SIGN CHANGES IN $\pi_{q,a}(x) - \pi_{q,b}(x)$

Kevin Ford
Richard H. Hudson

1. Introduction and summary.

Let

$$\mathrm{li}(x) = \lim_{\epsilon \to 0^+} \int_0^{1-\epsilon} \frac{dt}{\log t} + \int_{1+\epsilon}^{x} \frac{dt}{\log t}$$

and let $\pi(x)$ denote the number of primes $\leqslant x$. Also, $\pi_{q,a}(x)$ denotes the number of primes $\leqslant x$ lying in the progression $a \bmod q$. In 1792, Gauss observed that $\pi(x) < \mathrm{li}(x)$ for $x < 3,000,000$ (see e.g. [E]) and the question of whether or not there are any sign changes of $\pi(x) - \mathrm{li}(x)$ remained open until 1914 when J.E. Littlewood [Li] showed that there exists a positive constant k such that infinitely often both $\pi(x) - \mathrm{li}(x)$ and $\mathrm{li}(x) - \pi(x)$ exceed

$$\frac{kx^{1/2} \log\log\log x}{\log x}.$$

Sign changes are, nonetheless, quite rare and it was not until 1955 that any upper bound was obtained for the first sign change. The upper bound of

$$10^{10^{10^{34}}}$$

was obtained by Skewes [Sk1] on the assumption of the Riemann Hypothesis, and in 1955 [Sk2] he provided the first unconditional upper bound for the first sign change, namely

$$10^{10^{10^{10^3}}}.$$

In 1966, Lehman [Leh] developed a new method based on an explicit formula for $\mathrm{li}(x) - \pi(x)$ averaged by a Gaussian kernel and knowledge of zeros of the Riemann zeta function $\zeta(s)$ in the region $|\Im s| \leqslant 12000$. Lehman's method drastically improves the upper bound for the first sign change. In particular, he proved that it must occur before 1.5926×10^{1165}

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and his method was used by te Riele [tR] to lower the bound to 6.6658×10^{370} and by Bays and Hudson [BH5] to lower it further to 1.39822×10^{316}.

In this paper, we generalize Lehman's method, enabling one to compare the number of primes $\le x$ in any two arithmetic progressions $qn + a$ and $qn + b$. For reasons given in, e.g., [H2], [RS], negative values of $\pi_{q,b}(x) - \pi_{q,a}(x)$ may be relatively infrequent if b is a quadratic non-residue of q and a a quadratic residue. This phenomenon, first noted by Chebyshev in 1853 for the case $q = 4$, is known as "Chebyshev's bias". It is quite pronounced when $q|24$, $1 < b < q$, $(b, q) = 1$ and $a = 1$, and these cases have been studied extensively from a numerical point of view ([BH1], [BH2], [BH3], [BH4], [Lee], [Sh]) and from a theoretical point of view ([BFHR], [H2], [K1], [K2], [K3], [KT1], [KT2], [Li], [RS]). For example, Bays and Hudson [BH2] showed in 1978 that the smallest x with $\pi_{3,2}(x) < \pi_{3,1}(x)$ is $x = 608,981,813,029$.

Section 2 is devoted to the development of the analog of Lehman's theorem. Our bounds are considerably sharper than in [Leh], but as a consequence the bounds are a bit more complex. In §3 we apply the theorem for $q|24$ and $a = 1$. Our present knowledge of the zeros of these L-functions is due to Rumely ([Ru1], [Ru2]) and this is insufficient to obtain bounds which are anywhere near "best possible". The bounds, however, are in most cases adequate to localize negative values of $\pi_{q,b}(x) - \pi_{q,1}(x)$.

2. A generalization of Lehman's theorem

For non-real numbers z, define

$$\mathrm{li}(e^z) := e^z \int_0^\infty \frac{e^{-t}}{z-t}\,dt \tag{2.1}$$

and let

$$K(s;\alpha) = \sqrt{\frac{\alpha}{2\pi}} e^{-\alpha s^2/2}. \tag{2.2}$$

Also, for $\rho = \beta + i\gamma$, $0 < \beta < 1$, define

$$J(\rho) := \int_{\omega-\eta}^{\omega+\eta} K(u-\omega;\alpha) u e^{-u/2} \mathrm{li}(e^{\rho u})\,du.$$

Lemma 2.1. *If $\rho = \frac{1}{2} + i\gamma$ with $\gamma \ne 0$, $u \geqslant 1$ and $J \geqslant 1$, then*

$$\left| \frac{\mathrm{li}(e^{\rho u})}{e^{\rho u}} - \sum_{j=1}^{J} \frac{(j-1)!}{(\rho u)^j} \right| \leqslant \frac{J!}{u^{J+1}} \min\left(\frac{1}{|\gamma|^{J+1}}, \frac{2^{1.5J+2}}{(1+2|\gamma|)^{J+1}} \right).$$

Proof. By (2.1) and repeated integration by parts, we have for non-real z the identity

$$e^{-z}\mathrm{li}(e^z) - \sum_{j=1}^{J} \frac{(j-1)!}{z^j} = J! \int_0^\infty \frac{e^{-t}}{(z-t)^{J+1}}\, dt. \tag{2.3}$$

Now put $z = \rho u$. Since $|\rho u - t| \geqslant u|\gamma|$, the last integral is $\leqslant (u|\gamma|)^{-J-1}$. If $|\gamma|$ is small, we can do better by deforming the contour. If $\gamma > 0$ let C be the union of the straight line segments from 0 to $\frac{1}{2}(u - iu)$ to u to ∞ and if $\gamma < 0$ let C be the union of the line segments from 0 to $\frac{1}{2}(u + iu)$ to u to ∞. For $t \in C$, we have

$$|\rho u - t| \geqslant \frac{(1+2|\gamma|)u}{2^{3/2}}.$$

Together with the bound

$$\int_C |e^{-t}|\, dt \leqslant \sqrt{2},$$

this proves the lemma.

Lemma 2.2 (McCurley). *Let χ be a Dirichlet character of conductor k and denote by $N(T,\chi)$ the number of zeros of $L(s,\chi)$ lying in the region $s = \sigma + i\gamma$, $0 < \sigma < 1$, $|\gamma| \leqslant T$. Then*

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

where

$$C_2 = 0.9185, \qquad C_3 = 5.512.$$

Proof. This is Theorem 2.1 of [M] with $\eta = \frac{1}{2}$.

