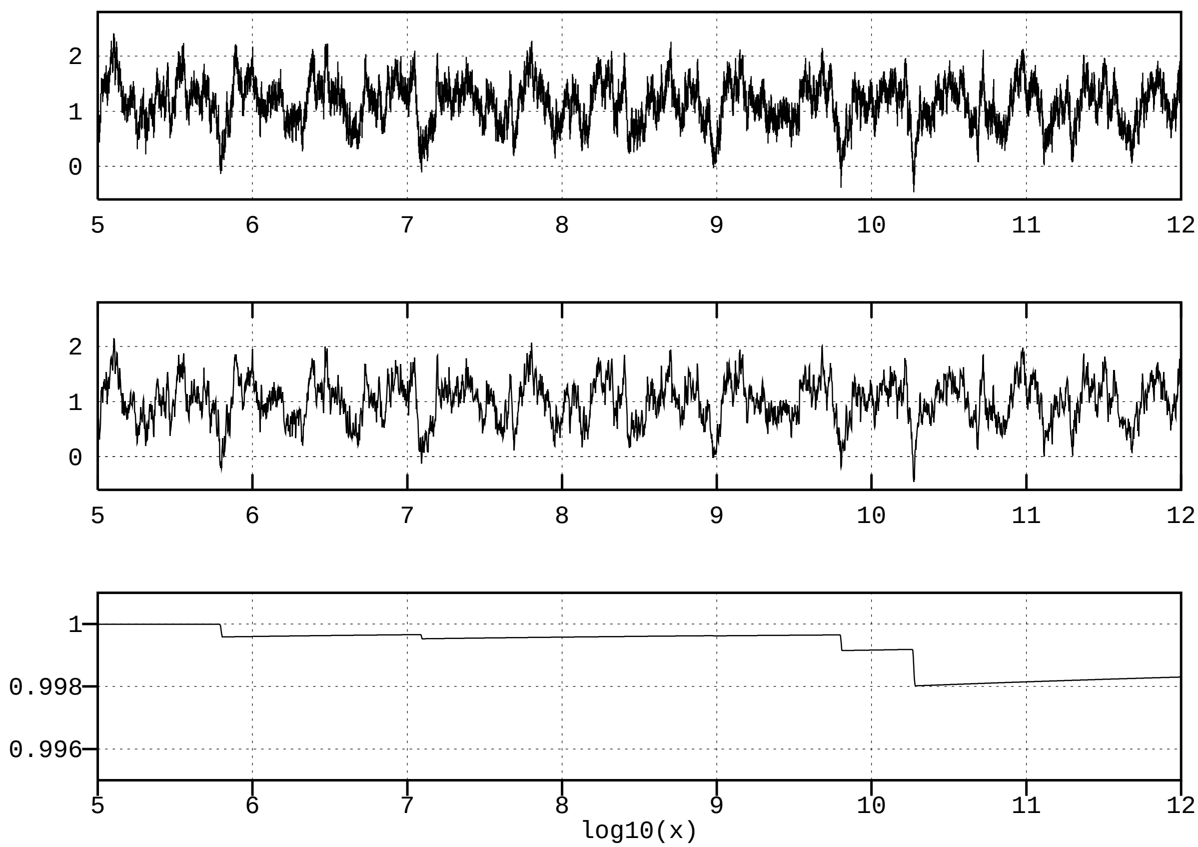

FIGURE 1. $P_{4,N,R}(x)$ (top), $P^*_{4,N,R}(x;10000)$ (middle), bias over $[1,x]$ (bottom).

Figure 1 depicts both $P_{4,N,R}(x)$ and $P^*_{4,N,R}(x;10000)$ for $x \leqslant 10^{12}$. The two functions are visually similar, and each region where $P_{4,N,R}(x) < 0$ is "detected" by the function $P^*_{4,N,R}(x;10000)$ (see also the table in §4). Figure 2 shows plots of $P^*_{q,N,R}(x;10000)$ for $q = 3$ and $q = 4$. These graphs should be a good predictor of the location of regions where $P_{q,N,R}(x)$ takes negative values. In particular, the next negative region for $q = 3$ should be at about 6.150×10^{12}, while there are probably no other negative regions before 10^{17}. Using an averaging argument,

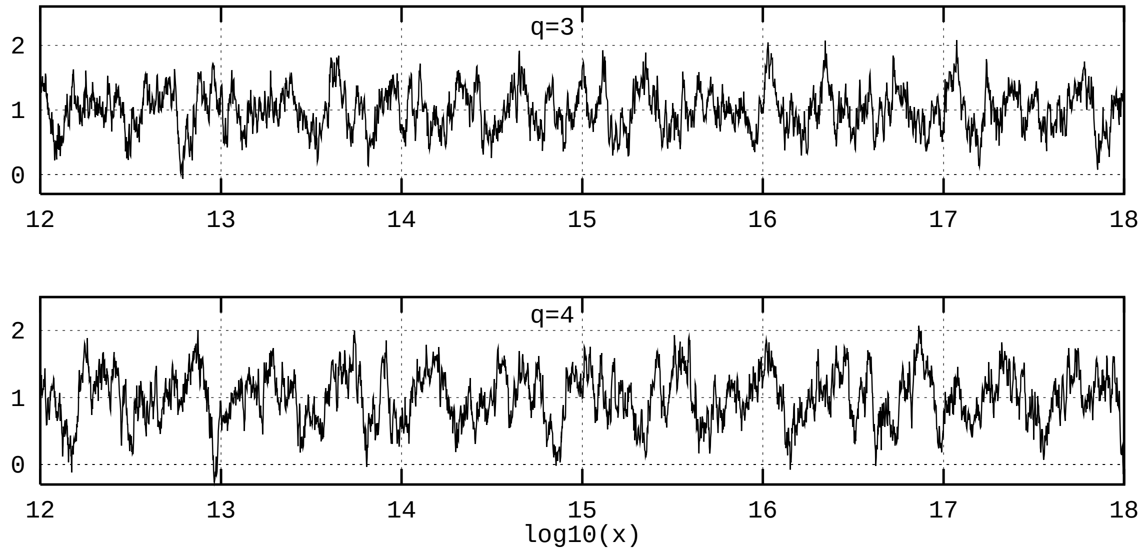

FIGURE 2. $P^*_{3,N,R}(x;10000)$, $P^*_{4,N,R}(x;10000)$.

