MATHEMATICS OF COMPUTATION
Volume 84, Number 295, September 2015, Pages 2433–2446
S 0025-5718(2015)02930-5
Article electronically published on February 12, 2015

A STILL SHARPER REGION WHERE $\pi(x) - \mathrm{li}(x)$ IS POSITIVE

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Abstract. We consider the least number x for which a change of sign of $\pi(x) - \mathrm{li}(x)$ occurs. First, we consider modifications of Lehman's method that enable us to obtain better estimates of some error terms. Second, we establish a new smaller upper bound for the first x for which the difference is positive. Third, we use numerical computations to improve the final result.

1. Introduction

The prime number theorem states that $\mathrm{li}(x) \sim \pi(x)$, where $\pi(x)$ counts the number of primes not exceeding x, and where $\mathrm{li}(x) = \lim_{\epsilon \to 0} \left\{ \int_0^{1-\epsilon} + \int_{1+\epsilon}^{x} \frac{dt}{\log t} \right\}$. It is known that $\pi(x) < \mathrm{li}(x)$ for $2 \leq x \leq 10^{14}$ [Kot08]. On the other hand, Littlewood [Lit14] proved in 1914 that $\pi(x) > \mathrm{li}(x)$ infinitely often, although he did not give an estimate on the first counterexample. The smallest number for which $\pi(x) > \mathrm{li}(x)$ is often called *Skewes' number*. For a history of refinements to Skewes' number, see [SD10, §1].

In 2010, Saouter and Demichel [SD10] proved that $\pi(x) > \mathrm{li}(x)$ in a new region around exp(727.951335792). The main approach there was to refine Lehman's method, first used in [Leh66]. They also remarked that a region around exp(727.951-335426) might contain a sign change; their theorems were not strong enough to prove this.

In this article, we derive a stronger version of Lehman's theorem involving a different weight function. This new theorem enables us to certify the preceding candidate region. We can then improve this region by appealing to a combination of theoretical results and numerical computations.

2. Preliminaries

Throughout this article the symbol ϑ will be used as a notation facility and will denote a complex number with $|\vartheta| \leq 1$, where each value of ϑ may be different at each occurrence. The same remark applies to symbols of the form ϑ_i. In this section, we gather some results that will be required in subsequent sections.

2.1. **The function** $\mathrm{li}(x)$.

Lemma 2.1. *Let w be a complex number such that $\mathrm{Im}(w) \neq 0$. Then for any integer $n \geq 1$, we have*

$$\mathrm{li}(e^w) = e^w \left\{ \sum_{k=1}^{n} \frac{(k-1)!}{w^k} + n! \int_0^{+\infty} \frac{e^{-t}}{(w-t)^{n+1}} dt \right\}. \tag{2.1}$$

Received by the editor June 11, 2013 and, in revised form, December 4, 2013.
2010 *Mathematics Subject Classification.* Primary 11-04, 11A15, 11M26, 11Y11, 11Y35.
The second author was supported in part by ARC Grant DE120100173.

Proof. Lehman [Leh66, p. 402] proved this theorem in the case of $n = 1$ by integration by parts. Successive integrations by parts give the result. □

Though the sum in the right-hand side of (2.1) is not convergent, a judicious selection of n gives an approximation of $\mathrm{li}(e^w)$ that is sufficient in what follows. The following theorem provides approximations to $\mathrm{li}(e^w)$ in the case of real positive arguments.

Lemma 2.2. *Let $n \geq 1$ be an integer and, for $x > 1$, let $g_1(x) = \mathrm{li}(x) - x\sum_{k=1}^{n} \frac{(k-1)!}{(\log x)^k}$ and $g_2(x) = g_1(x) - x\frac{n!}{(\log x)^n}$. It follows that $g_1(x)$ is increasing for $x > e$ and $g_2(x)$ is decreasing for $x > e^{n+1}$.*

Proof. For $x > 1$, we have

$$g_1'(x) = \frac{1}{\log x} - \sum_{k=1}^{n} \frac{(k-1)!}{(\log x)^k} + \sum_{k=1}^{n} \frac{k!}{(\log x)^{k+1}} = \frac{n!}{(\log x)^{n+1}}.$$

Thus $g_1'(x)$ is positive when $x > 1$. We also have

$$g_2'(x) = g_1'(x) - \frac{n!}{(\log x)^n} + \frac{n.n!}{(\log x)^{n+1}} = \frac{n!}{(\log x)^{n+1}}(n + 1 - \log x).$$

Thus $g_2'(x)$ is negative when $x > e^{n+1}$. □

Lemma 2.3. *For $x > e^5$, we have*

$$\begin{aligned}
\frac{6x}{(\log x)^4} &< \mathrm{li}(x) - \frac{x}{\log x}\left\{1 + \frac{1}{\log x} + \frac{2}{(\log x)^2}\right\} < \frac{30x}{(\log x)^4},\\
\frac{2x}{(\log x)^3} &< \mathrm{li}(x) - \frac{x}{\log x}\left\{1 + \frac{1}{\log x}\right\} < \frac{8x}{(\log x)^3},\\
\frac{x}{(\log x)^2} &< \mathrm{li}(x) - \frac{x}{\log x} < \frac{13x}{5(\log x)^2},\\
\frac{x}{\log x} &< \mathrm{li}(x) < \frac{38x}{25\log x}.
\end{aligned}$$

Proof. The first inequality comes from applying Lemma 2.2 with $n = 4$ and from observing that $g_1(e^5) > 0$ and $g_2(e^5) < 0$. The others come from bounding the terms of the first equation with the hypothesis $x > e^5$. □

2.2. **The prime counting function $\pi(x)$.** Dusart proved the following theorem in [Dus98].