Corollary 2.3. *Suppose g is a continuous, positive, decreasing function for $t \geqslant T = \frac{2\pi e}{k}$, and $T_2 \geqslant T_1 \geqslant T$. Let χ be a Dirichlet character of conductor k and denote by γ the imaginary part of a generic non-trivial zero of $L(s,\chi)$. Then*

$$\left| \sum_{T_1 < |\gamma| \leqslant T_2} g(|\gamma|) - \frac{1}{\pi} \int_{T_1}^{T_2} g(t) \log\left(\frac{kt}{2\pi}\right) dt \right| \leqslant 2g(T_1)(C_2 \log kT_1 + C_3) + C_2 \int_{T_1}^{T_2} \frac{g(t)}{t}\, dt.$$

Proof. Lemma 2.2 and partial summation.

Corollary 2.4. *If $T \geqslant 150$, $n \geqslant 2$ and χ is a Dirichlet character of conductor $k \geqslant 3$, then*

$$\sum_{|\gamma|>T} \gamma^{-n} < \frac{T^{1-n}\log(kT)}{3}.$$

Proof. Letting $g(\gamma)=\gamma^{-n}$ in Corollary 2.3, we obtain

$$\begin{aligned}\sum_{|\gamma|>T} \gamma^{-n} &\leqslant T^{1-n}\left(\frac{\log\left(\frac{kT}{2\pi}\right)}{\pi(n-1)} + \frac{1}{\pi(n-1)^2} + \frac{2C_2\log(kT)+2C_3+C_2/n}{T}\right)\\ &\leqslant T^{1-n}\log(kT)\left(\frac{1}{\pi}+\frac{2C_2}{T}\right) + T^{1-n}\left(\frac{2C_3+C_2/2}{T} - \frac{\log(2\pi)}{\pi}\right)\\ &< \tfrac{1}{3}T^{1-n}\log(kT). \qquad \square.\end{aligned}$$

We also use the simple bound

$$\int_y^\infty K(u;\alpha)\,du < \sqrt{\frac{\alpha}{2\pi}}\int_y^\infty \left(\frac{u}{y}\right) e^{-\alpha u^2/2}\,du = \frac{K(y;\alpha)}{\alpha y} \qquad (y>0). \tag{2.4}$$

We now adopt a notational convention from [Leh]: The notation $f = \vartheta(g)$ means $|f| \leqslant |g|$.

Lemma 2.5. *Suppose*

$$\omega \geqslant 30, \quad 0<\eta\leqslant \omega/30, \quad |\gamma| \leqslant \frac{\alpha\eta}{2}. \tag{2.5}$$

If $\rho = \frac{1}{2}+i\gamma$, then

$$J(\rho) = e^{i\gamma\omega-\gamma^2/(2\alpha)}\left(\frac{1}{\rho}+\frac{1}{\omega\rho^2}+\frac{2}{\omega^2\rho^3}\right) + Q_1(\gamma)+Q_2(\gamma),$$

where

$$\begin{aligned}|Q_1(\gamma)| &\leqslant \frac{6}{(\omega-\eta)^3}\min\left(\frac{1}{\gamma^4}, \frac{64\sqrt{2}}{(1+2|\gamma|)^4}\right),\\ |Q_2(\gamma)| &\leqslant \frac{2.2K(\eta;\alpha)}{|\rho|\alpha\eta} + \frac{1.25}{\alpha\omega^3|\rho|^2} + \frac{1.27e^{-\gamma^2/(2\alpha)}}{\omega^2\alpha|\rho|}.\end{aligned}$$

Proof. Without loss of generality suppose $\gamma>0$. By Lemma 2.1 and the fact that $\int_{-\infty}^{\infty} K(u;\alpha)\,du = 1$,

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega;\alpha)ue^{-u/2}\mathrm{li}(e^{\rho u})\,du = I+E,$$

where

$$I = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega;\alpha) u e^{i\gamma u} \sum_{j=1}^{J} \frac{(j-1)!}{(\rho u)^j}\, du,$$
$$|E| \leqslant \frac{J!}{(\omega-\eta)^J} \min\left(\frac{1}{\gamma^{J+1}}, \frac{2^{1.5J+2}}{(1+2\gamma)^{J+1}} \right).$$

Now make the change of variables $u = \omega - s$ and take $J = 3$. By (2.5), $|s/\omega| \leqslant \frac{1}{30}$ and $|\rho\omega| \geqslant 15$, thus

$$\begin{aligned}
\frac{I}{e^{i\gamma\omega}} &= \int_{-\eta}^{\eta} K(s;\alpha) e^{-i\gamma s} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2(1-s/\omega)} + \frac{2}{\omega^2\rho^3(1-s/\omega)^2} \right) ds \\
&= \int_{-\eta}^{\eta} K(s;\alpha) e^{-i\gamma s} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3} + \frac{s}{\omega^2\rho^2} + \frac{4s}{\omega^3\rho^3} + \vartheta\left(\frac{1.25 s^2}{\omega^3\rho^2} \right) \right) ds \\
&= \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3} \right) I_0 + \frac{I_1}{\omega^2\rho^2}\left(1 + \frac{4}{\omega\rho} \right) + \vartheta\left(I_2' \frac{1.25}{\omega^3\rho^2} \right)
\end{aligned}$$

where

$$I_n = \int_{-\eta}^{\eta} K(s;\alpha) s^n e^{-i\gamma s}\, ds \qquad (n = 0, 1)$$

and

$$I_2' = \int_{-\infty}^{\infty} K(s;\alpha) s^2\, ds = 1/\alpha.$$

By (2.2) and (2.4), we have

$$\begin{aligned}
I_0 &= e^{-\gamma^2/(2\alpha)} + \vartheta\left(2\int_{\eta}^{\infty} K(s;\alpha)\, ds \right) \\
&= e^{-\gamma^2/(2\alpha)} + \vartheta\left(\frac{2K(\eta;\alpha)}{\alpha\eta} \right).
\end{aligned}$$

In addition, by (2.5) we have

$$\begin{aligned}
|I_1| &= \left| \frac{2i \sin\gamma\eta}{\alpha} K(\eta;\alpha) - \frac{i\gamma}{\alpha} I_0 \right| \\
&\leqslant \left(\frac{2}{\alpha} + \frac{2\gamma}{\alpha^2\eta} \right) K(\eta;\alpha) + \frac{\gamma e^{-\gamma^2/(2\alpha)}}{\alpha} \\
&\leqslant \frac{3K(\eta;\alpha) + \gamma e^{-\gamma^2/(2\alpha)}}{\alpha}.
\end{aligned}$$