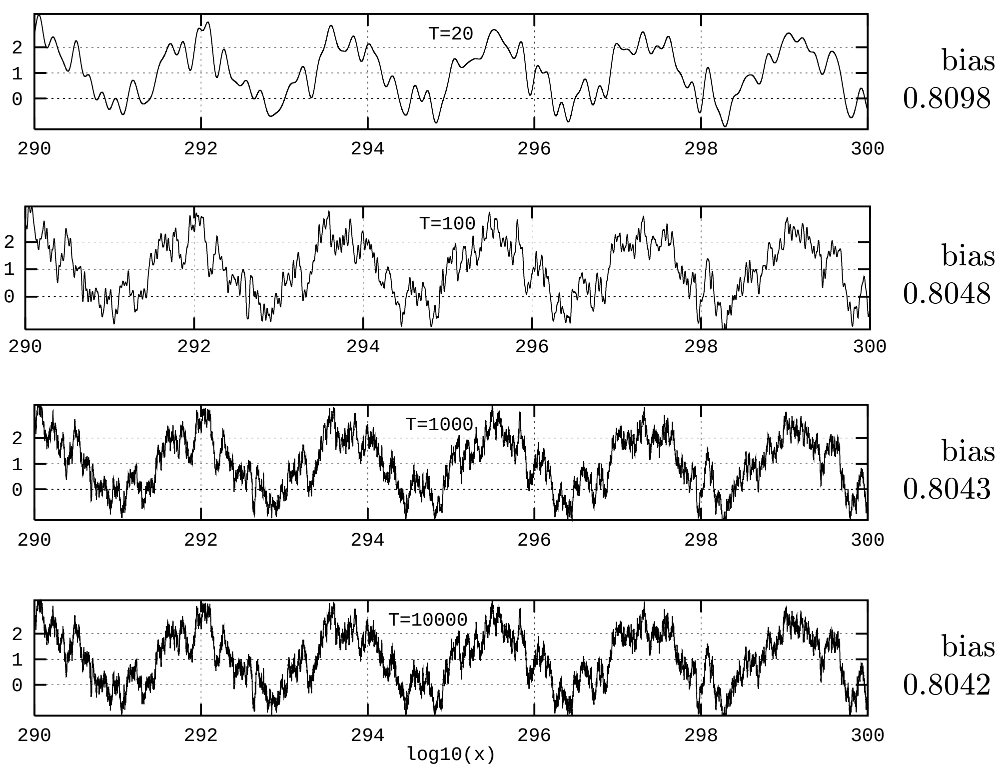

FIGURE 3. $P^*_{19,N,R}(x;T)$ for various T.

one can show that negative values of $P_{q,N,R}(x)$ in fact do exist near some points where $P^*_{q,N,R}(x;T)$ is negative (see [11]). Figure 3 shows $P^*_{19,N,R}(x;T)$ with three different values of T, together with the values of the bias obtained using (2.1) over $[10^{10}, 10^{300}]$. Figures 4, 5 and 6 show plots of $P_{q,N,R}(x)$ for $q = 3$, 5, 7, 11, 13, 19, 43, 67 and 163 obtained from a 4-day computer run. Although the bias for 5 $(0.9954\ldots)$ is very close to the bias for 4 $(0.9959\ldots)$, the first sign change in

