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PRIMES IN ARITHMETIC PROGRESSIONS

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ABSTRACT. Strengthening work of Rosser, Schoenfeld, and McCurley, we establish explicit Chebyshev-type estimates in the prime number theorem for arithmetic progressions, for all moduli $k \leq 72$ and other small moduli.

1. INTRODUCTION

In many applications it is useful to have explicit error bounds in the prime number theorem for arithmetic progressions. Furthermore, in numerical work, such estimates for small moduli are often the most critical. Let us recall the usual notation, where $x \geq 0$ is real:

$$\theta(x;k,l) = \sum_{\substack{p \equiv l(k) \\ p \leq x}} \ln(p), \qquad \text{where } p \text{ denotes a prime number;}$$

$$\psi(x;k,l) = \sum_{\substack{n \equiv l(k) \\ n \leq x}} \Lambda(n), \qquad \text{where } \Lambda(n) \text{ is Von Mangoldt's function.}$$

Here we obtain estimates of the type

$$(1-\epsilon)\frac{x}{\varphi(k)} \leq \theta(x;k,l) \leq \psi(x;k,l) \leq (1+\epsilon)\frac{x}{\varphi(k)}$$

for all moduli $k \leq 72$, all composite $k \leq 112$, and 48 other moduli; $\varphi(k)$ denotes Euler's function.

To obtain such estimates for the progression with modulus 1, Rosser and Schoenfeld ([8, 9, 11]) developed an analytic method which combines a numerical verification of the Riemann Hypothesis to a given height together with an explicit asymptotic zero-free region. McCurley ([3, 4, 5, 6]) adapted this method to progressions with modulus $k > 1$. However, except for $k = 3$, he got poor numerical results because of the paucity of numerical work on the Generalized Riemann Hypothesis. Recently, the second author [10] did such computations, and we get reasonably good results for all moduli accessible from his list. In fact, the results are better than one would expect, owing to a smoothing process implicit in the method, explained in §4.4.

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Our main theoretical result is Theorem 4.3.2, which provides an easy way to get applications like Theorem 1 below. In Theorem 3.6.2 we also establish a zero-free region for Dirichlet L-functions, valid for heights $|t| \geq 1000$, which improves somewhat on the region found by McCurley [4].

Finally, we mention that this paper is an important step in a forthcoming paper by the first author, in which it is proved that *every* even integer can be written as a sum of at most 6 primes.

Our main numerical result is the following:

Theorem 1. *For any triple (k, ε, x_0) given by Table 1 (see §5), and any l prime to k, we have*

$$\max_{1\leq y\leq x} |\theta(y;k,l) - \frac{y}{\varphi(k)}| \leq \varepsilon \frac{x}{\varphi(k)} \quad \text{for } x \geq x_0,$$
$$\max_{1\leq y\leq x} |\psi(y;k,l) - \frac{y}{\varphi(k)}| \leq \varepsilon \frac{x}{\varphi(k)} \quad \text{for } x \geq x_0.$$

For example, if $k = 1$,

$$\varepsilon = 0.000213 \ \text{ for } \ x_0 = 10^{10}, \quad \varepsilon = 0.000015 \ \text{ for } \ x_0 = 10^{13},$$
$$\varepsilon = 0.000001 \ \text{ for } \ x_0 = 10^{30}.$$

If $k \leq 13$, one can take

$$\varepsilon = 0.004560 \ \text{ for } \ x_0 = 10^{10}, \quad \varepsilon = 0.002657 \ \text{ for } \ x_0 = 10^{13},$$
$$\varepsilon = 0.002478 \ \text{ for } \ x_0 = 10^{30}, \quad \varepsilon = 0.002020 \ \text{ for } \ x_0 = 10^{100}.$$

If $k \leq 72$, one can take

$$\varepsilon = 0.023269 \ \text{ for } \ x_0 = 10^{10}, \quad \varepsilon = 0.011310 \ \text{ for } \ x_0 = 10^{13},$$
$$\varepsilon = 0.010484 \ \text{ for } \ x_0 = 10^{30}, \quad \varepsilon = 0.008672 \ \text{ for } \ x_0 = 10^{100}.$$

We have supplemented these analytic results with a tabulation up to 10^{10}, obtaining surprisingly uniform bounds:

Theorem 2. *For all moduli k in Table 1, and all l prime to k, uniformly for $1 \leq x \leq 10^{10}$,*

$$\max_{1\leq y\leq x} \left|\theta(y;k,l) - \frac{y}{\varphi(k)}\right| \leq 2.072\sqrt{x},$$
$$\max_{1\leq y\leq x} \left|\psi(y;k,l) - \frac{y}{\varphi(k)}\right| \leq 1.745\sqrt{x}.$$

In particular, for a bound of the type in Theorem 1 when $x_0 \leq x \leq 10^{10}$, one can take

$$\varepsilon = 2.072\varphi(k)/\sqrt{x_0}.$$

Sharper bounds for individual moduli are given in Table 2 (see §5). Especially, for $k = 5$ or $k \geq 7$, the constant 1.745 in the error bound for $\psi(x;k,l)$ can be replaced by 1.000, and for $k = 1$ it can be replaced by $\sqrt{2}$.

2. Numerical results about the GRH

Throughout the paper, p always stands for a prime and the gcd of k and l is written (k,l).

The letter ρ always denotes a nontrivial zero of a Dirichlet L-function, i.e., a zero with $0<\Re\rho<1$. We will always write $\rho=\beta+i\gamma$.

Given a Dirichlet L-function $L(s,\chi)$, the set of its zeros with $0<\beta<1$ will be denoted by $\mathcal{Z}(\chi)$. Thus, if χ' is induced by χ, then $\mathcal{Z}(\chi')=\mathcal{Z}(\chi)$.

Given a nonnegative real number H, we will say that $L(s,\chi)$ satisfies GRH(H), the Generalized Riemann Hypothesis to height H, if all its nontrivial zeros with $|\gamma|\le H$ verify $\beta=\frac{1}{2}$.

It is possible to prove or disprove GRH(H) for any given H and $L(s,\chi)$ with only a finite amount of computation. Rumely [10] did such computations, obtaining:

Theorem 2.1.1.

∘ *Every L-function associated with a Dirichlet character of conductor* $k\le 13$ *satisfies GRH*(10000).

∘ *Every L-function associated with a Dirichlet character of conductor in the sets*

$$\{k\le 72\},$$
$$\{k\le 112, k \text{ not prime}\},$$
$$\{116,117,120,121,124,125,128,132,140,143,144,$$
$$156,163,169,180,216,243,256,360,420,432\}$$

satisfies GRH(2500).

Sharper results for individual moduli, together with bounds for the sums

$$\sum_{\substack{|\mathrm{Im}(\rho)|\le H\\ \rho\in\mathcal{Z}(\chi)}}\frac{1}{|\rho|}$$

may be found in Tables 1 and 5 of [10]; these results were used in computing Table 1 below. The following facts about the Riemann zeta function were also used:

$\zeta(s)$ satisfies GRH(545439823.215)
(van de Lune, te Riele, and Winter [2]);

for $H=12030$, $\displaystyle\sum_{|\mathrm{Im}(\rho)|\le H}\frac{1}{|\rho|}\le 9.056$
(R. S. Lehman, cf. Rosser and Schoenfeld [9]).

3. Zero-free regions for L-functions

This part follows McCurley [4] and some evaluations are taken directly from McCurley's paper without being re-established. We employ a device due to Stechkin [12] to widen the zero-free region.

Let $s=\sigma+it$ and $s_1=\sigma_1+it$ be complex numbers with $|t|\ge 1000$ satisfying

$$\begin{cases} 1<\sigma\le\dfrac{1+\sqrt{2}}{2}\le\sigma_1\le\dfrac{1+\sqrt{5}}{2},\\ \sqrt{\sigma(\sigma-1)}+\sqrt{\sigma_1(\sigma_1-1)}=1 \end{cases}\tag{3.1}$$

and put $\kappa(\sigma) = \frac{1+\frac{4}{5}\sqrt{\sigma-1}}{\sqrt{5}}$. Note that $1/\sqrt{5} \le \kappa(\sigma) \le 0.61004$, and that $\sigma \ge \kappa(\sigma)\sigma_1$.

These assumptions on σ and σ_1 will hold throughout the paper.

We define the auxiliary function

$$f(t,\chi) = \Re\left(\sum_{n\ge 1}\Lambda(n)\left(\frac{1}{n^{\sigma}} - \frac{\kappa(\sigma)}{n^{\sigma_1}}\right)\frac{\chi(n)}{n^{it}}\right) \tag{3.2}$$

and introduce constants

$$\begin{cases}\varepsilon_1 = 0.0067,\\ \varepsilon_2 = 10^{-6},\end{cases} \qquad \begin{cases} a_0 = 11.1859355312082048,\\ a_1 = 19.073344004352,\\ a_2 = 11.67618784,\\ a_3 = 4.7568,\\ a_4 = 1,\\ A = a_1+a_2+a_3+a_4 = 36.506331844352.\end{cases} \tag{3.3}$$

3.1. A device of Stechkin.

Lemma 3.1.1 (Stechkin)**.** *Let z be a complex number with $0 \le \Re z \le 1$. Put*

$$F(s,z) = \Re\Big\{\frac{1}{s-z} + \frac{1}{s-(1-\bar z)}\Big\}.$$

Then

$$F(s,z) \ge \kappa(\sigma)F(s_1,z).$$

Moreover, if $\Im z = \Im s$ and $\frac12 \le \Re z \le 1$, and if $S(\sigma) = -\frac{1}{\sigma} + \kappa(\sigma)\left(\frac{1}{\sigma_1} + \frac{1}{\sigma_1-1}\right)$, then

$$-\Re\left(\frac{1}{s-(1-\bar z)}\right) + \kappa(\sigma)F(s_1,z) \le S(\sigma).$$

Proof. The first inequality is implicit in Stechkin [12]: see the top line on p.132 of the English translation. For the second inequality, note that when $\Im z = \Im s = t$, then, writing $z = \beta + it$, the left side of the inequality becomes

$$-\frac{1}{\sigma-1+\beta} + \kappa(\sigma)\left(\frac{1}{\sigma_1-\beta} + \frac{1}{\sigma_1-1+\beta}\right).$$

For $\frac12 \le \beta \le 1$, both terms are increasing with β. Taking $\beta = 1$ we obtain the result. □

As will be seen later, we will only need to consider σ in the interval $[1, 1.062]$. Although we will not use this, it can be shown that on $[1, 1.062]$

$$S(\sigma) = 2\sqrt{\Delta} + \frac{86}{25}\Delta + \mathcal{O}(\Delta^{3/2}),$$

where $\Delta = \sigma - 1$ and the implied constant can be taken as 18. Furthermore, throughout the interval,

$$2\sqrt{\Delta} + 3\Delta \le S(\sigma) \le 2\sqrt{\Delta} + 5\Delta.$$

3.2. Handling the Γ-factor.

Lemma 3.2.1. *If $0 \le a \le 2$, $\varepsilon_1 = 0.0067$ and $\varepsilon_2 = 10^{-6}$, then for $|t| \ge 1000$*

$$\frac{1}{2}\Re\left\{\frac{\Gamma'}{\Gamma}(\frac{s+a}{2}) - \kappa(\sigma)\frac{\Gamma'}{\Gamma}(\frac{s_1+a}{2})\right\} \le \frac{1-\kappa(\sigma)}{2}\left(\ln\left(\frac{|t|}{2}\right) + \varepsilon_1 - 10\varepsilon_2\right).$$