We thus obtain

$$\begin{aligned}
&\left| I - e^{i\gamma\omega - \gamma^2/(2\alpha)} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3} \right) \right| \\
&\qquad \leqslant \frac{1.27\gamma e^{-\gamma^2/(2\alpha)}}{\omega^2|\rho|^2\alpha} + \frac{1.25}{\alpha\omega^3|\rho|^2} + \left(\frac{3.8}{\omega^2|\rho|^2\alpha} + \frac{2.16}{|\rho|\alpha\eta} \right) K(\eta;\alpha).
\end{aligned}$$

By (2.5), $\omega^2|\rho| \geqslant 450\eta$, and the lemma follows. $\square$

The next lemma, essentially due to Lehman ([Leh], §5), shows how to deal with the contribution from large γ without needing to assume the truth of Riemann Hypothesis.

Lemma 2.6. *Suppose that*

$$|\gamma| \geqslant 100, \quad \omega \geqslant 30, \quad \eta \leqslant \omega/15, \quad 1 \leqslant N \leqslant \min\left(\frac{|\gamma|\eta}{2}, \frac{\alpha\omega^2}{100}\right). \tag{2.6}$$

Writing $\rho = \beta + i\gamma$, *with* $0 < \beta < 1$, *we have*

$$|J(\rho)| \leqslant e^{(\beta-1/2)(\omega+\eta)} \left(\frac{2.4\sqrt{\alpha}e^{-\alpha\eta^2/8}}{\gamma^2} + \frac{2.8\sqrt{N}}{|\gamma|^{N+1}}\left(\frac{N\alpha}{e}\right)^{N/2}\right).$$

Proof. By Lemma 2.5, we expect that $|J(\rho)|$ is about $|\rho|^{-1}e^{(\beta-1/2)\omega-\gamma^2/(2\alpha)}$. Suppose without loss of generality that $\gamma > 100$. As in [Leh], we begin by considering the function

$$f(s) := \rho s e^{-\rho s}\mathrm{li}(e^{\rho s})e^{-\alpha(s-\omega)^2/2}$$

in the region $-\pi/4 \leqslant \arg s \leqslant \pi/4$, $|s| > 1$. This function is analytic in this sector because $\gamma > 100$. Then

$$J(\rho) = \frac{1}{\rho}\sqrt{\frac{\alpha}{2\pi}}I_1, \quad I_1 = \int_{\omega-\eta}^{\omega+\eta} e^{(\rho-1/2)u}f(u)\,du.$$

By repeated integration by parts,

$$I_1 = \sum_{n=0}^{N} \frac{(-1)^n e^{(\rho-\frac12)\omega}}{(\rho-\frac12)^{n+1}}\left(e^{(\rho-\frac12)\eta}f^{(n)}(\omega+\eta) - e^{-(\rho-\frac12)\eta}f^{(n)}(\omega-\eta)\right) + \frac{(-1)^N}{(\rho-\frac12)^N}\int_{\omega-\eta}^{\omega+\eta} e^{(\rho-\frac12)u}f^{(N)}(u)\,du.$$

Choose $r \leqslant \omega/10$. Then

$$f^{(n)}(u) = \frac{n!}{2\pi i}\oint_{|s-u|=r}\frac{f(s)}{(s-u)^{n+1}}\,ds. \tag{2.7}$$

By (2.3) we have

$$f(s) = e^{-\alpha(s-\omega)^2/2}\left(1 + \frac{1}{\rho s} + \vartheta\left(\frac{2|\rho s|}{|\Im \rho s|^3}\right)\right).$$

Since $|\rho s|\geqslant 2000$ and $|\Im \rho s|\geqslant \frac{1}{2}|\rho s|$, it follows that

$$|f(s)|\leqslant 1.001e^{-(\alpha/2)\Re(s-\omega)^2}.$$

Writing $s=u+re^{i\phi}$ and using (2.7), we deduce

$$|f^{(n)}(u)|\leqslant \frac{1.001n!}{2\pi r^n}\int_{-\pi}^{\pi} e^{(\alpha/2)(r^2-r^2\cos^2\phi-(r\cos\phi+u-\omega)^2)}\,d\phi. \tag{2.8}$$

When $u=\omega\pm\eta$, we take $r=\eta/2$ and get

$$\begin{aligned}|f^{(n)}(u)| &\leqslant \frac{1.001n!}{2\pi(\eta/2)^n}e^{-\alpha\eta^2/8}\int_{-\pi}^{\pi} e^{-(\alpha\eta^2/4)(1-\cos\phi)^2}\,d\phi\\ &\leqslant 1.001n!(2/\eta)^n e^{-\alpha\eta^2/8},\end{aligned}$$

since the integrand above is $\leqslant 1$. We then obtain

$$|I_1|\leqslant e^{(\beta-\frac12)(\omega+\eta)}\left(\frac{2.002e^{-\frac18\alpha\eta^2}}{\gamma}\sum_{n=0}^{N} n!\left(\frac{2}{\gamma\eta}\right)^n+\gamma^{-N}\int_{\omega-\eta}^{\omega+\eta}|f^{(N)}(u)|\,du\right).$$

Since $n!\leqslant 2(N/2)^n$ for $n\leqslant N$ and $N/(\gamma\eta)\leqslant\frac12$, the sum on n is $\leqslant 3$. By (2.8),

$$\begin{aligned}\int_{\omega-\eta}^{\omega+\eta}|f^{(N)}(u)|\,du &\leqslant \frac{1.001N!}{2\pi r^N}e^{\alpha r^2/2}\int_{-\pi}^{\pi}e^{-\frac{\alpha}{2}r^2\cos^2\phi}\int_{-\eta}^{\eta}e^{-\frac{\alpha}{2}(t+r\cos\phi)^2}\,dt\,d\phi\\ &\leqslant \frac{1.001N!}{2\pi r^N}e^{\alpha r^2/2}\int_{-\pi}^{\pi}\int_{-\infty}^{\infty}e^{-\frac{\alpha}{2}t^2}\,dt\,d\phi\\ &= \frac{1.001N!}{r^N}e^{\alpha r^2/2}\sqrt{\frac{2\pi}{\alpha}}.\end{aligned}$$