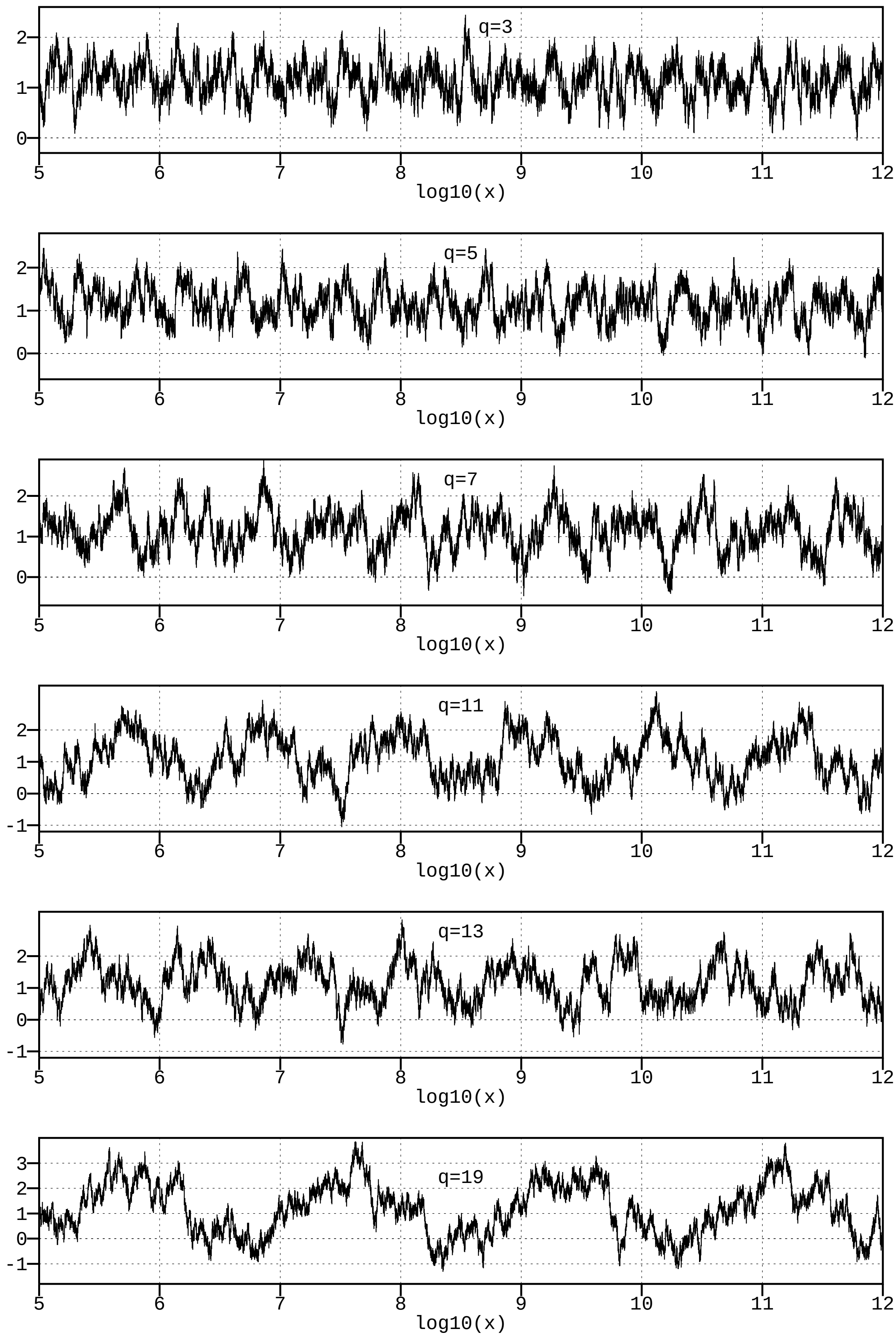

FIGURE 4. $P_{q,N,R}(x)$ for $q = 3, 5, 7, 11, 13, 19$.

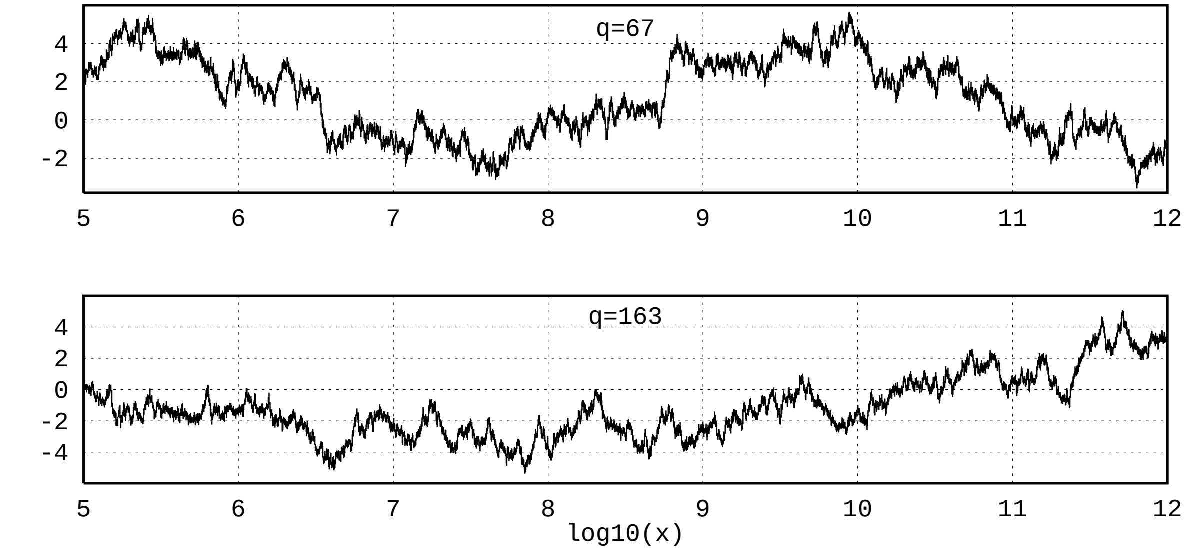

FIGURE 5. $P_{67,N,R}(x)$ and $P_{163,N,R}(x)$.

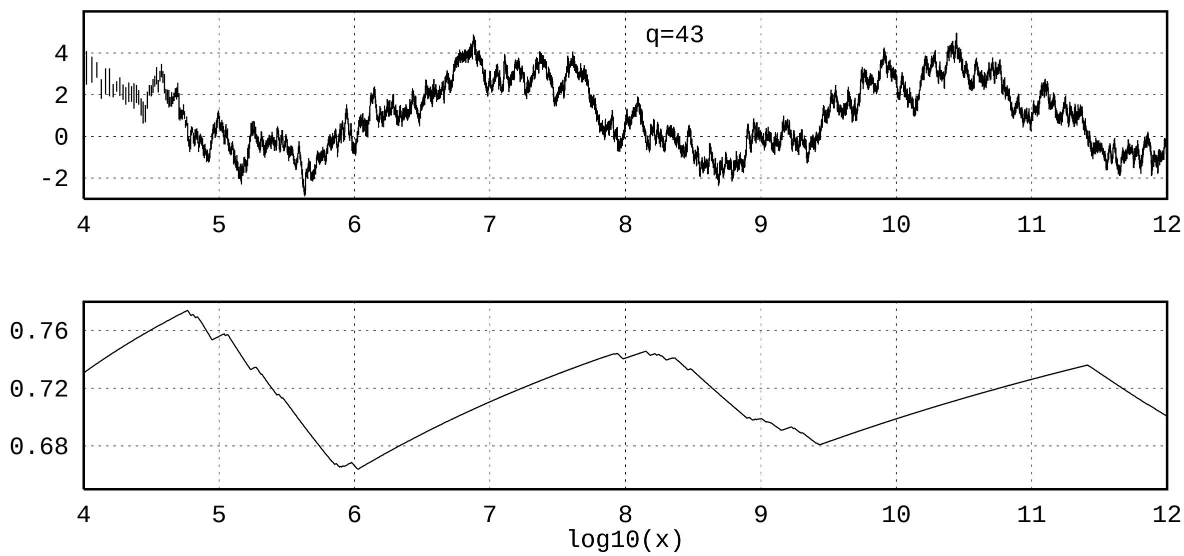

FIGURE 6. $P_{43,N,R}(x)$ (top) and bias over $[1,x]$(bottom).