Proof. We follow Lemma 2 of McCurley ([4]). Since $\Re\left(\frac{\Gamma'}{\Gamma}(z)\right)$ is invariant under $z \to \bar{z}$, we have for $z = x + iy$, with $x > 0$:

$$\Re\frac{\Gamma'}{\Gamma}\left(\frac{z+a}{2}\right) = \ln\left(\frac{|y|}{2}\right) + \frac{1}{2}\ln\left|1 + \left(\frac{x+a}{y}\right)^2\right| - \frac{x+a}{(x+a)^2+y^2} + \Theta(y) \tag{3.2.1}$$

where $|\Theta(y)| \le \frac{1}{|y|}\cdot\left[\frac{\pi}{2} - \arctan\left(\frac{x+a}{|y|}\right)\right] \le \left|\frac{\pi}{2y}\right|$. We apply this, taking $z = s, s_1$. Using $\sigma \ge \kappa(\sigma)\sigma_1$, we find

$$\begin{cases} -\dfrac{\sigma+a}{(\sigma+a)^2+t^2} + \kappa(\sigma)\dfrac{\sigma_1+a}{(\sigma_1+a)^2+t^2} \le 0, \\ \dfrac{1}{4}\ln\left|1+\left(\dfrac{\sigma+a}{t}\right)^2\right| \le \dfrac{2.58}{t^2}, \\ \dfrac{1}{2}(1+\kappa(\sigma))\Theta(t) \le \dfrac{1.26453}{|t|}. \end{cases}$$

These facts, together with $(1-\kappa(\sigma))/2 \ge 0.19498$, yield the result. □

3.3. Approximating $f(t,\chi)$. Here the character which is the argument of $f(t,\cdot)$ is assumed to be primitive.

Lemma 3.3.1. *If χ_0 is the trivial character and*

$$E(\sigma) = 1.08699 + 1.40018\sqrt{\sigma-1} + 1.86576(\sigma-1) + 2.32244(\sigma-1)^{3/2},$$

then for $1 < \sigma \le 1.062$,

$$f(0,\chi_0) \le \frac{1}{\sigma-1} - E(\sigma).$$

Proof. We follow McCurley's Lemma 3 ([4]). We have for any complex number z

$$-\frac{\zeta'}{\zeta}(z) = \frac{1}{z-1} - \frac{\ln(\pi)}{2} + \frac{\Gamma'}{2\Gamma}(\frac{z+2}{2}) - \sum_{\rho\in\mathcal{Z}(\chi_0)}\frac{1}{z-\rho}, \tag{3.3.1}$$

where $\sum_\rho$ is to be understood as $\lim_{T\to\infty}\sum_{\rho,|\gamma|\le T}$. We use (3.3.1) for $z = \sigma$. Since for any zero of ζ, we have $|\gamma| \ge 10 \ge \sigma - \beta$, we see that

$$\frac{\sigma-\beta}{(\sigma-\beta)^2+\gamma^2} \ge \frac{1-\beta}{(1-\beta)^2+\gamma^2}. \tag{3.3.2}$$

It follows that

$$f(0,\chi_0) = -\frac{\zeta'}{\zeta}(\sigma) + \kappa(\sigma)\frac{\zeta'}{\zeta}(\sigma_1)$$
$$\le \frac{1}{\sigma-1} - \frac{\ln(\pi)}{2} + \frac{\Gamma'}{2\Gamma}\big(\frac{\sigma+2}{2}\big) - \Re\left(\sum_{\rho\in\mathcal{Z}(\chi_0)}\frac{1}{1-\rho}\right) + \kappa(\sigma)\frac{\zeta'}{\zeta}(\sigma_1).$$

We recall McCurley's estimate (taken from the proof of Lemma 3 of [4])

$$\frac{\Gamma'}{2\Gamma}\big(\frac{\sigma+2}{2}\big) \le 1 - \frac{C_0}{2} - \ln(2) + (\frac{\pi^2}{8}-1)(\sigma-1),$$

where $C_0 \cong 0.5772156649$ denotes Euler's constant. Further, by (Landau [1, §76, pp. 316-317]),

$$\sum_\rho \frac{1}{1-\rho} = \sum_\rho \frac{1}{\rho} = -\frac{1}{2}\ln(\pi) - \ln(2) + 1 + \frac{C_0}{2}. \tag{3.3.3}$$

Thus, we can take

$$E(\sigma) = C_0 - \left(\frac{\pi^2}{8}-1\right)(\sigma-1) + \kappa(\sigma)\left(-\frac{\zeta'}{\zeta}(\sigma_1)\right). \tag{3.3.4}$$

We now estimate $-(\zeta'/\zeta)(\sigma_1)$, which is a decreasing, nonnegative function of σ_1. As $\sigma \to 1^+$, σ_1 approaches $(1+\sqrt{5})/2$ from below. Writing $\Delta = \sigma - 1$, we have

$$\sigma_1 = \frac{1+\sqrt{5}\sqrt{1-(\frac{8}{5})\Delta^{1/2}+(\frac{4}{5})\Delta-\left(\frac{4}{5}\right)\Delta^{3/2}+((\frac{4}{5})\Delta^2+(\frac{1}{5})\Delta^{5/2})-\dots}}{2}.$$

For $0 \le \Delta \le 0.062$ the series inside the radical is alternating, with decreasing terms. Thus

$$\sigma_1 \le \frac{1+\sqrt{5}\sqrt{1-(\frac{8}{5})\Delta^{1/2}+(\frac{4}{5})\Delta}}{2}.$$

Upon expanding and using $\Delta \le 0.062$, we obtain

$$\sigma_1 \le \frac{1+\sqrt{5}\left(1-\frac{1}{2}\left(\frac{8}{5}\Delta^{1/2}-\frac{4}{5}\Delta\right)-\frac{1}{8}\left(\frac{8}{5}\Delta^{1/2}-\frac{4}{5}\Delta\right)^2\right)}{2}$$
$$\le \frac{1+\sqrt{5}(1-(\frac{4}{5})\Delta^{1/2}+(\frac{4}{25})\Delta)}{2}.$$

It follows that

$$(1+\sqrt{5})/2 - \sigma_1 \ge \left(\frac{2}{\sqrt{5}}\right)\Delta^{1/2} - \left(\frac{2}{5\sqrt{5}}\right)\Delta.$$

When $-(\zeta'/\zeta)(\sigma_1)$ is developed as a Taylor series about $(1+\sqrt{5})/2$, its coefficients alternate in sign. The first four coefficients satisfy

$$B_0 \ge 1.13991, \quad -B_1 \ge 2.48089, \quad B_2 \ge 4.20397, \quad -B_3 \ge 6.84664;$$

these values were obtained by expressing the coefficients in terms of the derivatives of the zeta function, which were computed using Euler-Maclaurin summation. Thus,

$$\begin{aligned}-(\zeta'/\zeta)(\sigma_1) &\geq 1.13991 + 2.48089\left(\frac{2\sqrt{\Delta}}{\sqrt{5}} - \frac{2}{5\sqrt{5}}\Delta\right)\\ &\quad + 4.20397\left(\frac{2\sqrt{\Delta}}{\sqrt{5}} - \frac{2}{5\sqrt{5}}\Delta\right)^2 + 6.84664(0.84988\sqrt{\Delta})^3\\ &\geq 1.13991 + 2.21897\sqrt{\Delta} + 2.91938\Delta + 2.85764\Delta^{3/2}.\end{aligned}$$

(Here we have again used that $0 \leq \Delta \leq 0.062$.) Inserting this in (3.3.4) yields

$$E(\sigma) \geq 1.08699 + 1.40018\Delta^{1/2} + 1.86576\Delta + 2.32244\Delta^{3/2}$$

and for the purposes of the lemma we can replace $E(\sigma)$ by its bound. □

Lemma 3.3.2. *If χ is a character of conductor k, then for $|t| \geq 1000$ and $\varepsilon_1 = 0.0067$,*

$$\begin{aligned}f(t,\chi) \leq &\frac{1-\kappa(\sigma)}{2}\left(\ln\left(\frac{k|t|}{2\pi}\right) + \varepsilon_1\right)\\ &- \Sigma'\,\Re\Big\{\frac{1}{s-\rho} + \frac{1}{s-(1-\bar{\rho})} - \frac{\kappa(\sigma)}{s_1-\rho} - \frac{\kappa(\sigma)}{s_1-(1-\bar{\rho})}\Big\},\end{aligned}$$

where Σ' denotes a sum over the zeros of $L(s,\chi)$ with $\beta \geq 1/2$ and where the zeros with $\beta = 1/2$ have a weight $\frac{1}{2}$.

Proof. We consider separately the cases $k = 1$ and $k > 1$.

First suppose $k = 1$. Using (3.3.1) with $z = s$, s_1, we get

$$\begin{aligned}f(t,\chi_0) = &\Re\left\{\frac{1}{s-1} - \frac{\kappa(\sigma)}{s_1-1}\right\} + \frac{1}{2}\Re\left\{\frac{\Gamma'}{\Gamma}\left(\frac{s+2}{2}\right) - \kappa(\sigma)\frac{\Gamma'}{\Gamma}\left(\frac{s_1+2}{2}\right)\right\}\\ &- \frac{1-\kappa(\sigma)}{2}\ln(\pi) - \frac{1}{2}\sum_{\rho\in\mathcal{Z}(\chi_0)}\left(F(s,\rho) - \kappa(\sigma)F(s_1,\rho)\right).\end{aligned} \tag{3.3.5}$$

By the functional equation of $\zeta(s)$, the last sum can be rewritten

$$\Sigma'\,\Re\left(\frac{1}{s-\rho} + \frac{1}{s-(1-\bar{\rho})} - \frac{\kappa(\sigma)}{s_1-\rho} - \frac{\kappa(\sigma)}{s_1-(1-\bar{\rho})}\right),$$

where the notation is as in the statement of the lemma.

Lemma 3.2.1, together with

$$\Re\left\{\frac{1}{s-1} - \frac{\kappa(\sigma)}{s_1-1}\right\} \leq \frac{\sigma-1}{t^2} \leq \varepsilon_2$$

and $(1-\kappa(\sigma))/2 \geq 0.19498$, yields the result.

Now suppose $k > 1$. The proof is similar to the previous one, apart from the absence of the pole at $s = 1$. Following McCurley's Lemma 5 ([4]), we have

$$\begin{aligned}f(t,\chi) = &\frac{1-\kappa(\sigma)}{2}\ln\left(\frac{k}{\pi}\right) + \frac{1}{2}\Re\left\{\frac{\Gamma'}{\Gamma}\left(\frac{s+a}{2}\right) - \kappa(\sigma)\frac{\Gamma'}{\Gamma}\left(\frac{s_1+a}{2}\right)\right\}\\ &- \Sigma'\left(F(s,\rho) - \kappa(\sigma)F(s_1,\rho)\right)\end{aligned}$$

with $a = (1-\chi(-1))/2$, and Lemma 3.2.1 gives the required estimate. □

Using Lemmas 3.1.1 and 3.3.2, we get

Lemma 3.3.3. *If χ is a character of conductor k, then for $|t| \geq 1000$ and $\varepsilon_1 = 0.0067$*

$$f(t,\chi) \leq \frac{1-\kappa(\sigma)}{2}(\ln\left(\frac{k|t|}{2\pi}\right)+\varepsilon_1)$$

and if $t=\gamma$ is the ordinate of a zero $\rho=\beta+i\gamma$ with $\beta > \frac{1}{2}$, then

$$f(t,\chi) \leq \frac{1-\kappa(\sigma)}{2}(\ln\left(\frac{k|t|}{2\pi}\right)+\varepsilon_1) - \frac{1}{\sigma-\beta} + S(\sigma).$$

3.4. The default to primitivity. Let χ be a primitive character of conductor k and let χ_m be the primitive character associated with χ^m, of conductor k_m. For a prime p dividing k we put

$$\begin{cases} c_p(\sigma) = \dfrac{1}{p^\sigma-1} - \dfrac{\kappa(\sigma)}{p^{\sigma_1}-1}, \\ D_p(k,\sigma,\chi) = a_0 c_p(\sigma) + \displaystyle\sum_{\substack{1\leq m\leq 4\\ p\nmid k_m}} a_m \left(\frac{1-\kappa(\sigma)}{2} v_p(\frac{k}{k_m}) - c_p(\sigma)\right), \end{cases} \tag{3.4.1}$$

where $v_p(x)$ is the p-adic valuation of x with $v_p(p)=1$. We seek a lower bound for

$$D(k,\sigma,\chi) = \sum_{p|k} \ln(p) D_p(k,\sigma,\chi).$$

This bound will be $D^*(k,\sigma)$, defined below: put

$$\begin{cases} D_2^*(\sigma) = 5.99\ c_2(\sigma), \\ D_3^*(\sigma) = 5.467\ c_3(\sigma), \\ D_p^*(\sigma) = a_0\ c_p(\sigma), \quad \text{for} \quad p\geq 5, \end{cases} \tag{3.4.2}$$

and

$$D^*(k,\sigma) = \sum_{p|k} \ln(p)\ D_p^*(\sigma). \tag{3.4.3}$$

Lemma 3.4.1. *The quantity $c_p(\sigma)$ is positive, and decreases as p increases or as σ increases.*