Theorem 2.4. *We have,* [Dus98, Thm. 1.10]

$$\begin{aligned}
\frac{x}{\log x}\left(1 + \frac{1}{\log x}\right) \underset{x\geq 599}{\leq} \pi(x) &\underset{x>1}{\leq} \frac{x}{\log x}\left(1 + \frac{1.2762}{\log x}\right),\\
\frac{x}{\log x - 1} \underset{x\geq 5393}{\leq} \pi(x) &\underset{x\geq 60184}{\leq} \frac{x}{\log x - 1.1},
\end{aligned}$$

$$\begin{aligned}
\frac{x}{\log x}\left(1 + \frac{1}{\log x} + \frac{1.8}{\log^2 x}\right) &\underset{x\geq 32299}{\leq} \pi(x)\\
&\underset{x\geq 355991}{\leq} \frac{x}{\log x}\left(1 + \frac{1}{\log x} + \frac{2.51}{\log^2 x}\right),
\end{aligned} \tag{2.2}$$

where subscripts describe the domains of the inequalities.

2.3. **The Gaussian kernel.** Let α be a positive real number. The Gaussian kernel we shall use is defined to be $K(y) = \sqrt{\frac{\alpha}{2\pi}}e^{-\alpha y^2/2}$. In [Leh66], Lehman proved

Lemma 2.5. *For $\eta > 0$,*

$$\int_{-\infty}^{+\infty} K(y)e^{i\gamma y}dy = e^{-\gamma^2/2\alpha}, \qquad \left|\int_{\eta}^{+\infty} K(y)e^{i\gamma y}dy\right| \leq \frac{2}{\gamma}K(\eta).$$

We will also need the following evaluation.

Lemma 2.6. *We have, for $\eta > 0$,*

$$\int_{-\eta}^{\eta} y\ K(y)e^{i\gamma y}dy = \frac{i\gamma}{\alpha}e^{-\gamma^2/2\alpha} + \frac{6\vartheta}{\alpha}K(\eta).$$

Proof. We have $K'(y) = -\alpha y K(y)$. Integrating by parts gives

$$\int_{-\eta}^{\eta} y\ K(y)e^{i\gamma y}dy = \left[-\frac{K(y)}{\alpha}e^{i\gamma y}\right]_{-\eta}^{\eta} + \frac{i\gamma}{\alpha}\int_{-\eta}^{\eta} K(y)e^{i\gamma y}dy.$$

The result follows from Lemma 2.5. □

2.4. **Summation over zeros of the Riemann zeta-function.** In §4, some error terms involve sums over zeros of the Riemann function in the critical strip. We denote the imaginary part of such a zero by γ. We recall some results used by Lehman.

Lemma 2.7. *Let $\phi(t)$ be a continuous positive and monotone decreasing function on the interval $[T_1, T_2]$ with $2\pi e \leq T_1 < T_2$, then*

$$\sum_{T_1<\gamma\leq T_2} \phi(\gamma) = \frac{1}{2\pi}\int_{T_1}^{T_2} \phi(t)\log\frac{t}{2\pi}dt + \vartheta\left\{4\phi(T_1)\log(T_1) + 2\int_{T_1}^{T_2}\frac{\phi(t)}{t}dt\right\}.$$

Lemma 2.8. *If $T \geq 2\pi e$, then, for $n \geq 2$,*

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

Lemmas 2.7 and 2.8 were proved using the classical estimate of $N(T)$ obtained by Backlund [Bac18]. This estimate has been refined, most recently by Trudgian [Tru12]. However, such a refinement does not lead to a substantial improvement in the application of Lemmas 2.7 and 2.8.

Using Lemma 2.8 and computations over the first 100 million zeros of the zeta-function, we obtained

Lemma 2.9. *We have*

$$\sum_{0<\gamma}\frac{1}{\gamma^2} < 2.31050 \times 10^{-2}, \quad \sum_{0<\gamma}\frac{1}{\gamma^3} < 7.29549 \times 10^{-4},$$
$$\sum_{0<\gamma}\frac{1}{\gamma^4} < 3.71726 \times 10^{-5}, \quad \sum_{0<\gamma}\frac{1}{\gamma^5} < 2.23119 \times 10^{-6}.$$

We will also need the following evaluation.

Lemma 2.10. *If $T \geq 2\pi e$, then*

$$\sum_{0<\gamma\leq T}\frac{1}{\gamma} = \frac{1}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + 0.9321\vartheta.$$

Proof. We use Lemma 2.7 with the function $\phi(t) = \frac{1}{t}$, whence

$$\begin{aligned}
\sum_{2\pi e<\gamma\leq T} \frac{1}{\gamma} &= \frac{1}{2\pi}\int_{2\pi e}^{T} \frac{1}{t}\log\frac{t}{2\pi}dt + \vartheta\left\{\frac{2\log(2\pi e)}{\pi e} + 2\int_{2\pi e}^{T}\frac{dt}{t^2}\right\} \\
&= \frac{1}{2\pi}\left[\frac{1}{2}\left(\log\frac{t}{2\pi}\right)^2\right]_{2\pi e}^{T} + \vartheta\left\{\frac{2\log(2\pi e)}{\pi e} + 2\left[-\frac{1}{t}\right]_{2\pi e}^{T}\right\} \\
&= \frac{1}{4\pi}\left\{\left(\log\frac{T}{2\pi}\right)^2 - 1\right\} + \vartheta\left\{\frac{2\log(2\pi e)+1}{\pi e}\right\} \\
&= \frac{1}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + 0.8614\vartheta.
\end{aligned}$$

For the summation to be over $0 < \gamma \leq T$, we add the contribution of zeros in the range $0 < \gamma \leq 2\pi e$; that is to say, the contribution of the first zero only. ☐

3. Main theorem

The first purpose of this paper is to prove the following theorem.