$P_{5,N,R}(x)$ occurs at $x = 2082927221$. The quasi-period effect can be seen visually in the plot of $P_{11,N,R}(x)$ (there is about one quasi-period in each power of ten), and also for $q = 19$, 43 and 67. Figure 6 shows both $P_{43,N,R}(x)$ (top graph) and the logarithmic density of $\{P_{43,N,R}(y) > 0\}$ over $2 \leqslant y \leqslant x$. The large quasi-period is visually obvious, and this illustrates why actual prime counts cannot be used to accurately estimate the bias for moduli with large quasi-periods (equivalently, moduli with small first zero of $L(s, \chi_q)$). Even more dramatic is the case $q = 163$. The interval $10^5 \leqslant x \leqslant 10^{10}$ represents only about 40% of the quasi-period, and Chebyshev's bias appears to be reversed for x in this range. In fact, on a natural scale, $P_{163,N,R}(x) < 0$ for more than 93% of the integers $\leqslant 10^{10}$. This can be explained with (1.3), since a low first zero γ_0 makes the first term in the sum about

$4\sin(\gamma_0 \log x + \pi/2)$, which is negative for $\pi/2 \leqslant \gamma_0 \log x \leqslant 3\pi/2$.

3. Use of the Chowla-Selberg formula to explain the small first zero for $q = 163$

In this section we use the Chowla-Selberg formula to explain the connection between small class number of $\mathbb{Q}(\sqrt{d})$ (negative d) and small first zero of $L(s, \chi_d)$, χ_d being the quadratic character modulo $-d$. Tables III–VIII make clear that low first zero, long quasi-period, and Chebyshev bias are closely connected. Among moduli with the same class number (1,2 or 3), there is a nearly monotone decrease in the lowest first zero of $L(s, \chi_d)$ and a corresponding decrease in Chebyshev's bias. This monotonicity is weaker for class numbers 4 and 5, and disappears if all prime moduli are listed in increasing order (regardless of class number) (Table VII, leftmost columns).

Let d be a negative integer, and let $h(d)$ be the class number of the imaginary quadratic number field $\mathbb{Q}(\sqrt{d})$. Let $\chi_d(n) = (\frac{d}{n})$ be Kronecker's extension of Legendre's symbol and let

$$\zeta_{\mathbb{Q}(\sqrt{d})}(s) = \zeta(s)\ L(s, \chi_d), \tag{3.1}$$

be the Dedekind zeta function of the quadratic field $\mathbb{Q}(\sqrt{d})$.

Observe that since the first zero of $\zeta(s)$ is near $\frac{1}{2} + 14.1347i$, the zeros of $\zeta_{\mathbb{Q}(\sqrt{d})}(s)$ that lie below this value correspond to zeros of $L(s, \chi_d)$.

Let $f_1(m,n), \dots, f_{h(d)}(m,n)$ be representatives for the $h(d)$ equivalence classes of binary quadratic forms of discriminant d. Each $f_j, j = 1, \dots, h(d)$, is of the form $a_j m^2 + b_j mn + c_j n^2$ with $b_j^2 - 4a_j c_j = d$. Then [10, Chapter 6]

$$\zeta_{Q(\sqrt{d})}(s) = \frac{1}{\omega} \sum_{j=1}^{h(d)} \sum{}' \Big(a_j m^2 + b_j mn + c_j n^2 \Big)^{-s}, \qquad \Re s > 1 \tag{3.2}$$

where

$$\omega = \begin{cases} 2 & d < -4, \\ 4 & d = -4, \\ 6 & d = -3, \end{cases}$$

and where $\sum{}'$ denotes the sums over all pairs $(m,n) \in \mathbb{Z}^2$, $(m,n) \neq (0,0)$.

The Chowla-Selberg formula [8] expresses a sum of the form

$$Z(s) = \sum{}' (am^2 + bmn + cn^2)^{-s}, \qquad \Re s > 1,$$

with $d = b^2 - 4ac < 0$, $a, c > 0$, as a series of K-Bessel functions. Specifically,

$$Z(s) = 2\zeta(2s)a^{-s} + \frac{2a^{s-1}\sqrt{\pi}}{\Gamma(s)\Big(|d|^{\frac{1}{2}}/2\Big)^{2s-1}}\ \zeta(2s-1)\Gamma(s-1/2) + Q(s) \tag{3.3}$$

where

$$Q(s) = \frac{8\pi^s 2^{s-\frac{1}{2}}}{a^{\frac{1}{2}}\Gamma(s)\ |d|^{\frac{2s-1}{4}}} \sum_{n=1}^{\infty} n^{s-\frac{1}{2}}\ \sigma_{1-2s}(n) \cos\Big(\frac{n\pi b}{a}\Big) K_{s-\frac{1}{2}}\Big(\frac{\pi n\ |d|^{\frac{1}{2}}}{a}\Big),$$

$$\sigma_\omega(n) = \sum_{m|n} m^\omega,$$

and

$$K_\omega(z) = \frac{1}{2}\int_0^\infty \exp\Big(-\frac{z}{2}(y+\frac{1}{y})\Big) y^{\omega-1}dy, \qquad \Re z > 0.$$

If $|d|^{\frac{1}{2}}/a$ is large, we can use this formula to approximate $Z(s)$ because $K_{s-\frac{1}{2}}(x)$ decreases exponentially fast as $x \to \infty$. Indeed, focusing on $\Re s = 1/2$,

$$K_{it}(x) = \frac{1}{2}\int_1^\infty \exp\Big(-\frac{x}{2}(y+\frac{1}{y})\Big)(y^{it}+y^{-it})\frac{dy}{y}$$

so that

$$|K_{it}(x)| \leqslant \int_1^\infty \exp\Big(-\frac{x}{2}(y+\frac{1}{y})\Big)\frac{dy}{y} < \sqrt{\frac{\pi}{2x}}e^{-x}. \tag{3.4}$$

The last inequality can be seen by writing $y + 1/y = (y^{1/2} - y^{-1/2})^2 + 2$, changing variables $u = x^{1/2}(y^{1/2} - y^{-1/2})$, and using $y^{1/2} + y^{-1/2} \geqslant 2$.