Proof. Easy. □

Lemma 3.4.2. *We have*

$$\begin{cases} \dfrac{1-\kappa(\sigma)}{c_2(\sigma)} - 1 \geq -0.298, \\ \dfrac{1-\kappa(\sigma)}{2c_3(\sigma)} - 1 \geq -0.328, \\ \dfrac{1-\kappa(\sigma)}{2} - c_5(\sigma) \geq 0. \end{cases}$$

Proof. If $\sigma^- \leq \sigma \leq \sigma^+$, then

$$\frac{1-\kappa(\sigma^+)}{2} - c_5(\sigma^-) \leq \frac{1-\kappa(\sigma)}{2} - c_5(\sigma) \leq \frac{1-\kappa(\sigma^-)}{2} - c_5(\sigma^+).$$

Cutting the interval $[1,(1+\sqrt{2})/2]$ into 10000 parts yields the third inequality in the lemma. The two other inequalities may be obtained similarly. □

Lemma 3.4.3. *For each prime $p \mid k$, we have $D_p(k,\sigma,\chi) \geq D_p^*(\sigma)$.*

Proof. If $p \geq 5$, then $c_5(\sigma) \geq c_p(\sigma)$, so by Lemma 3.4.2 and the fact that $k_1 = k$, we see that for each prime dividing k,

$$\begin{aligned} D_p(\kappa,\sigma,\chi) &= a_0 c_p(\sigma) + \sum_{\substack{m=2 \\ p\nmid k_m}}^{4} a_m \left(\frac{1-\kappa(\sigma)}{2} v_p\left(\frac{k}{k_m}\right) - c_p(\sigma)\right) \\ &\geq a_0 c_p(\sigma) = D_p^*(\sigma). \end{aligned}$$

The proof is analogous for $p = 2$ and $p = 3$. Note that when $p = 2$, if $p \nmid k_m$, then $v_p\left(\frac{k}{k_m}\right) \geq 2$. The constant in $D_2^*(\sigma)$ is $a_0 - 0.298(a_2+a_3+a_4)$, and the one in $D_3^*(\sigma)$ is $a_0 - 0.328(a_2+a_3+a_4)$. □

Combining Lemmas 3.4.1 and 3.4.2 gives the desired result:

Corollary 3.4.4. *For $1 \leq \sigma \leq (1+\sqrt{2})/2$, we have $D(k,\sigma,\chi) \geq D^*(k,\sigma)$. Furthermore, on this interval $D^*(k,\sigma)$ is a decreasing function of σ, with*

$$a_0 \sum_{p\mid k} \frac{\ln(p)}{p-1} \;\geq\; D^*(k,\sigma) \;\geq\; 0.$$

We finally need to go from an imprimitive character to a primitive one.

Lemma 3.4.5. *The notations being as above, we have*

$$f(0,\chi_0) = f(0,\chi^0) + \sum_{p\mid k} \ln(p) c_p(\sigma),$$

and

$$f(t,\chi_m) \geq f(t,\chi^m) - \sum_{\substack{p\mid k \\ p\nmid k_m}} \ln(p) c_p(\sigma).$$

Proof. We have for any real number t,

$$f(t,\chi_m) = f(t,\chi^m) + \sum_{\substack{p\mid k \\ p\nmid k_m}} \ln(p) \sum_{n\geq 1} \Re\left(\frac{\chi_m(p^n)}{p^{int}}\right)\left(\frac{1}{p^{n\sigma}} - \frac{\kappa(\sigma)}{p^{n\sigma_1}}\right).$$

If $\chi_m = \chi_0$ and $t = 0$, then $\chi_m(p^n)/p^{int} = 1$, otherwise its real part is ≥ -1. □

3.5. A positivity argument. The trigonometric polynomial

$$P(\theta) = \sum_{m=0}^{4} a_m \cos(m\theta)$$

is also given by

$$P(\theta) = 8(0.9126 + \cos\theta)^2 (0.2766 + \cos\theta)^2$$

and thus is nonnegative. We have

$$\sum_{m=0}^{4} a_m f(mt,\chi^m) = \sum_{n\geq 1} \Lambda(n)\left(\frac{1}{n^\sigma} - \frac{\kappa(\sigma)}{n^{\sigma_1}}\right) P(\arg(\chi(n)n^{-it})) \geq 0. \tag{3.5.1}$$

Recalling Lemma 3.4.5, we then get

$$\sum_{m=0}^{4} a_m f(mt,\chi_m) \geq a_0 \sum_{p\mid k} \ln(p) c_p(\sigma) - \sum_{m=1}^{4} a_m \sum_{\substack{p\mid k \\ p\nmid k_m}} \ln(p) c_p(\sigma). \tag{3.5.2}$$

Lemma 3.5.1. *We have*

$$a_0 f(0,\chi_0) + \sum_{m=1}^{4} a_m \left(f(mt,\chi_m) + \frac{1-\kappa(\sigma)}{2} \ln\left(\frac{k}{k_m}\right)\right) \geq D^*(k,\sigma).$$

Proof. By the definition of $D^*(k,\sigma)$, the inequality in the lemma follows from (3.5.2) if we have

$$\begin{aligned} a_0 \sum_{p|k} \ln(p) c_p(\sigma) - \sum_{m=1}^{4} a_m \sum_{\substack{p|k \\ p\nmid k_m}} \ln(p) c_p(\sigma) \\ \geq \sum_{p|k} \ln(p) D_p^*(\sigma) - \sum_{m=1}^{4} a_m \left(\frac{1-\kappa(\sigma)}{2}\right) \ln\left(\frac{k}{k_m}\right). \end{aligned} \tag{3.5.3}$$

However, by Lemma 3.4.3 we have, prime by prime,

$$a_0 c_p(\sigma) + \sum_{\substack{1\leq m\leq 4 \\ p|k, p\nmid k_m}} a_m \left(\frac{1-\kappa(\sigma)}{2} v_p\left(\frac{k}{k_m}\right) - c_p(\sigma)\right) \geq D_p^*(\sigma)$$

which certainly implies (3.5.3). □

3.6. The zero-free region. Inserting the bounds from Lemmas 3.3.1 and 3.3.3 in the expression from Lemma 3.5.1, if t is taken to be the ordinate of a zero $\beta+i\gamma$ with $\beta > 1/2$, and $|\gamma| \geq 1000$, we find that

$$\begin{aligned} a_0 \left[\frac{1}{\sigma-1} - E(\sigma)\right] + a_1 \left[\left(\frac{1-\kappa(\sigma)}{2}\right)(\ln\left(\frac{k|\gamma|}{2\pi}\right)+\varepsilon_1) - \frac{1}{\sigma-\beta} + S(\sigma)\right] \\ + \sum_{m=2}^{4} a_m \left[\left(\frac{1-\kappa(\sigma)}{2}\right)(\ln\left(\frac{k_m|m\gamma|}{2\pi}\right)+\varepsilon_1) + \left(\frac{1-\kappa(\sigma)}{2}\right)\ln\left(\frac{k}{k_m}\right)\right] \\ \geq D^*(k,\sigma). \end{aligned} \tag{3.6.1}$$

Recalling that $\kappa(\sigma) = \frac{1+\frac{4}{5}\sqrt{\sigma-1}}{\sqrt{5}}$, we can rewrite this as

$$u - \alpha u\sqrt{\sigma-1} - \frac{w}{\sigma-\beta} + \frac{1}{\sigma-1} - G \geq 0, \tag{3.6.2}$$

where

$$\begin{cases} u = \dfrac{1}{a_0}\dfrac{5-\sqrt{5}}{10}\displaystyle\sum_{m=1}^{4} a_m(\ln\left(\frac{km|\gamma|}{2\pi}\right)+\varepsilon_1), \\ \alpha = (\sqrt{5}+1)/5 \cong 0.647213595, \\ w = a_1/a_0 \cong 1.705118356, \\ G = E(\sigma) - wS(\sigma) + \dfrac{D^*(k,\sigma)}{a_0}. \end{cases} \tag{3.6.3}$$

Put $x = \sqrt{w}-1 \cong 0.305801806$. A near-optimal value for σ in (3.6.2) is $\sigma = 1+x/u$. Using this, and the fact that $|\gamma| \geq 1000$, we find that $1 \leq \sigma \leq 1.062$, validating the bounds used in our estimates for $E(\sigma)$ and $S(\sigma)$. Inserting $\sigma = 1 + x/u$ in (3.6.2) and replacing G by any lower bound $\overline{G} = \overline{G}(\sigma)$, we find

$$u - \alpha u\sqrt{x/u} - \frac{w}{1-\beta+x/u} + \frac{u}{x} - \overline{G} \geq 0.$$

Solving for $1-\beta$ and using $(1+1/x) = \sqrt{w}/x$ gives

$$1-\beta \geq \frac{w}{\frac{u\sqrt{w}}{x} - \alpha\sqrt{xu} - \overline{G}} - \frac{x}{u}.$$

Using $w - \sqrt{w} = x\sqrt{w}$ and cross-multiplying by u/x^2 yields

$$\frac{u}{x^2}(1-\beta) \geq \frac{1 + \frac{\alpha\sqrt{x}}{\sqrt{wu}} + \frac{1}{u\sqrt{w}}\overline{G}}{1 - \frac{\alpha x\sqrt{x}}{\sqrt{wu}} - \frac{x}{u\sqrt{w}}\overline{G}}.$$

Finally, using $x = \sqrt{w} - 1$, we obtain

$$1-\beta \geq \frac{1}{\frac{u}{x^2} - \frac{(\alpha/x)\sqrt{u/x}+(1/x^2)\overline{G}}{1+(\alpha/\sqrt{w})\sqrt{x/u}+(1/(x\sqrt{w}))(x/u)\overline{G}}}. \tag{3.6.4}$$

Note that

$$\frac{u}{x^2} = R\ln(k|\gamma|/C_1), \tag{3.6.5}$$

where

$$\begin{cases} R = \dfrac{1}{x^2}\dfrac{A}{a_0}\dfrac{5-\sqrt{5}}{10} \cong 9.645908801, \\ C_1 = 2\pi\exp\left(-\varepsilon_1 - (1/A)\displaystyle\sum_{m=2}^{4} a_m\ln(m)\right) \cong 4.171838431. \end{cases} \tag{3.6.6}$$

An especially useful choice for the lower bound $\overline{G}$ in (3.6.4) occurs when $D^*(k,\sigma)$ is replaced by a constant lower bound $\overline{D}$, giving

$$\overline{G} = \overline{G}(\sigma) = E(\sigma) - wS(\sigma) + \frac{\overline{D}}{a_0}. \tag{3.6.7}$$

In particular, we can always take $\overline{D} = 0$, or, if for some $H \geq 1000$ we are interested only in zeros $\beta + i\gamma$ with $|\gamma| \geq H$, then by Corollary 3.4.4 we can take $\overline{D}$ to be the value of $D^*(k,\sigma)$ corresponding to H. As will be seen, $\overline{G} \geq 0$ on $[1, 1.062]$.

Writing $\Delta = x/u$, and taking $\overline{G}$ as in (3.6.7), put

$$G_1(\Delta) = \frac{\alpha}{x}\sqrt{\frac{1}{\Delta}} + \frac{1}{x^2}\overline{G}(1+\Delta),$$
$$G_2(\Delta) = 1 + \frac{\alpha}{\sqrt{w}}\sqrt{\Delta} + \frac{1}{x\sqrt{w}}\cdot\Delta\cdot\overline{G}(1+\Delta).$$

Then $G_1(\Delta)/G_2(\Delta)$ is the fraction in the denominator of (3.6.4).