Theorem 3.1. *Let A be a positive number such that $\beta = \frac{1}{2}$ for all zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ for which $0 < \gamma \leq A$. Let α, η and ω be positive numbers for which $\omega - \eta > 25.6$ and for which*

$$4A/\omega \leq \alpha \leq A^2$$

and

$$2A/\alpha \leq \eta \leq \omega/2$$

hold. Let

$$K(y) = \sqrt{\frac{\alpha}{2\pi}}e^{-\alpha y^2/2}$$

and

$$I(\omega,\eta) = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\frac{u\{\pi(e^u) - \mathrm{li}(e^u)\}}{e^{u/2}(1+\frac{2}{u}+\frac{10.04}{u^2})}du.$$

Then for $2\pi e < T \leq A$,

$$\begin{aligned}
I(\omega,\eta) = &-1 + \frac{1}{1+\frac{2}{\omega}+\frac{10.04}{\omega^2}}\sum_{\rho,0<|\gamma|\leq T} e^{-\gamma^2/2\alpha}e^{i\gamma\omega}\left(\frac{1}{\rho}+\frac{1}{\rho^2\omega}\right) \\
&+ R_1 - R_2 - R_3 - R_4 - R_5,
\end{aligned}$$

where

$$\begin{aligned}
R_1 &= \frac{2}{\sqrt{\alpha}}K(\eta), \\
R_2 &= (\omega+\eta)(\log 2e^{-(\omega-\eta)/2} + 3e^{-(\omega-\eta)/6}), \\
R_3 &= 0.19K(\eta) + \frac{0.35}{\omega^2\sqrt{\alpha}}\left\{\left(\log\frac{A}{2\pi}\right)^2 + 11.81\right\} + \frac{2.92\times 10^{-3}}{(\omega-\eta)^2}, \\
R_4 &= e^{-T^2/2\alpha}\left(\frac{1}{T}+\frac{1}{T^2\omega}\right)\left\{\frac{\alpha}{\pi T}\log\frac{T}{2\pi} + 8\log T + \frac{4\alpha}{T^2}\right\}, \\
R_5 &= e^{(\omega+\eta)/2}A\log Ae^{-A^2/2\alpha}\{4\alpha^{-1/2}+15\eta\}.
\end{aligned}$$

If the Riemann hypothesis holds, the factor $e^{(\omega+\eta)/2}$ in R_5 can be replaced by 1.

This theorem is similar to the main theorem [Leh66, p. 399]. Originally, Lehman used the function $u/e^{u/2}$ as a weighing function. This function arises in his work as an approximation of function $2/\pi(e^{u/2})$. The previous theorem was obtained by using sharper approximations of the latter function given by Theorem 2.4.

4. Proof of the main theorem

We proceed as in Lehman [Leh66]. Let

$$\Pi(x) = \pi(x) + \frac{1}{2}\pi(x^{1/2}) + \frac{1}{3}\pi(x^{1/3}) + \dots$$

and let

$$\Pi_0(x) = \lim_{\varepsilon \to 0} \frac{1}{2}\Big\{\Pi(x+\varepsilon) + \Pi(x-\varepsilon)\Big\}.$$

The Riemann–von Mangoldt explicit formula states that, for $x > 1$,

$$\Pi_0(x) = \mathrm{li}(x) - \sum_{\rho} \mathrm{li}(x^{\rho}) + \int_x^{+\infty} \frac{du}{(u^2-1)u\log u} - \log 2,$$

where ρ runs over the non-trivial zeros of the zeta-function. We have

$$\frac{1}{3}\pi(x^{1/3}) + \frac{1}{4}\pi(x^{1/4}) + \dots \le \frac{1}{3}\pi(x^{1/3})\left\lfloor \frac{\log x}{\log 2}\right\rfloor,$$

whence

$$\pi(x) - \mathrm{li}(x) \ge -\frac{1}{2}\pi(x^{1/2}) - \sum_{\rho} \mathrm{li}(x^{\rho}) - \log 2 - 3x^{1/3}.$$

In Lehman's paper, the function $\pi(x^{1/2})$ is approximated by $\frac{x^{1/2}}{\log(x^{1/2})}$. We use Theorem 2.4 as it gives a better estimate. If $x \ge 1.3 \times 10^{11}$, we have

$$\pi(x) - \mathrm{li}(x) \ge -\frac{x^{1/2}}{\log x}\left(1 + \frac{2}{\log x} + \frac{10.04}{\log^2 x}\right) - \sum_{\rho} \mathrm{li}(x^{\rho}) - \log 2 - 3x^{1/3}.$$

Putting $x = e^u$, we have, for $u \ge 25.6$,

$$\frac{u\{\pi(e^u) - \mathrm{li}(e^u)\}}{e^{u/2}\left(1 + \frac{2}{u} + \frac{10.04}{u^2}\right)} \ge -1 - \sum_{\rho} \frac{u\mathrm{li}(e^{\rho u})}{e^{u/2}\left(1 + \frac{2}{u} + \frac{10.04}{u^2}\right)} - \frac{u(\log 2 + 3e^{u/3})}{e^{u/2}\left(1 + \frac{2}{u} + \frac{10.04}{u^2}\right)}. \tag{4.1}$$

Let $\omega > \eta > 0$ and $\omega - \eta \ge 25.6$. We wish to multiply each term on the right-hand side of (4.1) by $K(u-\omega)$ and integrate. First, note that

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)du = 1 - 2\int_{\eta}^{\infty} K(u)du = 1 - \mathrm{erfc}(\eta\sqrt{\alpha/2}). \tag{4.2}$$

When $x > 0$, we have $\sqrt{\frac{2}{\pi}}e^{-x^2} < \mathrm{erfc}(x)$, whence

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)du > 1 - \sqrt{\frac{2}{\pi}}e^{-\alpha\eta^2/2} > 1 - \frac{2K(\eta)}{\sqrt{\alpha}}.$$

Second, we have, for $\omega-\eta \geq 25.6$,

$$\begin{aligned}
(4.3)\qquad \left|\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\frac{u(\log 2+3e^{u/3})}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du\right| \\
&\leq \max_{u\in[\omega-\eta,\omega+\eta]}\frac{u(\log 2+3e^{u/3})}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)} \\
&\leq (\omega+\eta)(\log 2e^{-(\omega-\eta)/2}+3e^{-(\omega-\eta)/6}).
\end{aligned}$$

Equations (4.1), (4.2) and (4.3) show that, for $\omega-\eta \geq 25.6$,

$$\begin{aligned}
\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\frac{u\{\pi(e^u)-\mathrm{li}(e^u)\}}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du &\geq -1+\frac{2K(\eta)}{\sqrt{\alpha}} \\
&-(\omega+\eta)(\log 2e^{-(\omega-\eta)/2}+3e^{-(\omega-\eta)/6}) \\
&-\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\left(\sum_\rho \frac{u\ \mathrm{li}(e^{\rho u})}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}\right)du.
\end{aligned}$$