Taking $r=\sqrt{N/\alpha}$ and using the inequality $N!\leqslant e^{1-N}N^{N+1/2}$ gives

$$\int_{\omega-\eta}^{\omega+\eta}|f^{(N)}(u)|\,du\leqslant 1.001e\sqrt{\frac{2\pi N}{\alpha}}\left(\frac{\alpha e}{N}\right)^{-N/2}.$$

The lemma now follows. □

Theorem 1. *Suppose χ is a primitive Dirichlet character of conductor k, and all the nontrivial zeros $\rho=\beta+i\gamma$ of $L(s,\chi)$ with $|\gamma|\leqslant A$ have real part $\beta=\frac12$. Suppose that*

$$150\leqslant T\leqslant A,\quad \omega\geqslant 30,\quad \eta\leqslant\omega/30,\quad \frac{2A}{\eta}\leqslant\alpha\leqslant A^2. \tag{2.9}$$

Then

$$\sum_\rho J(\rho) = \sum_{|\gamma|\leqslant T} e^{i\gamma\omega-\gamma^2/(2\alpha)} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3}\right) + \sum_{i=1}^4 R_i(\chi, T),$$

where

$$|R_1(\chi,T)| \leqslant \frac{6}{(\omega-\eta)^3} \sum_\rho \min\left(\frac{1}{\gamma^4}, \frac{64\sqrt{2}}{(1+2|\gamma|)^4}\right),$$

$$|R_2(\chi,T)| \leqslant \left(\frac{2.2K(\eta;\alpha)}{\alpha\eta} + \frac{1.27}{\alpha\omega^2}\right) \sum_{|\gamma|\leqslant A} \frac{1}{|\rho|} + \frac{1.25}{\alpha\omega^3} \sum_\rho \frac{1}{|\rho|^2},$$

$$|R_3(\chi,T)| \leqslant e^{-T^2/(2\alpha)} \log(kT) \left(\frac{\alpha}{\pi T^2} + \frac{4.3}{T}\right),$$

$$|R_4(\chi,T)| \leqslant e^{(\omega+\eta)/2} \log(kA) \left(\frac{0.8\sqrt{\alpha}e^{-\alpha\eta^2/8}}{A} + 2.56A\alpha^{-1/2}e^{-A^2/(2\alpha)}\right).$$

If the Riemann Hypothesis is true for $L(s,\chi)$ *(i.e. all the nontrivial zeros have real part* $\frac{1}{2}$*), then the term* R_4 *may be omitted, as may the condition* $\alpha \leqslant A^2$*. Also, if* $A = T$*, then* $R_3(\chi,T) = 0$*.*

Proof. The main terms in the theorem come from the main terms of Lemma 2.5 for $|\gamma| \leqslant T$. The first part of the theorem follows by taking

$$R_i = R_i(\chi,T) = \sum_{|\gamma|\leqslant A} Q_i(\gamma), \qquad (i = 1, 2)$$

$$R_3 = R_3(\chi,T) = \sum_{T<|\gamma|\leqslant A} e^{i\gamma\omega-\gamma^2/(2\alpha)} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3}\right),$$

$$R_4 = R_4(\chi,T) = \sum_{|\gamma|>A} J(\rho).$$

The upper bounds for R_1 and R_2 follow from Lemma 2.5. Since $\omega \geqslant 30$, we have

$$\left|\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3}\right| \leqslant \frac{1}{\gamma}.$$

Thus, by Corollary 2.3, we find that

$$\begin{aligned}|R_3| &\leqslant \sum_{|\gamma|>T} \frac{e^{-\gamma^2/(2\alpha)}}{\gamma} \\ &\leqslant \int_T^\infty \frac{e^{-t^2/(2\alpha)}}{\pi t} \log\left(\frac{kt}{2\pi}\right) dt + \frac{2e^{-T^2/(2\alpha)}}{T}(C_2\log(kT) + C_3) \\ &\quad + C_2 \int_T^\infty \frac{e^{-t^2/(2\alpha)}}{t^2}\, dt.\end{aligned}$$

If $g(t)$ is positive and decreasing for $t \geqslant T$ we have

$$\int_T^\infty g(t)e^{-bt^2}\,dt < \frac{g(T)}{T}\int_T^\infty te^{-bt^2}\,dt = \frac{g(T)e^{-bT^2}}{2bT}.$$

Therefore,

$$|R_3| \leqslant e^{-T^2/(2\alpha)}\left(\frac{\alpha\log(kT/(2\pi))}{\pi T^2} + \frac{2C_2\log(kT)+2C_3}{T} + \frac{\alpha C_2}{T^3}\right).$$

The desired bound for R_3 now follows from the bounds $kT \geqslant 100$ and

$$\frac{\alpha C_2}{T^3} \leqslant \frac{\alpha\log(2\pi)}{\pi T^2}.$$

Lastly, Corollary 2.4 and Lemma 2.6 give

$$\begin{aligned}|R_4| &\leqslant \sum_{|\gamma|>A}|J(\rho)| \\ &\leqslant e^{(\omega+\eta)/2}\log(kA)\left(\frac{0.8\sqrt{\alpha}e^{-\alpha\eta^2/8}}{A} + 0.94\sqrt{N}\left(\frac{N\alpha}{eA^2}\right)^{N/2}\right).\end{aligned}$$

We take $N = \lfloor A^2/\alpha\rfloor$ and note that (2.9) implies (2.6). $\square$

Finally, we need explicit formulas for the number of primes in an arithmetic progression. For a primitive Dirichlet character χ modulo $k \geqslant 3$, let $a = 0$ if $\chi(-1) = 1$ and $a = 1$ if $\chi(-1) = -1$. By an analog of the Riemann-von Mangoldt formula ([La, p. 532]), if $L(s,\chi)$ has no positive real zeros then

(2.10)
$$\begin{aligned}S(\chi;x) &:= \sum_{\substack{p,m\\ p^m\leqslant x}}\frac{\chi(p)^m}{m} \\ &= -\sum_\rho \mathrm{li}(x^\rho) + \int_x^\infty \frac{dy}{y^{1-a}(y^2-1)\log y} + (1-a)\log\log x + K_a,\end{aligned}$$

where

$$K_0 = C - \log\left(\frac{\tau(\chi)\pi}{2k}L(1,\overline{\chi})\right),$$

$$K_1 = \log\left(\frac{\tau(\chi)}{i\pi}L(1,\overline{\chi})\right),$$

and

$$\tau(\chi) = \sum_{m=1}^q \chi(m)e^{2\pi i m/q}.$$

Here $C = 0.5772\dots$ is the Euler-Mascheroni constant and $\log z$ refers to the principal branch of the logarithm. The values of $L(1,\chi)$ are computed easily by means of the formula

$$\tau(\chi)L(1,\overline{\chi}) = -\sum_{j=1}^{k-1} \chi(j)\log(1-e^{2\pi ij/k}).$$