Lemma 3.6.1. *For each $\overline{D} \geq 0$, the functions $G_1(\Delta)/G_2(\Delta)$ and $\overline{G}(1+\Delta)$ as given by* (3.6.7) *are nonnegative and decreasing on* $[0, 0.062]$.

Proof. First suppose $\overline{D} = 0$. Note that

$$E(\sigma) = 1.08699 + 1.40018\sqrt{\Delta} + 1.86576\Delta + 2.32244\Delta^{3/2}$$

and that (after some manipulations)

$$S(\sigma) = -\frac{1}{1+\Delta} + \frac{\left(1 + \frac{4}{5}\sqrt{\Delta}\right)\sqrt{1 - \frac{8}{5}\sqrt{\Delta^2+\Delta} + \frac{4}{5}(\Delta^2+\Delta)}}{\left(1 - \sqrt{\Delta^2+\Delta}\right)^2}.$$

It follows that the derivatives of $\overline{G}(1+\Delta)$, $G_1(\Delta)$ and $G_2(\Delta)$ are sums and quotients of various terms monotonic on $[0, 0.062]$. Thus, on any given subinterval, rigorous upper bounds for $\overline{G}'(1+\Delta)$ and $G_1'(\Delta)$, and a rigorous lower bound for $G_2'(\Delta)$, can be obtained. Dividing $[0, 0.062]$ into subintervals of length 0.001, it was found that $\overline{G}'(1+\Delta) < 0$ and $G_1'(\Delta) < 0$ throughout the interval, and $G_2'(\Delta) > 0$ on $[0, 0.057]$.

Graphically it is clear that $G_2(\Delta)$ has a maximum at about 0.0590 and then slowly decreases. To deal with the interval $[0.057, 0.062]$, multiply through by $\sqrt{\Delta}$. The derivatives of $\sqrt{\Delta}\cdot G_1(\Delta)$ and $\sqrt{\Delta}\cdot G_2(\Delta)$ are sums and quotients of monotonic terms. Dividing $[0, 0.062]$ into subintervals of length 0.001, it was found that $(\sqrt{\Delta}\cdot G_1(\Delta))' < 0$ on $[0.047, 0.062]$ and $(\sqrt{\Delta}\cdot G_2(\Delta))' > 0$ throughout $[0, 0.062]$.

Combining these facts yields the monotonicity of $G_1(\Delta)/G_2(\Delta)$. Its nonnegativity and that of $\overline{G}(1+\Delta)$ follow by evaluation at $\Delta = 0.062$.

Now let $\overline{D} \geq 0$ be arbitrary; let $g_1(\Delta)$, $g_2(\Delta)$ denote $G_1(\Delta)$ and $G_2(\Delta)$ when $\overline{D} = 0$. By the discussion above, it follows that $g_2 \cdot g_1' - g_1 \cdot g_2' < 0$ and $g_1' < 0$ on $[0, 0.062]$. Applying the quotient rule to $G_1(\Delta)/G_2(\Delta)$, it is easily seen that for $G_1(\Delta)/G_2(\Delta)$ to be decreasing, it suffices to have

$$g_2' + \frac{x}{\sqrt{w}} g_1 > 0.$$

This was checked by the same means as before. □

Theorem 3.6.2. *If χ is a character of conductor k, and $R = 9.645908801$, then any zero $\beta + i\gamma$ of $L(s,\chi)$ with $|\gamma| \geq 1000$ satisfies*

$$1 - \beta \geq \frac{1}{R\ln\left(\frac{k|\gamma|}{4.1718}\right) - 3.2356\sqrt{\ln\left(\frac{k|\gamma|}{4.1718}\right)}}\ .$$

Proof. When $\beta > \frac{1}{2}$, the result follows from (3.6.4), taking $\overline{G} = 0$ (which is permissible by Lemma 3.6.1); here $3.2356 \leq \alpha\sqrt{R/x}/(1 + (\alpha/\sqrt{w})\sqrt{0.062})$. It is easy to check that the bound is decreasing in k and $|\gamma|$; when $k = 1$ and $|\gamma| = 1000$, it is less than 0.02194. Thus the inequality holds when $\beta \leq \frac{1}{2}$ as well. □

Taking $\overline{D} = D^*(k,\sigma)$ in (3.6.7), we obtain a result better suited to the needs of this paper: recall that $\alpha = (\sqrt{5}+1)/5$, $w = a_1/a_0$ and $x = \sqrt{w} - 1$.

Theorem 3.6.3. *If χ is a character of conductor k, and $H \geq 1000$, then any zero $\beta + i\gamma$ of $L(s,\chi)$ with $|\gamma| \geq H$ satisfies*

$$1 - \beta \geq \frac{1}{R \ln(k|\gamma|/C_1(\chi))},$$

where

$$C_1(\chi) = C_1(\chi, H) = C_1 \cdot \exp\left(\frac{1}{R} \cdot \frac{\frac{\alpha}{x}\sqrt{\frac{1}{\Delta}} + \frac{1}{x^2}\overline{G}(1+\Delta)}{1 + \frac{\alpha}{\sqrt{w}}\sqrt{\Delta} + \frac{1}{x\sqrt{w}} \cdot \Delta \cdot \overline{G}(1+\Delta)}\right)$$

with $\Delta = 1/(xR \cdot \ln(kH/C_1))$, $\overline{G}$ given by (3.6.7), *and $\overline{D} = D^*(k, 1+\Delta)$ by* (3.4.3).

Proof. When $\beta > \frac{1}{2}$, the result follows from (3.6.4) and Lemma 3.6.1. To see that it holds for $\beta \leq \frac{1}{2}$, one can use the upper bound $11.624 \geq \frac{1}{x^2}(E(\sigma) - wS(\sigma))$, the upper and lower bounds for $D^*(k,\sigma)$ from Corollary 3.4.4, and the fact that $|\gamma| \geq 1000$ to show that

$$R \ln(k|\gamma|/C_1(\chi)) \geq 15. \quad \square$$

Some examples :

For $k = 1$,	$\|\gamma\| \geq 545000000$,	$1 - \beta \geq 1/(R \cdot \ln(k\|\gamma\|/38.31))$.
For $k = 3$,	$\|\gamma\| \geq 10000$,	$1 - \beta \geq 1/(R \cdot \ln(k\|\gamma\|/20.92))$.
For $k = 12$,	$\|\gamma\| \geq 10000$,	$1 - \beta \geq 1/(R \cdot \ln(k\|\gamma\|/29.68))$.
For $k = 17$,	$\|\gamma\| \geq 2500$,	$1 - \beta \geq 1/(R \cdot \ln(k\|\gamma\|/20.90))$.
For $k = 420$,	$\|\gamma\| \geq 2500$,	$1 - \beta \geq 1/(R \cdot \ln(k\|\gamma\|/56.59))$.

4. L-functions, $\psi(X;k,l)$ and $\theta(X;k,l)$

Before drawing consequences from Theorem 3.6.3, we need some lemmas.

In the following, we assume that the L-function under examination has no zero satisfying

$$\begin{cases} |\gamma| \geq H \geq 1000, \\ \beta > 1 - \dfrac{1}{R \ln(k|\gamma|/C_1(\chi))} \end{cases} \tag{4.1}$$

for some positive constants R and $C_1(\chi)$ such that

$$R \cdot \ln\left(\frac{kH}{C_1(\chi)}\right) \geq 2. \tag{4.2}$$

When $R = 9.645908801$, then taking $k = 1$ and $\gamma = 1000$ in Theorem 3.6.2 shows we can always use $C_1(\chi) = 9.14$; Theorem 3.6.3 gives sharper results.

4.1. Preparatory lemmas. We restate McCurley's results before using them.

First of all, let us note the following consequence of McCurley [5] :

Lemma 4.1.1 (McCurley)**.** *If χ is a Dirichlet character of conductor k, if $T \geq 1$ is a real number, and if $N(T,\chi)$ denotes the number of zeros $\beta + i\gamma$ of $L(s,\chi)$ in the rectangle $0 < \beta < 1$, $|\gamma| \leq T$, then*

$$|N(T,\chi) - \frac{T}{\pi}\ln\left(\frac{kT}{2\pi e}\right)| \leq C_2 \ln\,(kT)\ + C_3$$

with $C_2 = 0.9185$ and $C_3 = 5.512$.

Our values of C_2 and C_3 correspond to the choice $\eta = \frac{1}{2}$ in McCurley's notation and are undoubtedly not optimal. (Note that our C_2 is his C_1, and our C_3 is his C_2.) If $k > 1$, Lemma 4.1.1 follows immediately from ([5, Theorem 2.1]). When $k = 1$, it follows from the theorem of Rosser cited in ([5, formula 2.17]).

Lemma 4.1.2. *If k is the conductor of χ, and $L(s,\chi)$ satisfies $GRH(H)$ for some $H \geq 1$, then*

$$\sum_{\substack{|\gamma|\leq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{1}{|\rho|} \leq \tilde{E}(H),$$

with

$$\tilde{E}(H) = \frac{1}{2\pi}\ln^2(H) + \frac{\ln\left(\frac{k}{2\pi}\right)}{\pi}\ln(H) + C_2 + 2\left(\frac{\ln\left(\frac{k}{2\pi e}\right)}{\pi} + C_2\ln(k) + C_3\right). \tag{4.1.1}$$

Proof. We consider what happens for $|\gamma| \leq 1$ and for $|\gamma| > 1$.

For $|\gamma| \leq 1$, using GRH(1), we have

$$\sum_{\substack{|\gamma|\leq 1\\ \rho\in\mathcal{Z}(\chi)}} \frac{1}{|\rho|} \leq 2N(1,\chi). \tag{4.1.2}$$

For $|\gamma| > 1$, one gets

$$\begin{aligned}\sum_{\substack{1<|\gamma|\leq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{1}{|\rho|} &\leq \sum_{\substack{1<|\gamma|\leq H\\ \rho\in\mathcal{Z}(\chi)}} \left(\int_{|\gamma|}^{H}\frac{dt}{t^2} + \frac{1}{H}\right)\\ &= \int_1^H \frac{N(t,\chi) - N(1,\chi)}{t^2}dt + \frac{N(H,\chi) - N(1,\chi)}{H},\end{aligned}$$

thus

$$\sum_{\substack{1<|\gamma|\leq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{1}{|\rho|} \leq \int_1^H \frac{N(t,\chi)}{t^2}dt + \frac{N(H,\chi)}{H} - \frac{N(1,\chi)}{1}. \tag{4.1.3}$$

Now we easily finish the proof on using Lemma 4.1.1. □

Lemma 4.1.3. *Let χ be a character with conductor k, let $m \geq 1$ be an integer and x, x_0 be two real numbers such that $x \geq x_0 \geq 1$ and $2R\ln^2(kH/C_1(\chi)) \geq \mathrm{Log}(x_0)$. Then*

$$\sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{x^\beta}{|\gamma|^{m+1}} + \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\bar\chi)}} \frac{x^\beta}{|\gamma|^{m+1}} \leq x(\tilde A + \tilde B) + \sqrt{x}(\tilde C + \tilde D),$$

where, with $C_2 = 0.9185$ and $C_3 = 5.512$, we have

$$\text{(4.1.4)}\qquad \begin{cases} \tilde A = \displaystyle\int_H^\infty \left\{ \frac{\ln\left(\frac{kt}{2\pi}\right)}{\pi} + \frac{C_2}{t}\right\} \frac{\exp\left\{ -\frac{\ln(x_0)}{R\ln(kt/C_1(\chi))}\right\}}{t^{m+1}} dt,\\ \tilde B = \dfrac{1}{H^{m+1}} \exp\left\{ -\dfrac{\ln(x_0)}{R\ln(kH/C_1(\chi))}\right\} 2(C_2\ln(kH) + C_3),\\ \tilde C = \dfrac{1}{\pi m H^m}\left(\ln\left(\dfrac{kH}{2\pi}\right) + \dfrac{1}{m}\right),\\ \tilde D = \dfrac{1}{H^{m+1}}\left(2C_2\ln(kH) + 2C_3 + \dfrac{C_2}{m+1}\right). \end{cases}$$