Denote the integral on the right-hand side by J; §§5 and 6 are devoted to giving a good bound for J. The inversion of summation and integration is justified since the summation over the zeros of $\zeta(s)$ converges boundedly for $u \in [\omega-\eta,\omega+\eta]$. Thus, if we write

$$J_\rho = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)\frac{u\ \mathrm{li}(e^{\rho u})}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du,$$

then we may write $J=\sum_\rho J_\rho$. Recalling that, as in Theorem 3.1, A is the height to which the Riemann hypothesis has been verified, write

$$J = J_1+J_2 = \sum_{\rho,0<|\gamma|\leq A} J_\rho + \sum_{\rho,|\gamma|>A} J_\rho.$$

5. J_1: SUMMATION BELOW HEIGHT A

For any zero ρ in J_1, we have $\rho=\frac{1}{2}+i\gamma$, with $|\gamma|\leq A$. From Lemma 2.1 with $n=2$, we have

$$J_\rho = \int_{\omega-\eta}^{\omega+\eta}\frac{K(u-\omega)u\mathrm{li}(e^{\rho u})}{e^{u/2}\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{i\gamma u}\frac{\left(\frac{1}{\rho}+\frac{1}{\rho^2 u}+\frac{2\vartheta}{\gamma^3u^2}\right)}{\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du.$$

The error in the last term can be bounded above by writing

$$\left|\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{i\gamma u}\frac{\left(\frac{2\vartheta}{\gamma^3u^2}\right)}{\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du\right| \leq \frac{2}{\gamma^3(\omega-\eta)^2}.$$

Hence

$$J_\rho = \int_{\omega-\eta}^{\omega+\eta} K(u-\omega)e^{i\gamma u}\frac{\left(\frac{1}{\rho}+\frac{1}{\rho^2 u}\right)}{\left(1+\frac{2}{u}+\frac{10.04}{u^2}\right)}du + \frac{2\vartheta}{\gamma^3(\omega-\eta)^2}. \tag{5.1}$$

Now, we put $u=\omega+y$ so that

$$\frac{\left(\frac{1}{\rho}+\frac{1}{\rho^2(\omega+y)}\right)}{\left(1+\frac{2}{(\omega+y)}+\frac{10.04}{(\omega+y)^2}\right)} = \frac{\left(\frac{1}{\rho}+\frac{1}{\rho^2\omega}\right)}{\left(1+\frac{2}{\omega}+\frac{10.04}{\omega^2}\right)} + \frac{y}{\omega^2}\left\{\frac{f(\omega,y)}{\rho}+\frac{g(\omega,y)}{\rho^2}\right\}, \tag{5.2}$$

where

$$f(\omega, y) = \frac{\omega^2\{2\omega^2 + 2\omega y + 10.04(2\omega + y)\}}{(\omega^2 + 2\omega + 10.04)(\omega^2 + 2\omega y + y^2 + 2\omega + 2y + 10.04)},$$
$$g(\omega, y) = \frac{\omega^2(10.04 - \omega y - \omega^2)}{(\omega^2 + 2\omega + 10.04)(\omega^2 + 2\omega y + y^2 + 2\omega + 2y + 10.04)}.$$

Now $w > 25.6$ and, if $\eta < \omega/2$, we have $|y| < \omega/2$. It is easy to see that both $f(\omega, y)$ and $|g(\omega, y)|$ are decreasing functions in y. Moreover,

$$f(\omega, -\omega/2) \le f(25.6, -12.8) \le 4.78, \quad |g(\omega, y)| = -g(\omega, y) \le g(\omega, -\omega/2) \le 1.46.$$

Substituting all of this in (5.2), we obtain

$$\frac{\left(\frac{1}{\rho} + \frac{1}{\rho^2(\omega+y)}\right)}{\left(1 + \frac{2}{(\omega+y)} + \frac{10.04}{(\omega+y)^2}\right)} = \frac{\left(\frac{1}{\rho} + \frac{1}{\rho^2\omega}\right)}{(1 + \frac{2}{\omega} + \frac{10.04}{\omega^2})} + \frac{y}{\omega^2}\left(\frac{4.78\vartheta_1}{\rho} + \frac{1.46\vartheta_2}{\rho^2}\right),$$

which, when added to (5.1), gives

$$\begin{aligned} J_\rho &= e^{i\gamma\omega}\frac{\left(\frac{1}{\rho} + \frac{1}{\rho^2\omega}\right)}{(1 + \frac{2}{\omega} + \frac{10.04}{\omega^2})}\int_{-\eta}^{\eta} K(y)e^{i\gamma y}dy \\ &\quad + \frac{e^{i\gamma\omega}}{\omega^2}\int_{-\eta}^{\eta} yK(y)e^{i\gamma y}\vartheta_1\left(\frac{4.78}{\rho} + \frac{1.46}{\rho^2}\right)dy + \frac{2\vartheta_2}{\gamma^3(\omega-\eta)^2} \\ &= e^{i\gamma\omega}\frac{\left(\frac{1}{\rho} + \frac{1}{\rho^2\omega}\right)}{(1 + \frac{2}{\omega} + \frac{10.04}{\omega^2})}\int_{-\eta}^{\eta} K(y)e^{i\gamma y}dy \\ &\quad + \frac{\vartheta_1}{\omega^2}\sqrt{\frac{2}{\pi\alpha}}\left(\frac{4.78}{\gamma} + \frac{1.46}{\gamma^2}\right) + \frac{2\vartheta_2}{\gamma^3(\omega-\eta)^2}, \end{aligned}$$

since $|\int_{-\eta}^{\eta} yK(y)\,dy| \le 2\int_0^\infty yK(y) = \sqrt{2/(\pi\alpha)}$. Using Lemma 2.5 to estimate the above integral and Lemmas 2.9 and 2.10 to estimate the sums over the zeros we obtain

$$\begin{aligned} J_1 &= \frac{1}{(1 + \frac{2}{\omega} + \frac{10.04}{\omega^2})}\sum_{\rho, 0<|\gamma|\le A} e^{-\gamma^2/2\alpha}e^{i\gamma\omega}\left(\frac{1}{\rho} + \frac{1}{\rho^2\omega}\right) + 0.19\vartheta_1 K(\eta) \\ &\quad + \frac{0.35\vartheta_2}{\omega^2\sqrt{\alpha}}\left\{\left(\log\frac{A}{2\pi}\right)^2 + 11.81\right\} + \frac{2.92\times 10^{-3}\vartheta_3}{(\omega-\eta)^2}. \end{aligned}$$