It was conjectured by Gauss that there are exactly nine imaginary quadratic number fields with $h(d) = 1$ (namely $d = -3, -4, -7, -8, -11, -19, -43, -67, -163$), and Stark ([36], [38]) proved this conjecture. Returning to (3.2), for such d, we have

$$\zeta_{\mathbb{Q}(\sqrt{d})}(s) = \frac{1}{\omega}Z(s),$$

with

$$am^2 + bmn + cn^2 = \begin{cases} m^2 + mn + \frac{1-d}{4}n^2 & d \equiv 1 \pmod 4, \\ m^2 - \frac{d}{4}n^2, & d \equiv 0 \pmod 4, \end{cases}$$

being a representative form of discriminant d. Note that in both cases, $a = 1$, so that $|d|^{\frac{1}{2}}/a$ is, for a given d, as large as possible.

Rather than $\zeta_{\mathbb{Q}(\sqrt{d})}(s)$, it is more elegant to consider

$$\Big(\frac{|d|^{\frac{1}{2}}}{2\pi}\Big)^s \Gamma(s)\zeta_{\mathbb{Q}(\sqrt{d})}(s) = \frac{1}{\omega}\Big(\frac{|d|^{\frac{1}{2}}}{2\pi}\Big)^s \Gamma(s)\ Z(s), \tag{3.5}$$

which is real on the critical line by the functional equation for $\zeta_{\mathbb{Q}(\sqrt{d})}(s)$ (note that the gamma factor is as above since we are only considering imaginary quadratic fields).

Using (3.3) and (3.4) we find that (3.5) is

$$\frac{2}{\omega}\Big(\frac{|d|^{\frac{1}{2}}}{2}\Big)^s \pi^{-s}\Gamma(s)\zeta(2s) + \frac{2}{\omega}\Big(\frac{|d|^{\frac{1}{2}}}{2}\Big)^{1-s} \pi^{(1-2s)/2}\zeta(2s-1)\ \Gamma(s-1/2) + r_d(s)$$

where, on $\Re(s) = 1/2$,

$$|r_d(s)| \leqslant \frac{4}{\omega} \sum_{n=1}^{\infty} \frac{\sigma_0(n)}{n^{1/2}} e^{-n\pi|d|^{1/2}} \leqslant 2e^{-\pi|d|^{1/2}} + 4\frac{e^{-2\pi|d|^{1/2}}}{1 - e^{-\pi|d|^{1/2}}} \leqslant 2.02e^{-\pi|d|^{1/2}}$$

(for the 2nd to last inequality we used $\omega \geqslant 2$ and $\sigma_0(n) < 2n^{1/2}$ for $n \geqslant 2$, and, for the last inequality, $|d| \geqslant 3$). The error term $r_d(s)$ is smallest for the largest $|d|$, i.e. $|d| = 163$.

On the critical line, using the functional equation for $\zeta(s)$, the main terms may be written as

$$\frac{4}{\omega} \Re\left(\left(\frac{|d|^{\frac{1}{2}}}{2\pi}\right)^{1/2+it} \Gamma(1/2 + it)\ \zeta(1 + 2it)\right). \tag{3.6}$$

Hence, the low zeros of $\zeta_{\mathbb{Q}(\sqrt{d})}(s)$ will be close to those determined by (3.6). However, as $|t|$ grows, by Stirling's formula $|\Gamma(1/2 + it)| \sim \sqrt{2\pi}\ e^{-\pi|t|/2}$, and (3.6) quickly becomes smaller than $r_d(1/2 + it)$ as $|t|$ surpasses $2|d|^{\frac{1}{2}}$.

In Table III we give a comparison of the first few zeros of $\zeta_{\mathbb{Q}(\sqrt{d})}(s)$ and values obtained using (3.6) when $h(d) = 1$. For $d = -43$, -67, and -163 the results are quite striking.

Observe that (3.6) is zero when

$$\arg\left(\left(\frac{|d|^{\frac{1}{2}}}{2\pi}\right)^{it} \Gamma(1/2 + it)\ \zeta(1 + 2it)\right) \tag{3.7}$$

is an odd multiple of $\frac{\pi}{2}$. Now, for $|t|$ small,

$$\arg \Gamma(1/2 + it) \approx -1.96351t + 2.8048t^3 + O(t^5)$$

and

$$\arg \zeta(1 + 2it) \approx -\pi/2 + 1.15443t - .137836t^3 + O(t^5), \qquad t \neq 0$$

(computed using Maple) so that (3.7) equals

$$-\pi/2 + ((1/2) \log |d| - 2.64696)t + 2.66696t^3 + O(t^5) \pmod{2\pi}.$$

(the $-2.64696...$ here is equal to $\gamma - \log(8\pi)$). Ignoring the terms of degree higher than t^3, the above expression starts at $-\pi/2$ at $t = 0$ (this corresponds to the pole of ζ), moves away, then returns to $-\pi/2$, encountering the first zero at approximately $t = \sqrt{.9925 - 0.18748 \log |d|}$ (with less accuracy the larger this value is).

Remarks:

1) Had there been a $|d| > 199$ with $h(d) = 1$, then the coefficient of t in the Maclaurin expansion of (3.7) would be positive, and its first zero would actually be quite high, since the first multiple of $\pi/2$ encountered would then be $\pi/2$ rather than $-\pi/2$. The low zero phenomenon is not something that would have persisted. This is not surprising since the linear term in the series expansion for (3.7) is closely related to the value of $L(1/2, \chi_d)$ and hence to the GRH. As is shown in [8, §9],