Proof. The functional equation of the L-functions enables us to write

$$\text{(4.1.5)}\qquad \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{x^\beta}{|\gamma|^{m+1}} + \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\bar\chi)}} \frac{x^\beta}{|\gamma|^{m+1}} = \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \left(\frac{x^{1-(1-\beta)}}{|\gamma|^{m+1}} + \frac{x^{1-\beta}}{|\gamma|^{m+1}}\right).$$

One of β and $1-\beta$ is at most $\frac{1}{2}$, the other is less than

$$1 - \frac{1}{R\ln(k|\gamma|/C_1(\chi))}.$$

We can split our upper bound in two pieces. For the first,

$$\text{(i)}\qquad \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{1}{|\gamma|^{m+1}},$$

an integration by parts assures that this sum is bounded by $\tilde C + \tilde D$. For the second,

$$\text{(ii)}\qquad \tilde S(x) = \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \frac{x}{|\gamma|^{m+1}} \exp\left\{ -\frac{\ln(x)}{R\ln(k|\gamma|/C_1(\chi))}\right\},$$

we have $\tilde S(x)/x \leq \tilde S(x_0)/x_0$, hence it remains to evaluate $\tilde S(x_0)/x_0$. Let us define

$$\varphi_m(t) = \frac{1}{t^{m+1}} \exp\left\{ -\frac{\ln(x_0)}{R\ln(kt/C_1(\chi))}\right\}$$

and integrate it by parts:

$$\text{(4.1.6)}\qquad \frac{\tilde S(x_0)}{x_0} = \sum_{\substack{|\gamma|\geq H\\ \rho\in\mathcal{Z}(\chi)}} \int_{|\gamma|}^\infty -\varphi_m'(t)dt = \int_H^\infty (N(t,\chi) - N(H,\chi))\,(-\varphi_m'(t))\,dt.$$

But

$$\frac{\varphi_m'(t)}{\varphi_m(t)} = \frac{m+1}{t\ln^2(kt/C_1(\chi))}\left[-\ln^2(kt/C_1(\chi)) + \frac{\ln(x_0)}{(m+1)R}\right]$$

and our hypothesis gives us $-\varphi_m'(t) \geq 0$ for $t \geq H$.

Lemma 4.1.1 gives us an upper bound for $N(t,\chi)$ and we integrate back by parts. □

Lemma 4.1.4. *If k is the conductor of χ, and $L(s,\chi)$ satisfies GRH(1), we have*

$$\sum_{\rho\in\mathcal{Z}(\chi)} \frac{2}{|\rho(2-\rho)|} \leq 3.94\ln(k) + 12.7.$$

Proof. The contribution to the sum of the zeros with $|\gamma| \leq 1$ is at most $\frac{8}{3}N(1,\chi)$. The contribution of the remaining ones is not more than

$$4\int_1^\infty \frac{N(t,\chi)-N(1,\chi)}{t^3}dt = -2N(1,\chi) + 4\int_1^\infty \frac{N(t,\chi)}{t^3}dt,$$

and on using Lemma 4.1.1, we obtain the result. □

4.2. Computing $\tilde{A}$. The constant $\tilde{A}$ is the dominant term in Lemma 4.1.3. However, the integral defining $\tilde{A}$ converges slowly, and care is needed in evaluating it. This was forcefully brought home to us when we initially sought to compute $\tilde{A}$ using the pre-programmed numerical integration of PARI. Lionel Reboul of the University of Lyon kindly verified the values by independent computations with MAPLE. To our surprise, the values were the same for $\ln(x_0) \geq 40$, but they were not close for small x_0 (for instance 0.032 instead of 0.034).

We will first give a simple lemma (Lemma 4.2.1) which gives a rather good upper bound for $\tilde{A}$. Then we will describe a way for accurately computing $\tilde{A}$ advocated by Rosser, Schoenfeld, and McCurley, which involves transforming the given integral to a sum of rapidly convergent incomplete Bessel integrals.

For $m \geq 2$ let us define $h_m(t)$ by

$$h_m(t) = \frac{1}{\pi(m-1)t^{m-1}}(\ln\left(\frac{kt}{2\pi}\right) + \frac{1}{m-1}) + \frac{C_2}{mt^m}. \tag{4.2.1}$$

Lemma 4.2.1. *We have, under the hypothesis of Lemma 4.1.3, but with in addition $R\ln^2(kH/C_1(\chi)) \geq \ln(x_0)$ and $m \geq 2$,*

$$\begin{cases} \tilde{A} \leq \dfrac{h_m(H)}{H}\exp(-\dfrac{\ln(x_0)}{R\ln(kH/C_1(\chi))}), \\ \tilde{A} \geq h_{m+1}(H)\exp(-\dfrac{\ln(x_0)}{R\ln(kH/C_1(\chi))}). \end{cases}$$

Proof. Let us define

$$g_m(t) = \frac{\ln(\frac{kt}{2\pi})}{\pi t^m} + \frac{C_2}{t^{m+1}}. \tag{4.2.2}$$

Then, we readily see that $h'_m(t) = -g_m(t)$. We also have

$$\begin{aligned}\tilde{A} =& \int_H^\infty g_m(t) \exp(-\frac{\ln(x_0)}{R\ln(kt/C_1(\chi))})\frac{dt}{t}\\ =& \frac{h_m(H)}{H}\exp(-\frac{\ln(x_0)}{R\ln(kH/C_1(\chi))})\\ &- \int_H^\infty \left(\ln^2(kt/C_1(\chi)) - \frac{\ln(x_0)}{R}\right)\exp(-\frac{\ln(x_0)}{R\ln(kt/C_1(\chi))})\frac{h_m(t)dt}{t^2\ln^2(kt/C_1(\chi))}\\ \le& \frac{h_m(H)}{H}\exp(-\frac{\ln(x_0)}{R\ln(kH/C_1(\chi))});\end{aligned}$$

the last inequality holds because our hypothesis ensures that

$$\left(\ln^2(kH/C_1(\chi)) - \frac{\ln(x_0)}{R}\right) \ge 0.$$

For the other inequality, we write

$$\tilde{A} = \int_H^\infty g_{m+1}(t)\exp(-\frac{\ln(x_0)}{R\ln(kt/C_1(\chi))})dt \tag{4.2.3}$$

and an integration by parts yields the result. □

We now turn to the accurate computation of $\tilde{A}$. Define

$$\begin{cases} K_n(z,w) = \dfrac{1}{2}\displaystyle\int_w^\infty u^{n-1}\exp[-\frac{z}{2}(u+\frac{1}{u})]du,\\ U_m = \sqrt{\dfrac{Rm}{\ln(x_0)}}\ln(\dfrac{kH}{C_1(\chi)}),\\ z_m = 2\sqrt{\dfrac{m\ln(x_0)}{R}}. \end{cases} \tag{4.2.4}$$

Then simple algebraic manipulations yield

Lemma 4.2.2. *There holds*

$$\begin{aligned}\tilde{A} =& \frac{2}{\pi}\frac{\ln(x_0)}{Rm}\left(\frac{k}{C_1(\chi)}\right)^m K_2(z_m,U_m)\\ &+ \frac{2}{\pi}\ln\left(\frac{C_1(\chi)}{2\pi}\right)\sqrt{\frac{\ln(x_0)}{Rm}}\left(\frac{k}{C_1(\chi)}\right)^m K_1(z_m,U_m)\\ &+ 2C_2\sqrt{\frac{\ln(x_0)}{R(m+1)}}\left(\frac{k}{C_1(\chi)}\right)^{m+1} K_1(z_{m+1},U_{m+1}).\end{aligned}$$

The tails in the integrals K_1 and K_2 can be estimated as follows. Write

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt. \tag{4.2.5}$$

Lemma 4.2.3 (Rosser and Schoenfeld). *Put* $y = \frac{\sqrt{w}-1/\sqrt{w}}{\sqrt{2}}$ *for* $w \geq 1$. *Then*

$$K_1(z,w) < \frac{e^{-z}}{2z}\big\{(1+\frac{3\sqrt{2}}{8}y)e^{-zy^2} + (\frac{3}{8\sqrt{z}}+\sqrt{z})\sqrt{\frac{\pi}{2}}\operatorname{erfc}(y\sqrt{z})\big\},$$

and

$$K_2(z,w) < \frac{e^{-z}}{2z}\big\{[\frac{35\sqrt{2}}{64}y^3 + 2y^2 + (\frac{105}{128z}+\frac{15}{8})\sqrt{2}y + 2 + \frac{2}{z}]e^{-zy^2} + (\frac{105}{128z}+\frac{15}{8}+z)\sqrt{\frac{\pi}{2z}}\operatorname{erfc}(y\sqrt{z})\big\}.$$

Lemma 4.2.4. *Assume* $z > 0$.

The integrand in $K_1(z,w)$ *is decreasing in* u *for* $u \geq 1$.

The integrand in $K_2(z,w)$ *is increasing for* $1 \leq u \leq \frac{1+\sqrt{1+z^2}}{z}$ *and decreasing in* u *afterwards.*

Lemma 4.2.3 is accurate if w is large. Thus, K_1 and K_2 can be computed by integrating numerically from w to some finite bound and then using Lemma 4.2.3. In computing Table 1, this method was used in conjunction with Simpson's rule to get a sharp rigorous upper bound for $\tilde{A}$ (within 1%). It should also be noted that R. Terras [13] has given a rapid continued fraction algorithm for computing integrals like K_1 and K_2. Although this algorithm does not produce a rigorous error bound, we have used it to give an independent check on the numerical integrations.

4.3. Estimating ψ and θ through L-functions. We are now in a position to prove Theorem 1. To do so we want to use Theorem 3.6 of McCurley [5]. But in that theorem, the notation $\mathcal{Z}(\chi)$ denotes the set of zeros of $L(s,\chi)$ with $0 \leq \beta < 1$, so it is necessary to pay careful attention to the distinction between conductor and modulus. In [5], the zeros with $\beta = 0$ are removed with some cumbersome arguments (cf. [5, (3.25), (3.26), (3.27) and (3.38)]). The troubles caused by the use of imprimitive characters can also be seen in ([5, (3.15)]).