We have thus obtained an expression giving J_1, contingent on a value of A. If A is so large as to prevent the computation of the summation in a reasonable time, we may stop at a height below A at the expense of an additional error term. Indeed, for $2\pi e < T \le A$, we have, by Lemma 2.7,

$$\begin{aligned} &\sum_{\rho, T<|\gamma|\le A} e^{-\gamma^2/2\alpha}\left(\frac{1}{\gamma} + \frac{1}{\gamma^2\omega}\right) \\ &\qquad \le \frac{1}{\pi}\int_T^A e^{-t^2/2\alpha}\left(\frac{1}{t} + \frac{1}{t^2\omega}\right)\log\frac{t}{2\pi}dt + 8e^{-T^2/2\alpha}\left(\frac{1}{T} + \frac{1}{T^2\omega}\right)\log T \\ &\qquad + 4\int_T^A e^{-t^2/2\alpha}\left(\frac{1}{t^2} + \frac{1}{t^3\omega}\right)dt, \end{aligned}$$

whence we obtain

$$\left|\frac{1}{\left(1+\frac{2}{\omega}+\frac{10.04}{\omega^2}\right)}\sum_{\rho, T<|\gamma|\le A} e^{-\gamma^2/2\alpha}e^{i\gamma\omega}\left(\frac{1}{\rho}+\frac{1}{\rho^2\omega}\right)\right|$$
$$\le e^{-T^2/2\alpha}\left\{\frac{\alpha}{\pi}\left(\frac{1}{T^2}+\frac{1}{T^3\omega}\right)\log\frac{T}{2\pi}+8\left(\frac{1}{T}+\frac{1}{T^2\omega}\right)\log T+4\alpha\left(\frac{1}{T^3}+\frac{1}{T^4\omega}\right)\right\}.$$

6. J_2: Summation beyond height A

Following Lehman's approach [Leh66, §5] we introduce the function

$$f_\rho(s)=\frac{\rho s e^{-\rho s}\mathrm{li}(e^{\rho s})}{\left(1+\frac{2}{s}+\frac{10.04}{s^2}\right)}e^{-\alpha(s-\omega)^2/2}. \tag{6.1}$$

Define $D=\{s:\ -\frac{\pi}{4}\le\arg(s)\le\frac{\pi}{4},\quad |s|\ge 14\}$. Since all zeros in $0<\beta<1$ have $|\gamma|\ge 14$ it follows that, for $s\in D$, $\frac{\pi}{6}<|\mathrm{Arg}(\rho s)|<\frac{3\pi}{4}$, whence the numerator in (6.1) is a regular analytic function on D. Moreover, the polynomial $s^2+2s+10.04$ has roots at t_0 and $\overline{t_0}$, where $t_0=-1+i\sqrt{9.04}$, which are outside D. Thus $f_\rho(s)$ is a regular analytic function on D.

We now proceed to proving an upper bound for $f_\rho(s)$. Applying Lemma 2.1 with $n=1$ gives

$$|\rho s e^{-\rho s}\mathrm{li}(\rho s)|\le\left|1+\rho s\int_0^{+\infty}\frac{e^{-t}}{(\rho s-t)^2}dt\right|\le 1+\frac{|\rho s|}{(\mathrm{Im}(\rho s))^2}.$$

Since $|s-t_0|\ge|s|-|t_0|\ge|s|-4.01>0$, and likewise for $|s-\overline{t_0}|$, we have

$$|s^2+2s+10.04|=|s-t_0||s-\overline{t_0}|\ge(|s|-4.01)^2.$$

Finally, on D we have $|\frac{\rho s}{\mathrm{Im}(\rho s)}|\le 2$ and $|\rho s|>152$, so that

$$|f_\rho(s)|\le 1.99|e^{-\alpha(s-\omega)^2/2}|<2|e^{-\alpha(s-\omega)^2/2}|.$$

In [Leh66], Lehman obtained the same bound for his candidate function $f_\rho(s)$. As a consequence, we can follow his bounding strategy to conclude that, if $A^2/\alpha\ge 1$, $A/\alpha\le\omega/4$ and $\eta\ge 2A/\alpha$, then

$$|J_2|\le e^{(\omega+\eta)/2}A\log A e^{-A^2/2\alpha}\{4\alpha^{-1/2}+15\eta\}.$$

This latter result establishes Theorem 3.1.

7. Roundoff error

Zeros with $|\gamma|\le A$ lie on the critical line and appear as conjugate pairs. Thus if we denote the expression to be computed by S, we have

$$S=\frac{1}{1+\frac{2}{\omega}+\frac{10.04}{\omega^2}}\sum_{\rho,0<\gamma\le T}e^{-\gamma^2/2\alpha}\left\{e^{i\gamma\omega}\left[\frac{1}{1/2+i\gamma}+\frac{1}{(1/2+i\gamma)^2\omega}\right]\right.$$
$$\left.+e^{-i\gamma\omega}\left[\frac{1}{1/2-i\gamma}+\frac{1}{(1/2-i\gamma)^2\omega}\right]\right\} \tag{7.1}$$

$$= \frac{1}{1+\frac{2}{\omega}+\frac{10.04}{\omega^2}} \sum_{\rho, 0<\gamma\le T} e^{-\gamma^2/2\alpha} \left\{ \frac{4\cos(\gamma\omega)+8\gamma\sin(\gamma\omega)}{1+4\gamma^2} + \frac{8\cos(\gamma\omega)+32\gamma\sin(\gamma\omega)-32\gamma^2\cos(\gamma\omega)}{(1+4\gamma^2)^2\omega} \right\}.$$