Also, the integral in (2.10) is less than $1/x$ for $x > 10$. The last formula we need is

$$\pi_{q,a}(x) = \frac{1}{\phi(q)} \sum_{\chi \bmod q} \overline{\chi}(a) S(\chi;x) - \sum_{\substack{p,m \\ p^m \leqslant x, m \geqslant 2 \\ p^m \equiv a \pmod q}} \frac{1}{m}. \tag{2.11}$$

In practice the $m = 2$ terms will be very significant, while the terms with $m \geqslant 3$ will be negligible. In fact, we have

$$\sum_{\substack{p^m \leqslant x \\ m \geqslant 3}} \frac{1}{m} \leqslant \frac{1.3x^{1/3}}{\log x}, \qquad (x \geqslant e^{30}) \tag{2.12}$$

which follows easily from the inequality

$$\pi(x) \leqslant \frac{x}{\log x} + \frac{1.5x}{\log^2 x} \qquad (x > 1)$$

given by Theorem 1 of Rosser and Schoenfeld [RoS]. Lastly, if χ_0 is the primitive character (of order q_0) which induces χ, then

$$\begin{aligned} |S(\chi_0;x) - S(\chi;x)| &\leqslant \sum_{\substack{p^m \leqslant x \\ p|q, p\nmid q_0}} \frac{1}{m} \leqslant \sum_{p|q, p\nmid q_0} \left(1 + \log\frac{\log x}{\log p}\right) \\ &\leqslant \left|\{p : p|q, p \nmid q_0\}\right| (\log\log x + 1 - \log 2). \end{aligned} \tag{2.13}$$

Here we have used the inequality $\sum_{n \leqslant x} \frac{1}{n} \leqslant 1 + \log x$.

3. Primes in progressions modulo 3, 4, 8, 12 and 24

For brevity, write

$$\Delta_{q,b,1}(x) := \pi_{q,b}(x) - \pi_{q,1}(x).$$

In this section we give new results on the location of negative values of $\Delta_{q,b,1}(x)$. Throughout we assume $q|24$, $1 < b < q$ and $(b,q) = 1$. As noted previously, such negative values are quite rare. The smallest x giving

$\Delta_{4,3,1}(x) < 0$ is $x = 26861$, discovered by Leech [Lee] in 1957. Shanks [Sh] computed $\Delta_{8,b,1}(x)$ for $b = 3, 5, 7$ and $x \leqslant 10^6$ and found that none of the functions takes negative values. Extensive computations by Bays and Hudson in the 1970s ([BH1],[BH2],[BH3],[BH4]) for $x \leqslant 10^{12}$ led to the discovery of several more "negative regions" for $\Delta_{4,3,1}(x)$, as well as a single region for $\Delta_{3,2,1}(x)$, a single region for $\Delta_{24,13,1}(x)$ and two regions for $\Delta_{8,5,1}(x)$. By "negative region" we mean an interval $[x_1, x_2]$ where the corresponding function is negative a large percentage of time. It is not well-defined, but reflects the observation that negative values of the functions $\Delta_{q,b,1}(x)$ occur in "clumps". For example, $\Delta_{3,2,1}(x) < 0$ for about 15.9% of the integers in the interval $[608981813029, 610968213796]$. On the other hand, the computations show that

$$\Delta_{q,b,1}(x) \geqslant 0 \qquad (x \leqslant 10^{12})$$

for

$$q = 8, b \in \{3, 7\} \qquad \text{and} \qquad q = 24, b \in \{5, 7, 11, 17, 19, 23\}. \tag{3.1}$$

With modern computers, the search could easily be extended to 10^{14} or even 10^{15}, and we will show that in fact there are regions in this range where $\Delta_{q,b,1}(x) < 0$ for some of the pairs q, b given in (3.1). Our method, though, takes only seconds versus weeks for an exhaustive search.

From a theoretical standpoint, Littlewood [Li] proved in 1914 that $\Delta_{4,3,1}(x)$ and $\Delta_{3,2,1}(x)$ change sign infinitely often. Knapowski and Turán (Part II of [KT1]) generalized this substantially, showing that $\Delta_{q,b,1}(x)$ changes sign infinitely often, whenever $q|24$, $1 < b < q$ and $(b, q) = 1$ (in addition to other q, b). Later papers ([KT1],[KT2]) deal with the frequency of sign changes, but the bounds for the first sign change are of the "towering exponentials" type, similar to Skewes' results.

In what follows, χ_k denotes the unique primitive character modulo k and $\chi_{k,i}$ $(i = 1, \dots, h)$ denote the primitive characters modulo k if there are more than one. In particular, $\chi_{8,1}(-1) = -1$ and $\chi_{24,1}(-1) = -1$. Table 1 below lists some parameters which we will need. Here

$$\Sigma_1 = \sum_\rho \frac{1}{|\rho|^2}, \quad \Sigma_2 = \sum_\rho \min\left(\frac{1}{\gamma^4}, \frac{64\sqrt{2}}{(1+2|\gamma|)^4}\right), \quad \Sigma_3 = \sum_{|\gamma| \leqslant 10000} \frac{1}{|\rho|}.$$

The entries in the second, third, and fourth columns are rigorous upper bounds, obtained from Rumely's lists of zeros [Ru2] and Corollary 2.4. The number N denotes the number of zeros with $0 < \gamma < 10000$. It is desirable in applications to know the zeros of all the required L-functions to the same height. Rumely [Ru1] originally computed zeros to height 10000 for characters with conductor $\leqslant 13$ and to height 2600 for other characters. For the two primitive characters modulo 24, Rumely's original programs were run to compute the zeros to height $T = 10000$, and the output was checked against his original list of zeros to height 2600. In all of our computations, we take $T = 10000$ for every character. Recently Rumely [Ru2] has extended the computations to height 100000 for characters of conductor < 10. So for such characters we may take $A = 100000$.