$\|d\|$	actual zeros	zeros of (3.6)	$\|d\|$	actual zeros	zeros of (3.6)
3	8.03973715	7.26668581	11	2.47724371	2.47563768
3	11.24920620	10.98289812	11	6.80070840	6.86524871
3	14.13472514	13.98189084	11	8.97128436	8.65385203
3	15.70461917	16.10467160	11	10.10833735	10.63557096
3	18.26199749	18.50496541	11	13.04011532	12.42259662
4	6.02094890	6.97468313	19	1.51608375	1.51607047
4	10.24377030	10.40228755	19	5.47661417	5.47743953
4	12.98809801	12.42264167	19	7.16067082	7.15644966
4	14.13472514	15.08382463	19	9.38332632	9.41292967
4	16.34260710	16.40456028	19	10.78581062	10.69731620
7	4.47573828	4.35854220	43	0.836400774	0.836400771
7	6.84549171	7.29023926	43	3.695326872	3.695326948
7	11.16018454	10.45963096	43	6.130223479	6.130221699
7	12.48960334	12.32965902	43	7.204421761	7.204428133
7	14.13472514	14.46550375	43	8.926634047	8.926603788
8	3.57615483	3.60366640	67	0.604314750	0.604314758
8	7.43447295	7.14485743	67	3.121420750	3.121420751
8	9.50320196	10.25200930	67	5.274587236	5.274587233
8	12.34050115	11.87421786	67	6.885631366	6.885631395
8	14.13472514	13.24028870	67	7.760383041	7.760382966
			163	0.202901337	0.202901337
			163	2.368533946	2.368533946
			163	4.055068538	4.055068538
			163	5.675975035	5.675975036
			163	6.903131581	6.903131581

TABLE III. Actual Zeros of $L(s,\chi_d)$ vs. those of (3.6) for $h(d) = 1$. Observe that the approximation is best for $|d| = 163$.

had there been a $|d| > 199$ with $h(d) = 1$, the value of $L(1/2, \chi_d)$ would have been negative in violation of the GRH for $L(s, \chi_d)$ (since, by the class number formula, $L(1, \chi_d) > 0$, so a negative value at $s = 1/2$ would imply a zero somewhere on $(1/2, 1)$).

2) Let $1/2+i\gamma_d$ be the first zero (with γ_d smallest) of $L(s,\chi_d)$. From conjectures regarding the distribution of low lying zeros of L-functions [20], one expects, that, on average, $(\gamma_d/(2\pi))\log(|d|/\pi)$ should equal .78. (see [32]). So, the zero $1/2 + .202901337i$ of $L(s, \chi_{163})$ is indeed quite low (with its normalized value equal to .127524729).

3) One can also investigate what happens when $h(d) > 1$, $d < 0$. In that case, a set of representatives for the $h(d)$ equivalence classes of binary quadratic forms is

Some $h(d) = 3$ examples			Some $h(d) = 5$ examples		
$\lvert d\rvert$	actual zeros	zeros of (3.8)	$\lvert d\rvert$	actual zeros	zeros of (3.8)
23	2.87133984	2.87134326	47	2.217378213	2.22844809007
23	4.21518980	4.21501327	47	3.773974388	3.70387074661
23	6.73118915	6.73058016	47	5.023033964	5.15965904330
23	8.33484903	8.34313985	47	7.402618666	7.10350784569
23	10.63387123	10.60201591	47	8.118457993	8.41675763449
31	2.03498242	2.0349819103	79	1.466837987	1.47057672725
31	4.78968470	4.7896509428	79	3.441804066	3.39927010637
31	5.68644602	5.6864949507	79	5.019924093	5.36241173560
31	7.33591057	7.3361039491	79	6.257024678	5.66545017728
31	10.18385049	10.1796410431	79	6.762211042	7.12589602793
59	1.606455246	1.6088832927	787	0.631185188	0.63104761130
59	2.773359145	2.7652114200	787	1.390917921	1.39132633669
59	5.323877349	5.3590667021	787	2.798945295	2.79795419479
59	7.325391655	7.1447672724	787	4.286551977	4.29209340473
59	8.254212627	10.6399730880	787	4.973877955	4.96361223322
83	1.222920484	1.2231247949	947	0.289813660	0.28981220311
83	2.851649031	2.8501169772	947	2.021693610	2.02171726431
83	4.438368200	4.4427744279	947	2.742729316	2.74265875113
83	6.917592799	6.8733873005	947	3.604962603	3.60507568383
83	7.926910976	10.2046267235	947	4.677476492	4.67732014233
883	0.260999143	0.26150380157			
883	1.420753133	1.41924142972			
883	2.948889446	2.95571899768			
883	3.826164779	3.81211993259			
883	5.143970727	5.18011427328			
907	0.249926489	0.24965727136			
907	1.413631409	1.41441808670			
907	2.939204779	2.93563189434			
907	3.794263347	3.80159243875			
907	5.164186740	5.14422918306			

Table IV. Some class number 3 and 5 examples.

given by:

$$\{(a,b,c)\in\mathbb{Z}^3 \,|\, b^2-4ac=d, (a,b,c)=1, a>0, -a<b\leqslant a, c\geqslant a \text{ with } c>a \text{ if } b<0\}.$$

Substituting (3.3) into (3.2) for each such form and dropping the $Q(s)$ term, we are led to investigate

$$\sum_{j=1}^{h(d)} a_j^{-1/2} \Re\left(\left(\frac{|d|^{\frac{1}{2}}}{2\pi} \right)^{it} a_j^{-it} \; \Gamma(1/2+it) \; \zeta(1+2it) \right). \tag{3.8}$$

The latter step (dropping the $Q(s)$ term) is not valid for general d. However, each $a_j < \sqrt{|d|/3}$, and so each K_{it} term is, using (3.4), at most .002328 in size, if not much smaller. Furthermore, the presence of the $a_j^{1/2}$ in the denominator of $Q(s)$ helps slightly as does the $\cos(n\pi b_j/a_j)$ term which leads to cancellation as we sum over j. In short, it seems, numerically, that (3.8) can be used to study the low zeros of $L(s,\chi_d)$ to the first 2-3 decimal places. However, as d increases or h increases, the approximation (3.8) becomes less accurate. See Table IV where actual zeros are compared to those of (3.8) for several values of $d<0$. Observe, however, in Table IV that the nearly monotone decrease in the size of the first zero as $|d|$ increases is not just a class number 1 phenomenon, though it weakens as h increases.

$\lvert d\rvert$	actual zeros	zeros of (3.8)
1000000103	0.345939372	0.34383231663
1000000103	0.411877310	0.41441458500
1000000103	0.877544016	0.87587286032
1000000103	1.246499176	1.25028137102
1000000663	0.092368733	0.09155513661
1000000663	0.441328789	0.44209903514
1000000663	0.747623494	0.74670904731
1000000663	1.285017617	1.28793823979
1000011583	0.008057619	not detected!
1000011583	0.592419804	0.59357041358
1000011583	0.863743687	0.86095747438
1000011583	1.204354203	1.21162536229

TABLE V. Some examples with $|d|$ near 10^9.