We need to estimate the roundoff error arising from the precision with which the zeros of $\zeta(s)$ can be calculated. For a given zero $\rho = 1/2 + i\gamma$, we let $S_{\gamma+\varepsilon'}$ denote the value obtained for S using (7.1) if γ is replaced by $\gamma+\varepsilon'$. We suppose that we have $|\varepsilon'| < \varepsilon$, where ε is a positive value denoting the maximal roundoff error on the value of γ. We then have

$$|S - S_{\gamma+\varepsilon'}| \le \frac{\varepsilon}{1+\frac{2}{\omega}+\frac{10.04}{\omega^2}} \operatorname*{Max}_{t\in[\gamma,\gamma+\varepsilon']} \frac{\partial}{\partial t} \left\{ e^{-t^2/2\alpha} \left[\frac{4\cos(t\omega)+8t\sin(t\omega)}{1+4t^2} + \frac{(8-32t^2)\cos(t\omega)+32t\sin(t\omega)}{(1+4t^2)^2\omega} \right] \right\}.$$

We suppose that $\varepsilon < 0.1$, which, since $\gamma \ge 14.134$ implies that $t > 14$. Computing the derivative and bounding $\cos(tw)$ and $\sin(tw)$ trivially we obtain, since $\omega > 25.6$,

$$\begin{aligned} |S - S_{\gamma+\varepsilon'}| &\le 0.96\varepsilon \operatorname*{Max}_{t\in[\gamma,\gamma+\varepsilon']} \frac{t}{1+4t^2}(42\omega + 42/\alpha + 513) \\ &\le 0.96(42\omega+42/\alpha+513)\varepsilon \frac{\gamma+\varepsilon}{1+4(\gamma-\varepsilon)^2} \\ &\le 1.92(42\omega+42/\alpha+513)\varepsilon \frac{\gamma}{1+\gamma^2}. \end{aligned}$$

Suppose now that all zeros of $\zeta(s)$ with imaginary part less than T have been computed with a maximal error less than ε. Then the total roundoff error ΔS is such that

$$\begin{aligned} \Delta S &\le 1.92(42\omega+42/\alpha+513)\varepsilon \sum_{\rho,0<\gamma\le T} \frac{\gamma}{1+\gamma^2} \\ &\le 1.92(42\omega+42/\alpha+513)\varepsilon \sum_{\rho,0<\gamma\le T} \frac{1}{\gamma}. \end{aligned}$$

Then, with Lemma 2.10, we have

$$\Delta S \le 1.92(42\omega+42/\alpha+513) \left\{ \frac{1}{4\pi}\left(\log\frac{T}{2\pi}\right)^2 + 0.9321 \right\} \varepsilon. \tag{7.2}$$

8. Numerical applications

From [vdL01], the maximum value that A can take is $A_{MAX} = 3293531632.414$. In order to minimize the length of the interval, we set $\eta = 2A/\alpha$. We have $\omega \sim 727.95$. We set $A = 3.2 \times 10^9$, $\alpha = 10^{15}$ and $T = 2 \times 10^8$. The error term is then bounded by 5.82×10^{-9}. More precisely we have, $R_1 \sim 3.56 \times 10^{-8895}$, $R_2 \sim 4.46 \times 10^{-50}$, $R_3 \sim 1.63 \times 10^{-8}$, $R_4 \sim 2.84 \times 10^{-10}$ and $R_5 \sim 2.1 \times 10^{-2059}$. Concerning the roundoff error, values of the zeros were correct up to twenty decimal places. Thus we have $\varepsilon = 5 \times 10^{-21}$, and (7.2) gives $\Delta S \le 7.37 \times 10^{-15}$. We see that R_3 and R_4 dictate the final error value.

These values were used to compute values of $I(\omega, \eta)$ for ω between 727.9513354 and 727.951338; the result is depicted in Figure 1. Actually, two curves are depicted

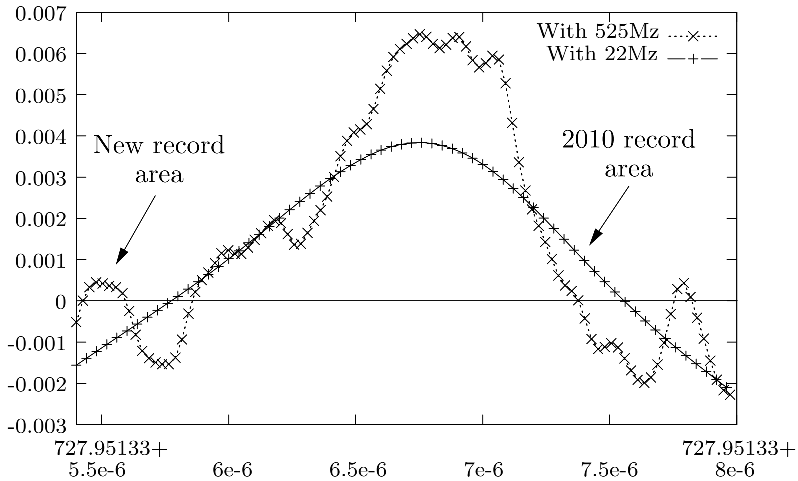

FIGURE 1. Comparison with previous work.

on the figure. The first was obtained with the use of 525 million zeros of the zeta-function using the equations of Theorem 3.1. The second is a reproduction at the same scale of [SD10, Fig. 4]. For the latter curve, only 22 million zeros were used, the formula was different, and the error term was larger. In both cases, the error term has been included to illustrate the worst case scenario. Together with the curves, the axis $I = 0$ is also represented. It is clear on the figure that a new record area is obtained for $\omega \simeq 727.9513355$.