However, it is possible to work from the beginning with primitive characters only. If χ is a character modulo k, let χ_1 be its associated primitive character. Given l prime to k, consider further

$$w_k(l,n) = \frac{1}{\varphi(k)}\sum_{\chi \bmod k}\chi_1(n)\bar{\chi}(l).$$

If K is the largest divisor of k coprime to n, we have

$$w_k(l,n) = \begin{cases} \frac{\varphi(K)}{\varphi(k)} & \text{if } n \equiv l \pmod K, \\ 0 & \text{otherwise,} \end{cases}$$

which can be proved as follows:

$$\begin{aligned}\varphi(k)w_k(l,n) &= \sum_{d|k}\sum_{\chi \bmod^* d}\chi(n)\bar{\chi}(l) \\ &= \sum_{d|K}\sum_{\chi \bmod^* d}\chi(n)\bar{\chi}(l) = \sum_{\chi \bmod K}\chi(n)\bar{\chi}(l),\end{aligned}$$

where $\sum_{\chi \bmod^* d}$ is a summation over the primitive characters modulo d. We now consider

$$\psi^*(x;k,l) = \sum_{n\le x} w_k(l,n)\Lambda(n).$$

We have $\psi(x;k,l) \le \psi^*(x;k,l) \le \psi(x;k,l) + f(k)\ln(x)$ for $x \ge 1$ with

$$f(k) = \sum_{p\mid k} \frac{1}{p-1}. \tag{4.3.1}$$

We remark that $f(k) \le 3.5$ if k has less than 12000 prime factors, which is true if $k \le \exp(127000)$, and in any case $f(k) = \mathcal{O}(\ln(\ln(\ln(k))))$. Thus, we can work with ψ^* instead of ψ with a small loss. Now McCurley's analysis ([5, §3]) goes through with characters replaced by primitive characters since ψ^* is also an increasing function. More precisely, McCurley's $m(\chi)$ now becomes the order of the zero of $L(s,\chi_1)$ at $s=0$, i.e. $m(\chi)=0$ if $\chi(-1)=-1$ or χ is the principal character, and $m(\chi)=1$ otherwise. In McCurley's notation, this yields $|d_2| \le 1/2$. Following the proof of Lemma 3.5 of [5], we find further that if $L(s,\chi)$ satisfies GRH(1) and χ is not principal, then

$$|b(\chi)| \le 1.57 + \sum_{\rho\in\mathcal{Z}(\chi)} \frac{2}{|\rho(2-\rho)|},$$

which, with Lemma 4.1.4 together with $|b(\chi_0)| = \ln(2\pi)$ yields "*If every L-function of modulus k satisfies* GRH(1)*, then* $|d_1+d_2| \le 3.94\ln(k)+12.7$" instead of Lemma 3.5 of [5]. Finally, the right-hand side of ([5, (3.21)]) becomes

$$(\delta x)^m \left[\frac{\ln(2)}{2} + \frac{\ln(2x)}{2} + 3.94\ln(k) + 12.7\right].$$

An additional error term comes from replacing ψ^* by ψ. The upper bound we get this way is an increasing function of x, so we can introduce the maximum $\max_{1\le y\le x}$ which is useful in practice. Thus we get

Theorem 4.3.1 (McCurley)**.** *Let $x \ge 1$ be a real number, $k \ge 1$ an integer, m a positive integer, δ a real number with $0 < \delta < \frac{x-2}{mx}$, and H a positive real number. Put*

$$A(m,\delta) = \frac{1}{\delta^m}\sum_{j=0}^{m}\binom{m}{j}(1+j\delta)^{m+1}.$$

Suppose that for each χ with modulus k, $L(s,\chi)$ satisfies GRH(1). Then

$$\frac{\varphi(k)}{x}\max_{1\le y\le x}|\psi(y;k,l) - \frac{y}{\varphi(k)}| < A(m,\delta)\sum_{\chi}\sum_{\substack{\rho\in\mathcal{Z}(\chi)\\ |\gamma|>H}}\frac{x^{\beta-1}}{|\rho(\rho+1)\ldots(\rho+m)|} + (1+\frac{m\delta}{2})\sum_{\chi}\sum_{\substack{\rho\in\mathcal{Z}(\chi)\\ |\gamma|\le H}}\frac{x^{\beta-1}}{|\rho|} + \frac{m\delta}{2} + \tilde{R},$$

where $\sum_\chi$ denotes the summation over all characters modulo k,

$$\tilde{R} = \frac{\varphi(k)}{x}\big[(f(k)+0.5)\ln(x) + 4\ln(k) + 13.4\big], \tag{4.3.2}$$

and $f(k)$ is given by (4.3.1).

We also wish to allow θ instead of ψ which can be done by recalling Theorem 6 of Rosser and Schoenfeld ([9]) :

$$0 \le \psi(x;k,l) - \theta(x;k,l) \le \psi(x) - \theta(x) \le 1.0012\sqrt{x} + 3x^{\frac{1}{3}} \quad \text{for} \quad x > 0. \tag{4.3.3}$$

Collecting our results, we finally get

Theorem 4.3.2. *Let $k \ge 1$ be an integer, and let $H \ge 1000$ be a real number such that every L-function with modulus k satisfies $GRH(H)$. Put $C = C_1(\chi_0, H)$, where χ_0 is the trivial character, and let x_0 be a real number such that $R \cdot \ln^2(H/C) \ge \ln(x_0)$. Let $m \ge 2$ be an integer, and let $\delta > 0$ be a real number such that $0 < \delta < (x_0 - 2)/(mx_0)$.*

Then for any $x \ge x_0$ we have

$$\frac{\varphi(k)}{x} \max_{1 \le y \le x} |\psi(y;k,l) - \frac{y}{\varphi(k)}| \le \frac{(1+(1+\delta)^{m+1})^m}{\delta^m} \frac{\varphi(k)}{2}((\tilde{A}+\tilde{B}) + \frac{1}{\sqrt{x_0}}(\tilde{C}+\tilde{D})) + (1+\frac{m\delta}{2})\frac{\varphi(k)}{\sqrt{x_0}}\tilde{E}(H) + \frac{m\delta}{2} + \tilde{R},$$

where $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ are those of Lemma 4.1.3 with $C_1(\chi)$ replaced by C and with $\tilde{A}$ estimated by Lemma 4.2.1, $\tilde{E}(H)$ given by Lemma 4.1.2, and $\tilde{R}$ given by (4.3.2) with $x = x_0$.

If $\tilde{\Delta} = \varphi(k)(1.0012x_0^{-1/2} + 3x_0^{-2/3})$, and $\tilde{Z}$ denotes the error bound above, then $\tilde{Z} + \tilde{\Delta}$ is an upper bound for

$$\frac{\varphi(k)}{x} \max_{1 \le y \le x} \left| \theta(y;k,l) - \frac{y}{\varphi(k)} \right|.$$

Proof. We use Theorem 4.3.1 and evaluate the sums over the zeros by appealing to Lemmas 4.1.2 and 4.1.3. We also remark (cf. [8]) that

$$A(m,\delta) \le \frac{(1+(1+\delta)^{m+1})^m}{\delta^m}. \quad \square \tag{4.3.4}$$

Theorem 4.3.2 has been stated in such a way as to make its implementation as simple as possible, and to minimize the numerical input required. For a stronger version which yields slightly better results, see Theorem 5.1.1 below.

4.4. Heuristic control of the values of m, δ and ε. Let $\varepsilon_k(m,\delta)$ denote the expression $\tilde{Z} + \tilde{\Delta}$ in Theorem 4.3.2, and let ε_k be its minimum value as m and δ vary. This optimization is achieved in practice by first minimizing over δ (with m held fixed) using any standard minimization algorithm, and then minimizing over m.

In this section we aim to heuristically estimate the optimal values of m and δ and the order of magnitude of ε_k, together with their dependence on k and H. Under the hypothesis of Theorem 4.3.2, we note that in the formula for $\tilde{Z} + \tilde{\Delta}$:

(1) $(1+(1+\delta)^{m+1})^m/\delta^m$ is equivalent to $2^m/\delta^m$ if $m\delta$ tends to 0.

(2) $(\tilde{A}+\tilde{B}+(\tilde{C}+\tilde{D})/\sqrt{x_0})$ can be approximated by $\ln\left(\frac{kH}{2\pi}\right)/(\pi m H^m)$ for large H and x_0.
(3) $(1+m\delta/2)\tilde{E}(H)x_0^{-1/2}$ is asymptotic to $x_0^{-1/2}\frac{\ln^2(kH)}{2\pi}$ as H goes to infinity and δ to 0. For large x_0 it is negligible.
(4) $\tilde{R}$ is $\mathcal{O}(k\ln(kx_0)/x_0)$ when x_0 goes to infinity. For x_0 large it is negligible.
(5) For large x_0, $\tilde{\Delta}$ is negligible.

Hence our ε_k can be approximated by

$$f(m,\delta)=\frac{m\delta}{2}+\frac{\varphi(k)}{2}\left(\frac{2}{\delta H}\right)^m\frac{\ln\left(\frac{kH}{2\pi}\right)}{\pi m}. \tag{4.4.1}$$

We reduce this expression once more; numerically, it happens that the values of m are almost always near 7. We replace the term $\left(\frac{2}{\delta H}\right)^m\frac{1}{m}$ by $\left(\frac{2}{\delta H}\right)^m\frac{1}{\bar{m}}$, where $\bar{m}$ is an estimation of the value of m and we finally consider

$$\bar{f}(m,\delta)=\frac{a}{(\delta B)^m}+\frac{m\delta}{2} \tag{4.4.2}$$

with

$$a=\frac{\varphi(k)}{2}\frac{\ln\left(\frac{kH}{2\pi}\right)}{\pi\bar{m}}\quad\text{and}\quad B=\frac{H}{2}. \tag{4.4.3}$$

We now let m vary continuously. Then

$$\frac{\partial\bar{f}}{\partial\delta}=\frac{\partial\bar{f}}{\partial m}=0$$

yields

$$\begin{cases}\dfrac{a}{(\delta B)^m}=\dfrac{\delta}{2},\\[2ex] \dfrac{a}{(\delta B)^m}\ln(\delta B)=\dfrac{\delta}{2},\end{cases}$$

hence

$$\delta=\frac{2e}{H},\qquad m=\ln(aH/e),$$
$$\bar{f}(m,\delta)=(m+1)\frac{\delta}{2}=\ln\left(\frac{H\varphi(k)}{2\pi\bar{m}}\ln\left(\frac{kH}{2\pi}\right)\right)\cdot\frac{e}{H}. \tag{4.4.4}$$

It is striking that in this approximation, δ depends neither on m nor on k. We have verified this numerically (δ is almost constant). The other striking thing is that $\bar{f}(m,\delta)$ (our ε_k) depends on k mainly through $\ln(\varphi(k))$; we find numerically that our ε_k's increase very slowly when k increases. This is rather surprising since there are $\varphi(k)$ sums to evaluate, so we might have expected ε_k to depend on k by a multiplicative factor $\varphi(k)$.

5. Numerical estimates for θ and ψ

In this section, we present the numerical estimates one can deduce from the results in §§2, 3, and 4. Since the analytic bounds only become useful for $x_0 \geq 10^{10}$, we have supplemented them with a tabulation for low heights.

The following notation is used throughout:

$$\begin{cases} \varepsilon(\theta, x, k) = \max\limits_{(l,k)=1} \dfrac{\varphi(k)}{x} \max\limits_{1\leq y\leq x} |\theta(y;k,l) - y/\varphi(k)|, \\ \varepsilon(\psi, x, k) = \max\limits_{(l,k)=1} \dfrac{\varphi(k)}{x} \max\limits_{1\leq y\leq x} |\psi(y;k,l) - y/\varphi(k)|. \end{cases} \tag{5.1}$$

The computations for the tables were performed on PCs using the Intel 80486 processor. The 80486-DX was used in Extended Precision mode, where it calculates with an 80-bit word having a 1-bit sign, a 15-bit exponent, and a 64-bit mantissa. It carries approximately 19.2 decimal digits of accuracy, and can represent numbers over the range 10^{-4392} to 10^{4392}. In Tables 1 and 2, the results are reported to 6 digits of accuracy, and were rounded up in their last digit.

As a verification, independent computations were done using the calculator GP of PARI, and some randomly chosen values were checked, with satisfying agreement.