Table V lists some of the zeros of $L(s,\chi_d)$ compared with the zeros of (3.8) for some large d. Observe that for $|d| = 1000011583$, one of the zeros is not detected by (3.8). This shows that, as d grows, we cannot ignore the importance of the K-Bessel terms in approximating $L(s,\chi_d)$. The column of actual zeros of $L(s,\chi_d)$ come from a computation done in [32]. Also note in Table IV the poor approximation for the 5th zeros for $|d| = 59, 83$. Here it seems that (3.8) skips over two of the zeros (i.e. misses one sign change) in each case. This is not too surprising since the K-Bessel sum becomes more significant as $\Im s$ increases.

Tables VI and VII tabulate information about the lowest zero of $L(s,\chi_d)$ for all d with class number $\leqslant 5$, as well as all prime $q \leqslant 67$. For values of $h(d)$ see [1], [2], [7]. For $q > 13$ and $h(-q) = 1$ the biases are computed using (2.1).

$h(-d)=1$		$h(-d)=2$		$h(-d)=3$		$h(-d)=5$	
d	γ_0	d	γ_0	d	γ_0	d	γ_0
163	0.2029	427	0.2499	907	0.1447	2683	0.1566
67	0.6043	403	0.2882	883	0.2609	2347	0.2698
43	0.8364	267	0.3488	643	0.3424	2203	0.1692
19	1.5160	235	0.4754	547	0.4460	1867	0.2242
11	2.4772	232	0.3106	499	0.3878	1747	0.3974
8	3.5761	187	0.5844	379	0.5053	1723	0.3689
7	4.4757	148	0.5048	331	0.5652	1123	0.4790
4	6.0209	123	0.6936	307	0.6568	1051	0.4120
3	8.0397	115	0.7969	283	0.6955	947	0.2898
		91	0.9184	211	0.7874	787	0.6311
		88	0.7546	139	1.0438	739	0.5695
		52	1.0926	107	1.0153	691	0.5557
		51	1.2678	83	1.2229	683	0.4304
		40	1.3205	59	1.6064	619	0.6099
		35	1.6232	31	2.0349	571	0.6977
		24	1.9771	23	2.8713	523	0.8967
		20	2.3589			443	0.6198
		15	3.0570			347	0.7398
						227	0.9838
						179	1.1174
						131	1.4899
						127	1.0356
						103	1.2047
						79	1.4668
						47	2.2173

$h(-d)=4$

d	γ_0	d	γ_0	d	γ_0
1555	0.1447	667	0.5860	291	0.7141
1507	0.2453	627	0.4460	280	0.6427
1435	0.1369	595	0.5420	259	0.9403
1411	0.0779	568	0.3839	228	0.6715
1387	0.2979	555	0.4525	219	0.8794
1243	0.3406	532	0.3995	203	0.8489
1227	0.1304	520	0.3846	195	0.9805
1027	0.3466	483	0.5364	184	0.8434
1012	0.1066	435	0.5552	168	0.8307
1003	0.4187	408	0.4124	155	1.0101
955	0.3122	388	0.5183	136	1.0345
795	0.3025	372	0.4515	132	0.9812
772	0.2568	355	0.7814	120	1.0388
763	0.5035	340	0.5616	84	1.3442
760	0.2158	328	0.5909	68	1.5009
723	0.3868	323	0.6102	56	1.7894
715	0.4862	312	0.5271	55	1.5980
708	0.1467	292	0.6428	39	2.1536

TABLE VI. The first zero of $L(s,\chi_d)$ (truncated) for d with $h(-d) \leqslant 5$.

q	γ_0	p
3	8.0397	0.7815
5	6.6484	0.9450
7	4.4757	1.4038
11	2.4772	2.5363
13	3.1193	2.0142
17	3.7281	1.6853
19	1.5160	4.1443
23	2.8713	2.1882
29	1.7938	3.5027
31	2.0349	3.0875
37	2.0572	3.0542
41	2.4753	2.5383
43	0.8364	7.5121
47	2.2173	2.8336
53	1.2871	4.8816
59	1.6064	3.9112
61	1.9445	3.2311
67	0.6043	10.3972
71	2.1795	2.8827
73	2.5980	2.4183
79	1.4668	4.2834

$h(-q) = 1$

q	γ_0	p	bias
3	8.0397	0.7815	99.90%
4	6.0209	1.0435	99.54%
7	4.4757	1.4038	97.82%
11	2.4772	2.5363	91.67%
19	1.5160	4.1443	80.65%
43	0.8364	7.5121	67.75%
67	0.6043	10.3972	63.79%
163	0.2029	30.9667	59.08%

TABLE VII. Smallest zero and quasi-period for prime $q \leqslant 79$; Chebyshev's bias, smallest zero of $L(s, \chi_d)$, and quasi-period for $h(-q) = 1$. γ_0=imaginary part of smallest zero of $L(s, \chi_q)$; p=quasi-period $= 2\pi/\gamma_0$. All values are truncated.

class number	largest $\|d\|$	first zero	smallest $\|d\|$	first zero
1	163	.202901337	3	8.03973715
3	907	.249926489	23	2.87133984
5	2683	.156678803	47	2.21737821
7	5923	.154845332	71	2.17958092
9	10627	.050291508	199	1.30027235
11	15667	.164688811	167	1.56701462
13	20563	.108750288	191	1.65670887
15	34483	.074760508	239	1.60129099
17	37123	.327102331	383	1.24749268
19	38707	.219545154	311	1.77809609
21	61483	.150744347	431	1.39727670
23	90787	.126125031	647	1.15586233

TABLE VIII. The first zero of $L(s, \chi_d)$ (truncated) for the largest and smallest discriminants with odd class number < 25. The values of the discriminant are taken from [1].