There are two reasons why this new record value cannot be found on the curve made with the 2010 data. First, the two curves are, in fact, averaging functions of $\pi(x) - \mathrm{li}(x)$. The 2010 curve corresponds to an average computed over an interval of length 4.6×10^{-5}. In this paper, the average was computed over an interval of length 1.3×10^{-5}. This shorter interval was obtained by considering larger values for the parameter α in our computations. From the expression of R_4, we deduce that larger values for T are therefore required. Thus in order to obtain shorter intervals it was necessary to consider more zeros of $\zeta(s)$. This enables the observation of the subtler behaviour of $\pi(x) - \mathrm{li}(x)$: the newly obtained curve has a shape more chaotic than that of [SD10].

The second reason is that the error term we obtain in this paper is smaller than that of [SD10]. Indeed, in this new work, the total error is less than 10^{-6}, while it was larger than 2.7×10^{-3} in the previous work. This improvement was obtained with the new weighing function we considered, which is more accurate in its approximation of $\pi(e^u) - \mathrm{li}(e^u)$ in the integral. As a consequence, the new record area is above the axis $I = 0$, while with the results of [SD10], the corresponding zone is below the axis.

Figure 2 gives a magnification of the new record region. Our data indicate that, in this interval, the least value of ω that gives a positive value for the average mean is equal to $\omega_0 = 727.951335426$, for which we have $J(\omega_0) = 0.0000070294 \pm 10^{-10}$. We considered then the value $E = J(\omega_0) + R_1 - R_2 - R_3 - R_4 - R_5$. The roundoff error was not added, since it only depends on the value ε which was kept small

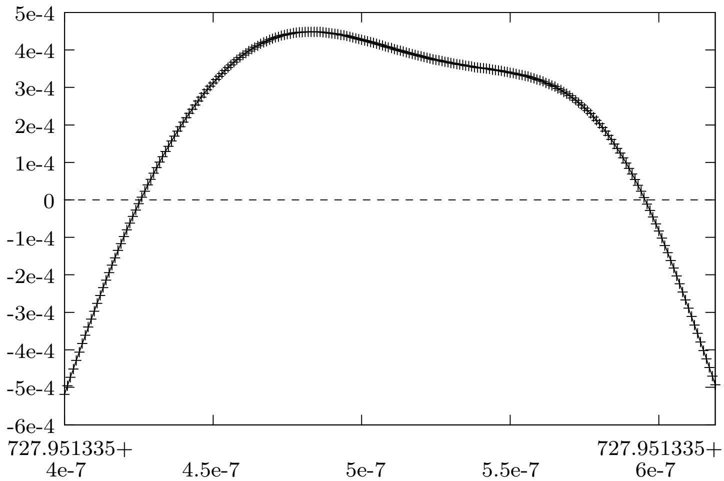

FIGURE 2. Shape of the new region.

enough to make the roundoff error negligible. Once ω and T have been fixed, the expression for E depends only on A and α. We have $\eta = 2A/\alpha$; thus if we treat η as a constant, it is possible to eliminate A in the expression of E, which then only depends on α.

We searched for maximum values of E by differentiating this value with respect to α and using Newton–Raphson iterations to find values of α at which the derivative is zero. When such a value, say α_0, is obtained, we need to verify whether the following conditions are met. First, the corresponding value for E has to be positive. Second, the corresponding value for A, i.e., $\eta\alpha_0/2$, has to be less than A_{MAX}.

We apply this strategy by fixing η in the interval $[10^{-6}, 10^{-5}]$ and searching by bisection for the least value for which the two previous conditions are verified. This search was greatly facilitated by the use of Maple™ [Map], which possesses general purpose differentiation and Newton–Raphson operators. Close to optimal values were found; we retain the following values $\alpha = 1.61 \times 10^{15}$ and $A = 1.13 \times 10^{9}$. This choice gives $\eta = 2A/\alpha \sim 1.4 \times 10^{-6}$ and we obtain $R_1 \geq 1.04 \times 10^{-689}$, $R_2 \leq 4.45 \times 10^{-50}$, $R_3 \leq 1.32 \times 10^{-8}$, $R_4 \leq 8.92 \times 10^{-7}$, $R_5 \leq 3.55 \times 10^{-9}$, and $\Delta S \leq 7.37 \times 10^{-15}$ so that $I(\omega_0, \eta) \geq 6.12 \times 10^{-6}$.

9. Sharpening the interval

Further improvements are possible using the technique of [SD10, §5]. Using Lemma 2.3 and Theorem 2.4, we can easily prove the following theorem.

Theorem 9.1. *If $x \geq 3.6 \times 10^5$, then*

$$|\pi(x) - \mathrm{li}(x)| \leq \frac{0.51x}{\log^3 x}.$$

From this result, if $0 < \eta_0 < \eta$ and $\omega + \eta_0 > 12.8$, we deduce that

$$\left| \int_{\omega+\eta_0}^{\omega+\eta} K(u-\omega) \frac{u(\pi(e^u) - \mathrm{li}(e^u))}{e^{u/2}(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right| \leq \left| \int_{\omega+\eta_0}^{\omega+\eta} K(u-\omega) \frac{0.51 e^{u/2}}{u^2(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right|$$
$$\leq 0.51(\eta - \eta_0) K(\eta_0) e^{(\omega+\eta)/2} (\omega + \eta_0)^{-2}.$$

Likewise, if $\omega - \eta > 12.8$, then

$$\left| \int_{\omega-\eta}^{\omega-\eta_0} K(u-\omega) \frac{u(\pi(e^u) - \mathrm{li}(e^u))}{e^{u/2}(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right| \leq 0.51(\eta - \eta_0) K(\eta_0) e^{(\omega-\eta_0)/2} (\omega - \eta)^{-2},$$

so that

$$|I(\omega, \eta) - I(\omega, \eta_0)| \leq 0.51(\eta - \eta_0) K(\eta_0) (e^{(\omega+\eta)/2} (\omega + \eta_0)^{-2} + e^{(\omega-\eta_0)/2} (\omega - \eta)^{-2}).$$

With previously chosen values and $\eta_0 = \eta/2.07$, this gives

$$|I(\omega_0, \eta) - I(\omega_0, \eta_0)| \leq 4.48 \times 10^{-8}.$$

If we invoke the Riemann hypothesis, better results are available. In fact, from [Sch76, p. 339] we have