5.1. Asymptotic results for $x_0 \geq 10^{10}$.

Theorem 1. *For any triple (k, ε, x_0) given by Table 1,*

$$\begin{cases} \varepsilon(\theta, x, k) \leq \varepsilon \quad \textit{for} \quad x \geq x_0, \\ \varepsilon(\psi, x, k) \leq \varepsilon \quad \textit{for} \quad x \geq x_0. \end{cases}$$

Table 1 contains the best known bounds for all the moduli covered by Rumely's L-series calculations. The bounds were computed using a strong form of Theorem 4.3.2, which broke the error term into its contributions from each individual L-series, and replaced the estimates for $\tilde{E}(H)$ by tabulated values:

Theorem 5.1.1. *Let $k \geq 1$ be an integer. For each character χ modulo k, let $H_\chi \geq 1000$ be such that $L(s,\chi)$ satisfies GRH(H_χ); we suppose $H_\chi = H_{\bar{\chi}}$ for all χ, and put $C_1(\chi) = C_1(\chi, H_\chi)$. Let $x_0 \geq 10$ be a real number such that for each d dividing k, and each χ with conductor d, $2R \cdot \ln^2(dH_\chi/C_1(\chi)) \geq \ln(x_0)$. Let m be a positive integer, and let $\delta > 0$ be a real number such that $0 < \delta < (x_0 - 2)/(mx_0)$. For each χ with conductor d, let $\tilde{A}_\chi$, $\tilde{B}_\chi$, $\tilde{C}_\chi$, $\tilde{D}_\chi$ be the constants from Lemma 4.1.3 computed using d and H_χ; let $\tilde{E}_\chi$ be a tabulated bound for $\sum_{\substack{\rho\in Z(\chi)\\ |\beta|\leq H_\chi}} 1/|\rho|$. Let $\tilde{R}$ be as in Theorem 4.3.1.*

Then for $x \geq x_0$

$$\varepsilon(\psi, x, k) \leq \frac{1}{2} A(m,\delta) \cdot \sum_\chi \left[\tilde{A}_\chi + \tilde{B}_\chi + (\tilde{C}_\chi + \tilde{D}_\chi)/\sqrt{x_0}\right] + \frac{(1 + m\delta/2)}{\sqrt{x_0}} \cdot \left(\sum_\chi \tilde{E}_\chi\right) + m\delta/2 + \tilde{R}.$$

TABLE 1. Analytic epsilons for $x \geq x_0$

The values reported are $\varepsilon = \max(\varepsilon(\theta, x_0, k), \varepsilon(\psi, x_0, k))$, and have been rounded up in the last decimal place (our notation is as in (5.1) of the paper).

k	10^{10}	10^{13}	10^{30}	10^{100}	k	10^{10}	10^{13}	10^{30}	10^{100}
1	0.000213	0.000015	0.000001	0.000001	46	0.012682	0.009592	0.009012	0.007046
2	0.000213	0.000015	0.000001	0.000001	47	0.018044	0.010720	0.010012	0.008148
3	0.002238	0.001951	0.001813	0.001310	48	0.011080	0.008876	0.008319	0.006373
4	0.002238	0.001943	0.001809	0.001324	49	0.017015	0.010461	0.009773	0.007891
5	0.002785	0.002250	0.002105	0.001606	50	0.012214	0.009447	0.008851	0.006861
6	0.002238	0.001951	0.001813	0.001310	51	0.014479	0.009803	0.009191	0.007312
7	0.003248	0.002406	0.002258	0.001770	52	0.012671	0.009058	0.008475	0.006656
8	0.002811	0.002257	0.002116	0.001634	53	0.019206	0.010734	0.010011	0.008188
9	0.003228	0.002380	0.002235	0.001759	54	0.011579	0.009061	0.008492	0.006572
10	0.002785	0.002250	0.002105	0.001606	55	0.016306	0.010159	0.009493	0.007591
11	0.004125	0.002590	0.002421	0.001954	56	0.012961	0.009462	0.008865	0.006969
12	0.002781	0.002241	0.002099	0.001610	57	0.015636	0.010300	0.009640	0.007691
13	0.004560	0.002657	0.002478	0.002020	58	0.014102	0.010007	0.009398	0.007440
14	0.003248	0.002406	0.002258	0.001770	59	0.020659	0.011057	0.010299	0.008451
15	0.008634	0.007628	0.007088	0.005045	60	0.010879	0.008740	0.008182	0.006204
16	0.008994	0.007938	0.007392	0.005393	61	0.021073	0.011080	0.010315	0.008475
17	0.010746	0.008587	0.008047	0.006203	62	0.014535	0.010088	0.009468	0.007527
18	0.003228	0.002380	0.002235	0.001759	63	0.015473	0.010048	0.009409	0.007510
19	0.011892	0.009442	0.008852	0.006838	64	0.014938	0.010019	0.009400	0.007530
20	0.008501	0.007465	0.006950	0.005024	65	0.018025	0.010412	0.009697	0.007837
21	0.009708	0.008143	0.007582	0.005625	66	0.011685	0.008844	0.008276	0.006357
22	0.004125	0.002590	0.002421	0.001954	67	0.022414	0.011252	0.010451	0.008620
23	0.012682	0.009592	0.009012	0.007046	68	0.014691	0.009884	0.009272	0.007412
24	0.008173	0.007107	0.006615	0.004775	69	0.017285	0.010536	0.009835	0.007944
25	0.012214	0.009447	0.008851	0.006861	70	0.012809	0.009431	0.008821	0.006862
26	0.004560	0.002657	0.002478	0.002020	71	0.023269	0.011310	0.010484	0.008672
27	0.011579	0.009061	0.008492	0.006572	72	0.012665	0.009118	0.008546	0.006759
28	0.009908	0.008298	0.007741	0.005800	74	0.015830	0.010323	0.009668	0.007768
29	0.014102	0.010007	0.009398	0.007440	75	0.016346	0.010341	0.009659	0.007724
30	0.008634	0.007628	0.007088	0.005045	76	0.015819	0.010331	0.009671	0.007751
31	0.014535	0.010088	0.009468	0.007527	77	0.020600	0.010854	0.010076	0.008235
32	0.011103	0.008857	0.008300	0.006399	78	0.012621	0.009108	0.008514	0.006625
33	0.011685	0.008844	0.008276	0.006357	80	0.014527	0.009700	0.009085	0.007218
34	0.010746	0.008587	0.008047	0.006203	81	0.019611	0.010834	0.010094	0.008264
35	0.012809	0.009431	0.008821	0.006862	82	0.016744	0.010524	0.009843	0.007953
36	0.009544	0.007900	0.007372	0.005563	84	0.012721	0.009304	0.008703	0.006792
37	0.015830	0.010323	0.009668	0.007768	85	0.021395	0.010990	0.010205	0.008353
38	0.011892	0.009442	0.008852	0.006838	86	0.017180	0.010598	0.009904	0.008025
39	0.012621	0.009108	0.008514	0.006625	87	0.019865	0.010903	0.010152	0.008278
40	0.010833	0.008627	0.008084	0.006183	88	0.016484	0.010131	0.009474	0.007646
41	0.016744	0.010524	0.009843	0.007953	90	0.012817	0.009413	0.008809	0.006884
42	0.009708	0.008143	0.007582	0.005625	91	0.023159	0.011148	0.010314	0.008484
43	0.017180	0.010598	0.009904	0.008025	92	0.017508	0.010574	0.009872	0.008009
44	0.011798	0.008871	0.008310	0.006440	93	0.020727	0.011013	0.010245	0.008375
45	0.012817	0.009413	0.008809	0.006884	94	0.018044	0.010720	0.010012	0.008148

TABLE 1 (continued)

k	10^{10}	10^{13}	10^{30}	10^{100}	k	10^{10}	10^{13}	10^{30}	10^{100}
95	0.023180	0.011282	0.010444	0.008570	144	0.018241	0.010486	0.009772	0.007976
96	0.014710	0.009886	0.009271	0.007395	150	0.016346	0.010341	0.009659	0.007724
98	0.017015	0.010461	0.009773	0.007891	154	0.020600	0.010854	0.010076	0.008235
99	0.020644	0.010823	0.010051	0.008238	156	0.018025	0.010363	0.009653	0.007827
100	0.016476	0.010310	0.009631	0.007737	162	0.019611	0.010834	0.010094	0.008264
102	0.014479	0.009803	0.009191	0.007312	163	0.044431	0.012935	0.011505	0.009799
104	0.018292	0.010424	0.009715	0.007922	168	0.017995	0.010459	0.009740	0.007882
105	0.017707	0.010434	0.009708	0.007787	169	0.042497	0.012769	0.011383	0.009670
106	0.019206	0.010734	0.010011	0.008188	170	0.021395	0.010990	0.010205	0.008353
108	0.015635	0.010079	0.009441	0.007589	174	0.019865	0.010903	0.010152	0.008278
110	0.016306	0.010159	0.009493	0.007591	180	0.018004	0.010482	0.009763	0.007903
111	0.023287	0.011261	0.010425	0.008589	182	0.023159	0.011148	0.010314	0.008484
112	0.018184	0.010498	0.009777	0.007942	186	0.020727	0.011013	0.010245	0.008375
114	0.015636	0.010300	0.009640	0.007691	190	0.023180	0.011282	0.010444	0.008570
116	0.020143	0.010962	0.010209	0.008353	198	0.020644	0.010823	0.010051	0.008238
117	0.023222	0.011135	0.010306	0.008499	210	0.017707	0.010434	0.009708	0.007787
118	0.020659	0.011057	0.010299	0.008451	216	0.023480	0.011154	0.010324	0.008542
120	0.014495	0.009785	0.009169	0.007257	222	0.023287	0.011261	0.010425	0.008589
121	0.031939	0.012053	0.010963	0.009223	234	0.023222	0.011135	0.010306	0.008499
122	0.021073	0.011080	0.010315	0.008475	242	0.031939	0.012053	0.010963	0.009223
124	0.021008	0.011055	0.010285	0.008436	243	0.043836	0.012879	0.011458	0.009740
125	0.029581	0.011885	0.010860	0.009072	250	0.029581	0.011885	0.010860	0.009072
126	0.015473	0.010048	0.009409	0.007510	256	0.036558	0.012394	0.011179	0.009461
128	0.022035	0.011123	0.010336	0.008526	286	0.033703	0.012101	0.010952	0.009218
130	0.018025	0.010412	0.009697	0.007837	326	0.044431	0.012935	0.011505	0.009799
132	0.016320	0.010123	0.009461	0.007593	338	0.042497	0.012769	0.011383	0.009670
134	0.022414	0.011252	0.010451	0.008620	360	0.028267	0.011631	0.010644	0.008854
138	0.017285	0.010536	0.009835	0.007944	420	0.027757	0.011602	0.010617	0.008766
140	0.017989	0.010523	0.009796	0.007898	432	0.039660	0.012542	0.011234	0.009519
142	0.023269	0.011310	0.010484	0.008672	486	0.043836	0.012879	0.011458	0.009740
143	0.033703	0.012101	0.010952	0.009218					

If $\tilde{\Delta} = \varphi(k)(1.0012x_0^{-1/2} + 3x_0^{-2/3})$, *and* $\tilde{Z}$ *denotes the above bound for* $\varepsilon(\psi, x, k)$, *then*

$$\varepsilon(\theta, x, k) \le \tilde{Z} + \tilde{\Delta}.$$

If k is not of the form $k = 2k'$ with k' odd, and $k \neq 1$, then the values reported in Table 1 are the minimal values of the expression $\tilde{Z} + \tilde{\Delta}$ in Theorem 5.1.1, when $2 \le m \le 14$ and δ ranges over its allowable values. The minima were found using Brent's golden section/parabolic interpolation algorithm ([7, p. 283]). It should be noted that as x_0 and the H_χ vary, different terms in the expression become dominant. Heuristically the best estimate is obtained using GRH data to height $H \cong 4e\pi \cdot \sqrt{x_0}/(\varphi(k) \cdot \ln(x_0))$. The values in Table 1 are minima over the following data sets:

(A) Rumely's L-series and zeta data, using $T = 2500$ data for $k \le 13$,
(B) Rumely's L-series and zeta data, using $T = 5000$ data for $k \le 13$,
(C) Rumely's L-series and zeta data,
(D) Rumely's L-series data + Lehman's zeta data, with $T = 12030$,

(E) Rumely's L-series data + vdL, teR, Winter zeta data to $T = 10^5$,
(F) Rumely's L-series data + vdL, teR, Winter zeta data to $T = 10^6$,
(G) Rumely's L-series data + vdL, teR, Winter zeta data to $T = 10^7$,
(H) Rumely's L-series data + vdL, teR, Winter zeta data to $T = 545439823$.

If $k = 2k'$ with k' odd, and if N is the order of 2 in $(\mathbb{Z}/k'\mathbb{Z})^\times$, then for $(k, l) = 1$

$$|\psi(x; k, l) - \psi(x; k', l)| \le (1/N)\ln(x) + \ln(2),$$
$$|\theta(x; k, l) - \theta(x; k', l)| \le \ln(2).$$

For the values of x_0 considered in Table 1, these inequalities yield estimates for $\varepsilon(\theta, x, k)$, $\varepsilon(\psi, x, k)$ better than those provided by Theorem 5.1.1 directly, and are the ones reported. It will be observed that the bounds for k and k' in Table 1 are always the same: the additional term in the error estimate was swallowed up when the values were rounded up to the nearest 10^{-6}.