Char.	Σ_1	Σ_2	Σ_3	N	a	$\tau(\chi)L(1,\overline{\chi})$	K_a
χ_3	0.114	0.00070	11.29	11891	1	$(\pi/3)i$	$-\log 3$
χ_4	0.156	0.00186	12.10	12349	1	$(\pi/2)i$	$-\log 2$
$\chi_{8,1}$	0.317	0.01336	14.14	13452	1	πi	0
$\chi_{8,2}$	0.236	0.00442	13.92	13452	0	$2\log(1+\sqrt{2})$	$1.6382\ldots$
χ_{12}	0.331	0.01120	15.12	14097	0	$2\log(2+\sqrt{3})$	$1.6420\ldots$
$\chi_{24,1}$	0.798	0.13683	17.61	15200	1	$2\pi i$	$\log 2$
$\chi_{24,2}$	0.553	0.04239	17.24	15200	0	$4\log(\sqrt{2}+\sqrt{3})$	$1.0877\ldots$

TABLE 1.

When $q|24$, all the characters modulo q are real, and furthermore the only quadratic residue modulo q is 1. When $x \geqslant e^{32.3}$, for each character in the table,

$$|(1-a)\log\log x + K_a| \leqslant |\log\log x + \log 3| \leqslant 0.00312\frac{x^{1/3}}{\log x}.$$

Further, if χ_0 is the primitive character (modulo q_0) which induces χ (for one of the seven characters in Table 1), then

$$(\log\log x + 0.31)\,|\{p : p|q, p\nmid q_0\}| \leqslant \log\log x + 0.31 \leqslant 0.0026\frac{x^{1/3}}{\log x}.$$

Together with (2.10), (2.11), (2.12) and (2.13), we obtain the formula

$$\text{(3.2)}\quad \pi_{q,b}(x) - \pi_{q,1}(x) = \frac{2}{\phi(q)} \sum_{\substack{\chi \bmod q \\ \chi(b)=-1}} \sum_{\rho} \mathrm{li}(x^\rho) + \frac{\pi(\sqrt{x})}{2} + \vartheta\left(\frac{1.31x^{1/3}}{\log x}\right).$$

We need a tight upper bound on $\pi(\sqrt{x})$, given by the next lemma.

Lemma 3.1. *For $x \geqslant 10^{14}$, we have $\pi(x) \leqslant 1.000011\,\mathrm{li}(x)$.*

Proof. From Table 3 of [Ri], we have $\pi(10^{14}) < \mathrm{li}(10^{14})$. Defining $\theta(x) = \sum_{p\leqslant x}\log p$, we have

$$|\theta(x) - x| \leqslant 0.0000055x \qquad (x \geqslant e^{32}),$$

which follows from Theorem 5.1.1 of [RR], upon taking $x = e^{32}$, $m = 18$, $H = 70000000$, and $\delta = 6.59668 \times 10^{-8}$. By partial summation, for $x \geqslant 10^{14}$ we obtain

$$\begin{aligned}\pi(x) &\leqslant \mathrm{li}(10^{14}) + \int_{10^{14}}^{x} \frac{d\theta(t)}{\log t} \\ &\leqslant (1 + 2(0.0000055))\mathrm{li}(x). \qquad \square\end{aligned}$$

Define

$$W(\chi; x) = \sum_{\rho} \mathrm{li}(x^{\rho}),$$

where the sum is over zeros ρ of $L(s,\chi)$ lying in the critical strip. Since we are primarily interested in locations where $\pi_{q,b}(x) - \pi_{q,1}(x)$ is negative, we apply Lemma 3.1 to obtain from (3.2) the inequality

$$\pi_{q,b}(x) - \pi_{q,1}(x) \leqslant \frac{2}{\phi(q)} \sum_{\substack{\chi \bmod q \\ \chi(b)=-1}} W(\chi; x) + \frac{1}{2}(1.000011)\,\mathrm{li}(\sqrt{x}) + \frac{1.31x^{1/3}}{\log x}.$$

It is easy to show that

$$\mathrm{li}(x) \leqslant \frac{x}{\log x}\left(1 + \frac{1}{\log x} + \frac{2}{\log^2 x} + \frac{h(x)}{\log^3 x}\right),$$

where

$$h(x) = \begin{cases} 8.326 & e^{16} \leqslant x < e^{21} \\ 7.538 & e^{21} \leqslant x \leqslant e^{29.3} \\ 7 & x \geqslant e^{29.3}. \end{cases}$$

By Theorem 1, we therefore have

Theorem 2. *Suppose that $\omega - \eta \geqslant 32.3$ and $0 < \eta \leqslant \omega/30$. Suppose $q|24$, $(b,q) = 1$ and $1 < b < q$. For each Dirichlet character χ modulo q with $\chi(b) = -1$, suppose that all the zeros of $L(s,\chi)$ which lie in the rectangle $0 < \Re s < 1, -A_{\chi} \leqslant \Im s \leqslant A_{\chi}$, actually lie on the critical line $\Re s = \frac{1}{2}$. Further suppose that*

$$150 \leqslant T_{\chi} \leqslant A_{\chi}, \qquad \frac{2A_{\chi}}{\eta} \leqslant \alpha \leqslant A_{\chi}^2$$

for every χ. Then

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega;\alpha) u e^{-u/2}(\pi_{q,b}(e^u) - \pi_{q,1}(e^u))\,du \leqslant$$

$$(1.000011)\left(1 + \frac{2}{\omega-\eta} + \frac{8}{(\omega-\eta)^2} + \frac{8h(e^{(\omega-\eta)/2})}{(\omega-\eta)^3}\right) + 1.31e^{-(\omega-\eta)/6}$$

$$+ \frac{2}{\phi(q)} \sum_{\substack{\chi \bmod q \\ \chi(b)=-1}} \left(\sum_{|\gamma| \leqslant T_{\chi}} e^{i\gamma\omega - \frac{\gamma^2}{2\alpha}} \left(\frac{1}{\rho} + \frac{1}{\omega\rho^2} + \frac{2}{\omega^2\rho^3}\right) + \sum_{i=1}^{4} |R_i(\chi, T_{\chi})| \right).$$

The error terms $R_i(\chi, T_\chi)$ are as given in Theorem 1, with $T = T_\chi$ and $A = A_\chi$. Furthermore, if $A_\chi = T_\chi$ then the corresponding $R_3(\chi, T) = 0$, and if the Riemann Hypothesis holds for $L(s,\chi)$, then we have $R_4(\chi, T) = 0$ and the condition $\alpha \leqslant A_\chi^2$ may be omitted.