We have observed that for class numbers 1,3,5,7, and 9 that the smallest first zero corresponds in every case with the largest $|d|$ and the largest first zero with the smallest $|d|$ (see Table VIII). In general, this is not always case. For example, when $h = 11$, $d = -13003$, the first zero is .0996261599, and when $h = 15$, $d = -17923$, the first zero is .03098579949. In the context of Chebyshev's bias, actual prime counts for these moduli (especially 10627 and 17923) are even more misleading than for $q = 163$ as they cover only a small portion of one quasi-period.

4. Sign changes of $\Delta_{q,a,b}(x)$ when $q = 3, 4, 5$, or 8

Sign changes of $\Delta_{4,3,1}(x)$ occur infrequently and $\Delta_{3,2,1}(x)$ even more infrequently. These sign changes occur in widely separated regions when the oscillatory terms in (2.1) overcomes the constant 1. The starting point x_f of these regions (the first value of x for which Δ is negative) in these regions are given below.

	Region	X_f	
	1	26,861	Leech [24], 1957
	2	616,841	Leech [24], 1957
	3	12,306,137	Lehmer 1969
$q = 4$	4	951,784,481	Lehmer 1969
	5	6,309,280,709	Bays and Hudson [4], 1979
	6	18,465,126,293	Bays and Hudson [4], 1979
	7	1,488,478,427,089	Bays and Hudson 1996

	Region	X_f	
$q = 3$	1	608,981,813,029	Bays and Hudson [3], 1978

In [4], Bays and Hudson computed $\Delta_{8,5,1}(x) = -1$ for $x = 588,067,889$. No further axis crossing regions were found for $\Delta_{8,b,1}(x)$ for $x < 10^{12}$. Indeed the bias for $q = 8$ is higher than for $q = 3$ or 4 because $c(q) = 3$ in (2.1) and the lowest zero for each of the three nonprincipal L-functions modulo 8 is relatively high; see [35], [21, p. 302]. In fact, the bias over $[1, 10^{12}]$ is exactly 1.000000. Figure 7 shows $P_{8,N,R}(x)$ and a plot of the first negative region for $P^*_{8,N,R}(x; 10000)$. The latter is possibly the first region where $P_{8,N,R}(x)$ becomes negative.

Sign changes for much larger x can be obtained through the use of (2.1) together with a generalization to arbitrary progressions of the method used by Lehman [25] to find sign changes of $\pi(x) - \mathrm{li}(x)$. Details will appear in [11].

Recently, the second author has succeeded in writing an efficient computer program to compute $\pi_{q,a}(x)$. It is based on Hudson's [14] generalization to arbitary arithmetic progressions of the well-known formula of E. Meissel [27] and the improvement of Meissel's algorithm given by Lagarias, Miller, and Odlyzko [22]. This will be discussed in detail in a future paper. These sign changes were found by first using the zeros of the L-functions (using a truncated form of (1.2)) to isolate potential sign changes, and then using the computer program to find exact values of $\pi_{q,a}(x)$. For example, the program required about 10 minutes on a Sun Ultra-10 workstation to find that $\pi_{8,1}(x) > \pi_{8,7}(x)$ at 1.9282×10^{14}.

The program can also be used to rapidly verify 3 new sign change regions which would take, at the least, many weeks (even years) to compute using the sieve of Eratosthenes. The values of x obtained are close to the minimum value of $P^*_{q,N,R}(x; 10000)$ in the region considered. The values were obtained by using the zeros of the relevant L -functions to identify "candidates" for sign changes and then using the generalized Meissel program to verify the sign changes. The 8th

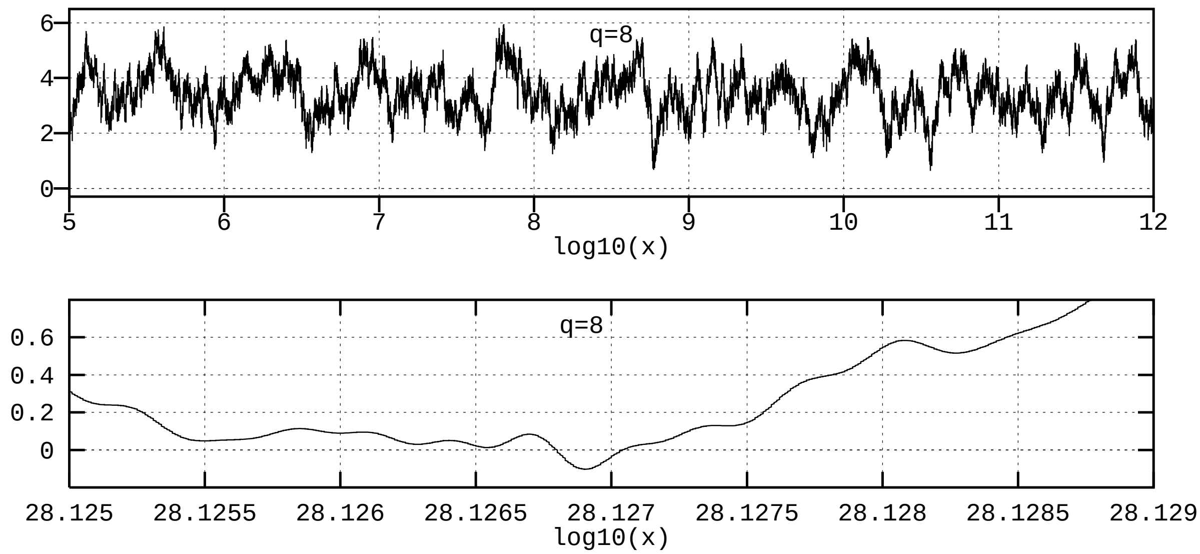

FIGURE 7. $P_{8,N,R}(x)$ (top); $P^*_{8,N,R}(x;10000)$ (bottom).

region of integers x with $\pi_{4,3}(x) < \pi_{4,1}(x)$ occurs for x in the neighborhood of $x = 9.318 \times 10^{12}$ (verified with Ford's program in a few minutes). The third region of integers x with $\pi_{3,2}(x) < \pi_{3,1}(x)$ likely occurs in the neighborhood of $3.96555843 \times 10^{19}$ (based on computations using (2.1)), a value computable using the generalized Meissel program but requiring considerable computer time.

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