Finally, when $k = 1, 2$ the $x_0 = 10^{10}$ entry in Table 1 is derived from the main table of Rosser and Schoenfeld ([9]), which gives $\varepsilon(\psi, e^{23}, 1) = 0.00020211$; this improves on the value 0.000272 given by Theorem 5.1.1.

5.2. Estimates over the range $0 - 10^{10}$. In Table 2 we compare $|\psi(x; k, l) - x/\varphi(k)|$ and $|\theta(x; k, l) - x/\varphi(k)|$ with $\sqrt{x}$, reporting the maximum ratio for $0 < x \le 10^{10}$ for each k. Tabulations over the subintervals $[10^n, 10^{n+1}]$ show that the results are remarkably stable and uniform over the entire range, so that Table 2 gives a good representation of the true error. The only exception is for very small moduli ($k \le 6$) where the initial primes distort the error estimates; more accurate asymptotic values are given at the end of the table for these moduli. Let $N(k, l)$ be the number of solutions to $a^2 \equiv l \pmod{k}$ with $0 \le a < k$. The function $(x - N(k, l)\sqrt{x})/\varphi(k)$ usually gives a better approximation to $\theta(x; k, l)$ than $x/\varphi(k)$; we have also tabulated the maximal ratios $|\theta(x; k, l) - (x - N(k, l)\sqrt{x})/\varphi(k)|\sqrt{x}$.

We can summarize the main results of Table 2 as follows:

Theorem 5.2.1. *For all the moduli in Table* 1*, uniformly over the range* $0 \le x \le 10^{10}$*, the following bounds hold:*

$$|\theta(x; k, l) - x/\varphi(k)| \le 2.072\sqrt{x},$$
$$\left|\theta(x; k, l) - \frac{x - N(k, l)\sqrt{x}}{\varphi(k)}\right| \le 1.174\sqrt{x},$$
$$|\psi(x; k, l) - x/\varphi(k)| \le 1.745\sqrt{x}.$$

If $k = 5$*,* $k \ge 7$ *or* $x \ge 224$*, then*

$$|\psi(x; k, l) - x/\varphi(k)| \le \sqrt{x};$$

for $k = 1, 3, 4$ *this holds if* $x \ge 14$*.*

Corollary 5.2.2. *For these moduli, over the range* $0 < x \le 10^{10}$*,*

$$\varepsilon(\theta, x, k) \le 2.072\frac{\varphi(k)}{\sqrt{x}}, \quad \varepsilon(\psi, x, k) \le 1.745\frac{\varphi(k)}{\sqrt{x}};$$

for $k = 5$ *or* $k \ge 7$*,* $\varepsilon(\psi, x, k) \le \varphi(k)/\sqrt{x}$*.*

TABLE 2. Tabulations $0 - 10^{10}$

k : The modulus.
θ : $\max_{(l,k)=1} \max_{(0,10^{10}]} |\theta(x;k,l) - x/\varphi(k)|/\sqrt{x}$
$\theta\#$: $\max_{(l,k)=1} \max_{(0,10^{10}]} |\theta(x;k,l) - (x - N(k,l)\sqrt{x})/\varphi(k)|/\sqrt{x}$,
(1) where $N(k,l)$ is the number of solutions to $a^2 \equiv l \pmod{k}$
ψ : $\max_{(l,k)=1} \max_{(0,10^{10}]} |\psi(x;k,l) - x/\varphi(k)|/\sqrt{x}$

Except for the ψ-values for a few small moduli, the bounds for θ, $\theta\#$ and ψ are remarkably good throughout the range $0 - 10^{10}$. All values have been rounded up in the last decimal place.

k	θ	$\theta\#$	ψ	k	θ	$\theta\#$	ψ
1	2.052818	1.052818	1.414214*	39	0.769446	0.666830	0.668572
2	2.071193	1.071193	1.744754*	40	1.076203	0.813546	0.816561
3	1.798158	1.053542	1.070833*	41	0.818620	0.818620	0.817634
4	1.780719	1.034832	1.118034*	42	1.130693	0.863011	0.813182
5	1.412480	0.912480	0.886346*	43	0.832936	0.785317	0.784932
6	1.798158	1.173049	1.322876*	44	0.873277	0.873277	0.871473
7	1.105822	0.829249	0.779283	45	0.844820	0.844820	0.844864
8	1.817557	1.000000	0.926535	46	0.973114	0.882205	0.881655
9	1.108042	0.899812	0.788900	47	0.744386	0.787865	0.790079
10	1.412480	0.912480	0.961267*	48	1.096688	0.870037	0.876180
11	0.976421	0.885771	0.878823	49	0.744132	0.696513	0.697158
12	1.735502	1.000000	0.906786*	50	0.821890	0.832182	0.762408
13	0.892444	0.741007	0.737610	51	0.817323	0.770458	0.771552
14	1.105822	0.829249	0.897528	52	0.884117	0.837232	0.837318
15	1.097307	0.769689	0.760264	53	0.829958	0.791497	0.725979
16	1.253606	0.771116	0.773805	54	0.881762	0.789677	0.794864
17	1.001057	0.876057	0.873548	55	0.795133	0.795133	0.798504
18	1.108042	0.899812	0.824180	56	0.981635	0.828677	0.833854
19	1.001556	0.911763	0.911536	57	0.834201	0.834201	0.833807
20	1.276501	0.776501	0.800391	58	0.793283	0.744371	0.745533
21	1.130693	0.863011	0.805421	59	0.710444	0.724352	0.710444
22	0.976421	0.885771	0.879312	60	1.056320	0.749787	0.748270
23	0.973114	0.882205	0.880877	61	0.719386	0.715829	0.717979
24	1.703144	1.000000	0.744935	62	0.771883	0.838550	0.845276
25	0.821890	0.832182	0.764098	63	0.847851	0.736979	0.750188
26	0.892444	0.744403	0.744403	64	0.842522	0.781042	0.779800
27	0.881762	0.789677	0.795451	65	0.753091	0.753091	0.753171
28	1.039662	0.764535	0.775919	66	0.797466	0.779343	0.788725
29	0.793283	0.744371	0.745590	67	0.708427	0.738730	0.731833
30	1.097307	0.769689	0.760264	68	0.803940	0.803940	0.805077
31	0.771883	0.838550	0.845276	69	0.740573	0.732708	0.733806
32	1.015064	0.866076	0.860459	70	0.865028	0.782493	0.779932
33	0.797466	0.779343	0.788725	71	0.750488	0.750488	0.750488
34	1.001057	0.876057	0.874371	72	1.062100	0.754145	0.765297
35	0.865028	0.782493	0.779932	74	0.867916	0.816491	0.815422
36	1.163674	0.830341	0.829482	75	0.729046	0.684061	0.685155
37	0.867916	0.816491	0.815422	76	0.771532	0.768761	0.702507
38	1.001556	0.911763	0.911624	77	0.690677	0.690677	0.690677

TABLE 2 (continued)

k	θ	$\theta\#$	ψ	k	θ	$\theta\#$	ψ
78	0.769446	0.666830	0.668572	130	0.753091	0.753091	0.753171
80	0.806030	0.774123	0.773105	132	0.834519	0.762402	0.763278
81	0.757028	0.757028	0.757028	134	0.708427	0.738730	0.731833
82	0.818620	0.818620	0.817634	138	0.740573	0.732708	0.733806
84	0.811175	0.805972	0.805906	140	0.737551	0.764606	0.769112
85	0.694146	0.694146	0.694146	142	0.750488	0.750488	0.750488
86	0.832936	0.785317	0.784932	143	0.713437	0.713437	0.713437
87	0.688240	0.759668	0.688240	144	0.753220	0.680366	0.680366
88	0.780273	0.742456	0.741766	150	0.729046	0.684061	0.685155
90	0.844820	0.844820	0.844864	154	0.690677	0.690677	0.690677
91	0.688707	0.688707	0.688707	156	0.789471	0.789471	0.790208
92	0.728679	0.720354	0.719766	162	0.757028	0.757028	0.757028
93	0.691390	0.758056	0.691390	163	0.719154	0.719154	0.719154
94	0.744386	0.787865	0.790048	168	0.699889	0.674579	0.674416
95	0.698739	0.732484	0.698739	169	0.718525	0.718525	0.718525
96	0.825985	0.744111	0.742971	170	0.694146	0.694146	0.694146
98	0.744132	0.696513	0.697303	174	0.688240	0.759668	0.688240
99	0.740587	0.691390	0.691390	180	0.723937	0.723937	0.723937
100	0.813770	0.813770	0.812489	182	0.688707	0.688707	0.688707
102	0.817323	0.770458	0.771552	186	0.691390	0.758056	0.691390
104	0.723333	0.767924	0.765581	190	0.698739	0.732484	0.698739
105	0.653897	0.653897	0.653897	198	0.740587	0.691390	0.691390
106	0.829958	0.791497	0.725979	210	0.653897	0.653897	0.653897
108	0.764890	0.722346	0.661992	216	0.698739	0.698739	0.698739
110	0.795133	0.795133	0.795133	222	0.698739	0.754294	0.698739
111	0.698739	0.754294	0.698739	234	0.698739	0.698739	0.698739
112	0.740472	0.740472	0.742195	242	0.711433	0.717617	0.711433
114	0.834201	0.834201	0.834201	243	0.719154	0.731499	0.719154
116	0.764606	0.751262	0.700136	250	0.709028	0.709827	0.709028
117	0.698739	0.698739	0.698739	256	0.714815	0.714815	0.714815
118	0.710444	0.724352	0.710444	286	0.713437	0.713437	0.713437
120	1.032367	0.672746	0.672746	326	0.719154	0.719154	0.719154
121	0.711433	0.717617	0.711433	338	0.718525	0.718525	0.718525
122	0.719386	0.715829	0.716087	360	0.707926	0.707926	0.707926
124	0.691390	0.749162	0.691390	420	0.688445	0.688445	0.688445
125	0.709028	0.709827	0.709028	432	0.717112	0.717112	0.717112
126	0.847851	0.736979	0.750188	486	0.719154	0.731499	0.719154
128	0.754709	0.817209	0.817799				

(*) The ψ-bounds for small k and x are distorted by powers of $p = 2, 3$. If the range $0 - 10^{10}$ is replaced by $1500 - 10^{10}$, the bounds are much improved, as shown below. Alternatively, a ψ-bound of 1.0 holds for $X_0 \le x \le 10^{10}$, with X_0 as below:

k	$\psi : 1500 - 10^{10}$	X_0
1	0.790594	8
2	0.805589	224
3	0.764104	14
4	0.879669	14
5	0.806086	0
6	0.785064	62
10	0.792735	0
12	0.862547	0

Table 2 was computed by using a sieve. First, θ and ψ were computed for each arithmetic progression. All three functions

$$[\theta(x,k,l) - x/\varphi(k)]/\sqrt{x}, \quad [\psi(x,k,l) - x/\varphi(k)]/\sqrt{x},$$
$$[\theta(x;k,l) - (x - N(k,l)\sqrt{x})/\varphi(k)]/\sqrt{x}$$

are monotone decreasing between their jumps at primes or prime powers. Thus, to determine their maximal absolute values over a given interval, it suffices to check their values at the endpoints of the interval, and their left and right limits at primes and prime powers within the interval.

Considerable roundoff error can accumulate in summing 10^9 or more floating point numbers. To assure the accuracy of the computations, upper and lower bounds for θ and ψ were computed by first rounding all the logarithms up and down to the nearest 2^{-30}. After this truncation, the upper and lower bounds could essentially be computed by integer arithmetic, e.g. without roundoff error, and θ and ψ were replaced by their bounds in such a way as to assure that Table 2 gave rigorous upper bounds. (This choice of the truncation would have allowed the computation to continue as high as 1.7×10^{10}, considerably beyond its actual limit of 10^{10}.) Finally, the values were rounded up in their last digit.

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