Locating likely candidates for regions where $\Delta_{q,b,1}(x)$ takes negative values is relatively simple. We search for values of ω for which

$$K^* = K^*(q,b;\omega) = \frac{\mathrm{li}(\sqrt{x})\log x}{2\sqrt{x}} + \frac{2}{\phi(q)} \sum_{\substack{\chi \bmod q \\ \chi(b)=-1}} \sum_{|\gamma| \leqslant T_\chi} \frac{e^{i\gamma\omega}}{\rho} < 0.$$

Heuristically, K^* is a good predictor for the average of $ue^{-u/2}\Delta_{q,b,1}(e^u)$ for u near ω. For example, $K^*(24, 13; \omega)$ reaches a relative minimum of -0.15873 at about $\omega = 27.617477$, while Bays and Hudson [BH3] computed at $x = 9.866 \times 10^{11} \approx e^{27.61753}$ the value $\Delta_{24,13,1}(x) = -6091 \approx -0.169357\frac{\sqrt{x}}{\log x}$ (It is possible that $\Delta_{24,13,1}(x)$ takes smaller values in this vicinity, but this is the smallest value listed in the paper). Using K^* as an approximation for $ue^{-u/2}\Delta_{q,b,1}(e^u)$ is also useful in computing a numerical value for Chebyshev's bias (see [RS], [BFHR]).

In practice, since ω is large, η is small, and T is large ($\geqslant 10000$), the most critical of the error terms is $R_4(\chi, T_\chi)$ because it controls the maximum practical value for α. We want to take α as large as possible, so the sums over $e^{i\gamma\omega - \gamma^2/(2\alpha)}/\rho$, which are required to be "large" negative, are not damped out too much by the $e^{-\gamma^2/(2\alpha)}$ factor.

The computations were performed with a C program running on a SUN Ultra-10 workstation using double precision floating point arithmetic, which provides about 16 digits of precision. The zeros of the L-functions in Rumely's lists are all accurate to within 10^{-12}. Values computed for the right side of the inequality in Theorem 2 were rounded up in the 4th decimal place.

Theorem 3. *For each row of Tables 2 and 3 for which a value of K is given, we have*

$$\min_{\omega-\eta \leqslant u \leqslant \omega+\eta} ue^{-u/2}(\pi_{q,b}(e^u) - \pi_{q,1}(e^u)) \leqslant K. \tag{3.3}$$

Proof. Take the indicated values of the parameters in Theorem 2. Here $T_\chi = 10000$ for every χ, $A_\chi = 100000$ in Table 2 and $A_\chi = 10000$ in Table 3. In the case where a value of K is not given, we could not prove that $K < 0$ with any choice of parameters. □

q	b	ω	K^*	η	α	K
3	2	45.12686	−0.0798	0.02	10^7	−0.0650
3	2	58.36855	−0.1710	0.02	10^7	−0.1525
4	3	2179.77584	−0.8109	0.05	4000000	−0.7761
4	3	78683.67818	−1.0480	2.00	120000	−0.8372
8	3	43.36630	−0.0249	0.02	10^7	−0.0013
8	3	54.94255	−0.0490	0.02	10^7	−0.0280
8	5	32.89388	−0.0716	0.02	10^7	−0.0503
8	5	34.46826	−0.0051			
8	5	57.48058	−0.2136	0.02	10^7	−0.1915
8	7	32.89284	−0.0136			
8	7	45.34991	−0.0868	0.02	10^7	−0.0508
8	7	48.79950	−0.1889	0.02	10^7	−0.1724
12	11	187.53674	−0.0410	0.02	10^7	−0.0191
12	11	191.89007	−0.0415	0.02	10^7	−0.0182

TABLE 2.

Example. The "error terms" R_3 and R_4 force α to be less than $\min(A^2/\omega, T^2)$ for practical purposes. For row 5 of Table 2, with the indicated values of the parameters, we compute (rounded in the last place after the decimal point)

char	sum on ρ	R_1	R_2	R_3	R_4
χ_4	−0.802723684	0.000000137	0.000000002	0.002303420	0
$\chi_{8,2}$	−1.308816425	0.000000326	0.000000003	0.002454092	0

Here the second column is the sum over $|\gamma| \leqslant T_\chi$ in Theorem 2. The first line of the right side of the inequality in Theorem 2 is computed as 1.0521043. All of these values are rounded in the last decimal place.

Corollary 4. *For each $b \in \{3,5,7\}$, $\pi_{8,b}(x) < \pi_{8,1}(x)$ for some $x < 5 \times 10^{19}$. For each $b \in \{5,7,11\}$, $\pi_{12,b}(x) < \pi_{12,1}(x)$ for some $x < 10^{84}$. For each $b \in \{5,7,11,13,17,19,23\}$, $\pi_{24,b}(x) < \pi_{24,1}(x)$ for some $x < 10^{353}$. Finally, if the zeros of $L(s,\chi_4)$ lying in the critical strip to height $A = 630000$ all have real part equal to $\frac{1}{2}$, then for some x in the vicinity of $e^{78683.7}$ we have*

$$\pi_{4,1}(x) - \pi_{4,3}(x) > \frac{\sqrt{x}}{\log x}.$$

The significance of the last statement is that we now know (once the zeros of $L(s,\chi_4)$ are computed to height 630000) a specific region where $\pi_{4,1}(x)$ runs ahead of $\pi_{4,3}(x)$ as much as it usually runs behind (This is the smallest x for which $K^* < -1$). The idea is that the terms on the right side of (3.2) corresponding to the zeros ρ are oscillatory, so that on average $\Delta_{q,b,1}(x)$ is about $\pi(\sqrt{x})/2 \approx \sqrt{x}/\log x$. Subject to certain