Theorem 9.2. *If the Riemann hypothesis holds and if $x \geq 2657$, then*

$$|\pi(x) - \mathrm{li}(x)| < \frac{1}{8\pi} \sqrt{x} \log x.$$

If $\omega - \eta > 7.89$ and the Riemann hypothesis holds, we then have

$$\left| \int_{\omega+\eta_0}^{\omega+\eta} K(u-\omega) \frac{u(\pi(e^u) - \mathrm{li}(e^u))}{e^{u/2}(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right| \leq \frac{1}{8\pi} \left| \int_{\omega+\eta_0}^{\omega+\eta} K(u-\omega) \frac{u^2}{(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right|$$
$$\leq 3.98 \times 10^{-2} (\eta - \eta_0) K(\eta_0) (\omega + \eta)^2$$

and

$$\left| \int_{\omega-\eta}^{\omega-\eta_0} K(u-\omega) \frac{u(\pi(e^u) - \mathrm{li}(e^u))}{e^{u/2}(1 + \frac{2}{u} + \frac{10.04}{u^2})} du \right| \leq 3.98 \times 10^{-2} (\eta - \eta_0) K(\eta_0) (\omega - \eta_0)^2$$

so that, finally we obtain

$$|I(\omega, \eta) - I(\omega, \eta_0)| \leq 3.98 \times 10^{-2} (\eta - \eta_0) K(\eta_0) ((\omega - \eta_0)^2 + (\omega + \eta)^2).$$

Choosing $\eta_0 = \eta/7.21$ we obtain

$$|I(\omega_0, \eta) - I(\omega_0, \eta_0)| \leq 4.57 \times 10^{-8},$$

which allows us to deduce the following result.

Lemma 9.3. *Let $\omega_0 = 727.951335426$ and $\eta = 1.41 \times 10^{-6}$. If the Riemann hypothesis is assumed, set $\eta_0 = \eta/7.21$; otherwise set $\eta_0 = \eta/2.07$. In both cases, we have*

$$I(\omega_0, \eta_0) \geq 6.07 \times 10^{-6}.$$

This allows us to deduce the following result.

Lemma 9.4. *With the same numerical values as in Lemma 9.3, the function $\pi(e^u) - \mathrm{li}(e^u)$ assumes a value larger than 9.85×10^{149} at least once in the interval $u \in [\omega_0 - \eta_0, \omega_0 + \eta_0]$.*

Proof. Since $|\int_{\omega-\eta_0}^{\omega+\eta_0} K(u-\omega)du| < 1$, then, for at least for one value $u \in [\omega - \eta_0, \omega + \eta_0]$, we necessarily have

$$\frac{u(\pi(e^u) - \mathrm{li}(e^u))}{e^{u/2}(1 + \frac{2}{u} + \frac{10.04}{u^2})} \geq 6.07 \times 10^{-6},$$

so that

$$\pi(e^u) - \mathrm{li}(e^u) \geq \frac{6.07 \times 10^{-6} e^{(\omega_0 - \eta_0)/2}}{\omega_0 + \eta_0}. \qquad \square$$

At this point we recall a result obtained in [SD10, Theorem 6.2].

Lemma 9.5. *Let x be a positive number such that $\pi(x) - \mathrm{li}(x) \geq N$. Then for any value y such that $0 < y < N \log x$, we have $\pi(x+y) - \mathrm{li}(x+y) > 0$.*

Together with Lemma 9.4, this lemma enables us to establish our last result.

Lemma 9.6. *There are more than 7.17×10^{152} successive integers x in the interval* $[\exp(727.951334744), \exp(727.951336108)]$ *such that the inequality $\pi(x) - \mathrm{li}(x) > 0$ holds. Moreover, if the Riemann hypothesis holds, the result is true on the interior interval* $[\exp(727.951335231), \exp(727.951335622)]$.

10. Conclusion

Improvements to our work are certainly possible. For instance, sharper estimates of the function $\pi(x)$ could be introduced to provide lower error bounds. Indeed, in what precedes, we essentially use the right-hand side of (2.2) of Theorem 2.4, which gives an estimate valid for $x \geq 3.6 \times 10^5$. However, it seems most probable that if we consider only $x \geq 10^{100}$, the constant 2.51 involved in (2.2) could be made very close to 2. Thus one could review Dusart's work to derive such an inequality and then apply it to lower the global error term. It could also be possible to improve previous works [Leh66, SD10]. However, the numerical impact of such revisions would be limited since obtained improvements affect error terms.

Unofficially the Riemann hypothesis has been verified to heights higher than that considered here. For instance, in 2005, Gourdon and Demichel [GD04] reached the 10^{13}-th zero. More recently, Platt [Pla12] computed the first 10^{11}-th zeros and put them online. But, although larger A values could be used to lower the global error bound, they could not be used to verify shorter intervals, and in fact, when we minimise the value η, we finally choose $A = 1.13 \times 10^9$ which is lower than the maximum allowed by van de Lune's result [vdL01]. Since $\eta = 2A/\alpha$, taking lower values for η requires considering larger values of α. On the other hand, the approximate order of R_4 is $e^{-T^2/2\alpha}$. Thus keeping a low error bound with larger α values requires us to consider larger values for T. In our work, the value for T is fixed; increasing it would greatly increase the time for computation.

Another curious point is the modest impact obtained if we consider the Riemann hypothesis. Indeed, in Lemma 9.6, the length of the interval obtained with the Riemann hypothesis is roughly three times less than that obtained unconditionally. This remark, together with the previous paragraph, suggests that the Skewes' problem is not much influenced by computational or theoretical results concerning the Riemann hypothesis.

The last point we shall address is the existence of smaller values of x for which $\pi(x) > \mathrm{li}(x)$. There is no practical way to test an isolated value of x. Analytical methods, such as the one described here, can only give intervals of positivity. Considering larger summations, it is certainly possible to tighten intervals given here. Moreover, in our work, we encounter a potential new record. The related value is $\omega = 727.951332982$. We decided to discard it because, we estimate that it would require the summation on the first 10^{12} zeros of the zeta-function. This seems an awful lot of work for a secondary result, however, it could be contemplated in a new large-scale verification of the Riemann hypothesis.

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