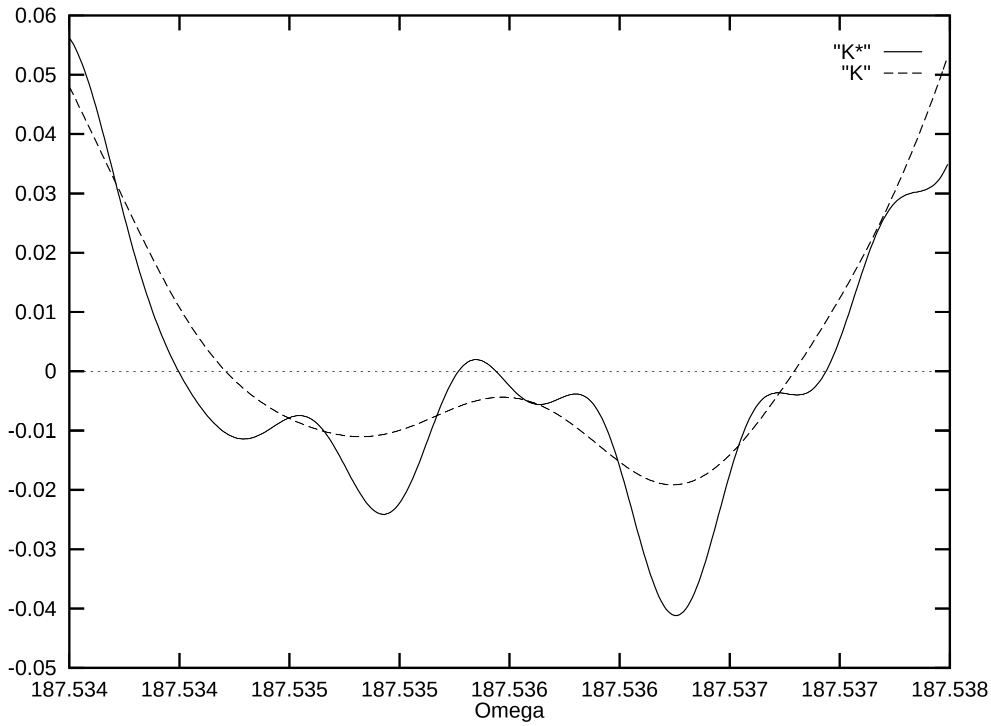
q	b	ω	K^*	η	α	K
12	5	39.12815	−0.0071			
12	5	69.00554	−0.0210			
12	5	73.93306	−0.0117			
12	5	88.98310	−0.0104			
12	5	102.08460	−0.0344			
12	5	103.73736	−0.0611	0.03	750000	−0.0445
12	7	39.12144	−0.2063	0.02	1550000	−0.1410
12	7	45.87795	−0.1468	0.02	1400000	−0.0871
24	5	161.18837	−0.1176	0.04	525000	−0.0920
24	7	92.49622	−0.0693	0.03	830000	−0.0530
24	11	111.54595	−0.0023			
24	11	812.63677	−0.0526	0.20	118000	−0.0104
24	13	34.14425	−0.4810	0.02	1700000	−0.3521
24	17	34.05708	−0.0387			
24	17	34.19749	−0.0208	0.02	1650000	−0.0110
24	19	34.20322	−0.1473	0.02	1650000	−0.1362
24	23	43.45318	−0.0204			
24	23	94.46170	−0.0376	0.03	800000	−0.0113

TABLE 3.

unproven hypotheses, this notion can be made very precise (e.g. [RS]). The two rows for $q = 4$ were chosen because of the large negative values of K^*.

In Tables 2 and 3, we have confined our calculations to locating regions with $x \geqslant e^{32.3} \approx 10^{14}$, smaller x being easily dealt with by exhaustive computer search. The listed values of K^* and K are rounded up in the last decimal place. For each pair (q, b) except $(4, 3)$, the first few likely regions of negative values of $\Delta_{q,b,1}(x)$ are listed. The lists continue until a region is found where a negative value can be proved with $A = 10000$. In some regions, a negative value can be proved with a larger value of A and in other regions no negative value could be proved even with $A = \infty$. These latter rows have no K value listed. However, when $\omega \leqslant 44$ or so, it is possible to find specific values of x with $\Delta_{q,b,1}(x) < 0$ by computing this function exactly by means of Hudson's extension of Meissel's formula [H1]. This formula makes it practical to compute exact values of $\pi_{q,a}(x)$ for x as large as 10^{20}. The first author is currently writing a computer program for this, and one preliminary result can be announced now. At $x = 1.9282 \times 10^{14}$ we have $\Delta_{8,7,1}(x) = -105$, and this computation took 10 minutes on a Sun Ultra-10 workstation.

For all pairs q, b, the values of ω given in Tables 2 and 3 represent the minimum of K, and this doesn't necessarily correspond to the minimum of K^*. The difference $|K - K^*|$ varies substantially, and this is expected due



GRAPH 1. K vs. K^*; $q = 12$, $b = 11$, $\eta = 0.02$, $\alpha = 10^7$, $A = 100000$.

to the factors $e^{-\gamma^2/(2\alpha)}$ in Theorem 2. To illustrate the difference, Graph 1 depicts the functions K and K^* for $q = 12$, $b = 11$ in the vicinity of $e^{187.536}$. Also as expected, larger values of A, which permit larger values of α, narrow the difference appreciably.

A shortcoming of our method is the inability to compare three or more progressions. For example, Shanks [Sh] asked if $\pi_{8,1}(x)$ will ever be greater than each of $\pi_{8,3}(x)$, $\pi_{8,5}(x)$ and $\pi_{8,7}(x)$ simultaneously. Based on computations of the functions K^*, it is likely that this occurs in the vicinity of $e^{389.3712}$, but this cannot be proved by the methods of this paper. It is, however, possible to detect negative values of any linear combination of the functions $\pi_{q,b}(x)$. For example, by Theorem 2 it follows that for some x with $|\log x - 158.64233| \leqslant 0.01$, we have

$$\pi_{8,1}(x) > \frac{1}{3}(\pi_{8,3}(x) + \pi_{8,5}(x) + \pi_{8,7}(x)). \tag{3.4}$$

We are really looking for negative values of $\frac{1}{3}(\Delta_{8,3,1}(x) + \Delta_{8,5,1}(x) + \Delta_{8,7,1}(x))$, and take $A = 100000$, $\alpha = 10^7$ and $\eta = 0.02$ and obtain $K < -0.0265$.

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DEPARTMENT OF MATHEMATICS, UNIVERSITY OF SOUTH CAROLINA, COLUMBIA, SOUTH CAROLINA 29208, USA

Current address: Department of Mathematics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF SOUTH CAROLINA, COLUMBIA, SOUTH CAROLINA 29208, USA

E-mail address: hudson@math.sc.edu