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On the Sign of the Difference $\pi(x) - \mathrm{li}(x)$

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Dedicated to Daniel Shanks on the occasion of his 70th birthday

Abstract. Following a method of Sherman Lehman we show that between 6.62×10^{370} and 6.69×10^{370} there are more than 10^{180} successive integers x for which $\pi(x) - \mathrm{li}(x) > 0$. This brings down Sherman Lehman's bound on the smallest number x for which $\pi(x) - \mathrm{li}(x) > 0$, namely from 1.65×10^{1165} to 6.69×10^{370}. Our result is based on the knowledge of the truth of the Riemann hypothesis for the complex zeros $\beta + i\gamma$ of the Riemann zeta function which satisfy $|\gamma| < 450{,}000$, and on the knowledge of the first 15,000 complex zeros to about 28 digits and the next 35,000 to about 14 digits.

1. Introduction. The prime number theorem, proved by Hadamard and de la Vallée Poussin in 1896, states that $\pi(x) \sim \mathrm{li}(x)$, as $x \to \infty$, where $\pi(x)$ is the number of primes $\leqslant x$ and $\mathrm{li}(x) = \int_0^x dt/\log t$. This result tells us that the ratio $\pi(x)/\mathrm{li}(x)$ tends to 1 as $x \to \infty$, but it does not say anything about the difference $\pi(x) - \mathrm{li}(x)$. This difference is known to be *negative* for all values of x for which $\pi(x)$ has been computed exactly ([3]; also cf. Bateman's remarks on p. 943 of [4]). However, already in 1914, Littlewood [5] proved that $\pi(x) - \mathrm{li}(x)$ changes sign infinitely often. More precisely, he proved the existence of a number $K > 0$ such that

$$\frac{\log(x)\{\pi(x) - \mathrm{li}(x)\}}{x^{1/2}\log(\log(\log(x)))}$$

is greater than K for arbitrarily large values of x and less than $-K$ for arbitrarily large values of x. In 1955, Skewes [11] obtained an upper bound for the smallest x for which $\pi(x) > \mathrm{li}(x)$, namely $\exp(\exp(\exp(\exp(7.705))))$. In 1966, Sherman Lehman [10] brought this bound down considerably by proving that between 1.53×10^{1165} and 1.65×10^{1165} there are more than 10^{500} successive integers for which $\pi(x) > \mathrm{li}(x)$. Sherman Lehman's method is described in Section 2. In order to prove his result, Sherman Lehman performed two major computations, namely a verification of the Riemann hypothesis for the first 250,000 zeros of the Riemann zeta function, i.e., for the complex zeros $\beta + i\gamma$ for which $|\gamma| < 170{,}571.35$, and the computation of the zeros $\frac{1}{2} + i\gamma$ of the Riemann zeta function for which $0 < \gamma < 12{,}000$ to about 7 decimal places.

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In Section 3 we will bring down Sherman Lehman's bound by showing that there are more than 10^{180} successive integers x between 6.62×10^{370} and 6.69×10^{370} for which $\pi(x) > \mathrm{li}(x)$. To that end, we use the knowledge of the truth of the Riemann hypothesis for the complex zeros $\beta + i\gamma$ with $|\gamma| < 450{,}000$ [9] and the knowledge of the first 15,000 complex zeros of the Riemann zeta function with an accuracy of about 28 digits [8] and the next 35,000 with an accuracy of about 14 digits. An error analysis is given which shows that our result could also have been obtained with a few digits less accuracy in the zeros of the Riemann zeta function.

In Section 3, we denote the imaginary part of the jth complex zero of the Riemann zeta function by γ_j ($\gamma_1 = 14.13\ldots$, $\gamma_2 = 21.02\ldots$, etc.).

2. Sherman Lehman's Method. In [10], Sherman Lehman derived an explicit formula for $ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\}$, averaged by a Gaussian kernel. He expressed it in the following

THEOREM [10]. *Let A be a positive number such that $\beta = \frac{1}{2}$ for all the zeros $\rho = \beta + i\gamma$ of the Riemann zeta function $\zeta(s)$ with $0 < \gamma \leqslant A$. Let α, η, and ω be positive numbers such that $\omega - \eta > 1$ and the conditions*

$$4A/\omega \leqslant \alpha \leqslant A^2 \tag{2.1}$$

and

$$2A/\alpha \leqslant \eta < \omega/2 \tag{2.2}$$

hold. Let

$$K(y) := (\alpha/2\pi)^{1/2} e^{-\alpha y^2/2}. \tag{2.3}$$

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

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega) ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\}\, du = -1 + H(T,\alpha,\omega) + R, \tag{2.4}$$

where

$$H(T,\alpha,\omega) = -\sum_{0<|\gamma|\leqslant T} \frac{e^{i\gamma\omega}}{\rho} e^{-\gamma^2/2\alpha} \tag{2.5}$$

and

$$|R| \leqslant \sum_{i=1}^{6} S_i$$

with

$$S_1 = 3.05/(\omega - \eta), \qquad S_2 = 4(\omega + \eta)\exp(-(\omega - \eta)/6),$$
$$S_3 = 2\exp(-\alpha\eta^2/2)/\left(\eta(2\pi\alpha)^{1/2}\right), \qquad S_4 = 0.08\alpha^{1/2}\exp(-\alpha\eta^2/2),$$
$$S_5 = \exp(-T^2/2\alpha)\left\{\frac{\alpha}{\pi T^2}\log\left(\frac{T}{2\pi}\right) + \frac{8\log T}{T} + \frac{4\alpha}{T^3}\right\} \quad \text{and}$$
$$S_6 = A\log A\exp\left(-A^2/2\alpha + (\omega + \eta)/2\right)\left(4\alpha^{-1/2} + 15\eta\right).$$

If the Riemann hypothesis holds true, then conditions (2.1) *and* (2.2) *and the last term* (S_6) *in the estimate for R may be omitted.* □

Sherman Lehman first looked for places where on heuristic grounds $\pi(x)$ could be expected to exceed $\mathrm{li}(x)$, namely, in the neighborhood of values of u for which the sum

$$S_T(u) := -\sum_{0<|\gamma|\leqslant T} \frac{e^{i\gamma u}}{\rho}, \tag{2.6}$$

which is the sum in (2.5) with the factor $e^{-\gamma^2/2\alpha}$ omitted, is somewhat larger than 1. He found three values of u, namely,

727.952, 853.853 and 2682.977,

for which $S_{1000}(u)$ is approximately 0.96. Next, after experiments with values of T greater than 1000, he finally concentrated on the third case. He computed

$$H(12000, 10^7, 2682 + 16005 \times 2^{-14}) \approx 1.00201,$$

and, moreover, he was able to prove that the computed value of H could not exceed the true value by more than 6.8×10^{-4}, so that

$$H(12000, 10^7, 2682 + 16005 \times 2^{-14}) \geqslant 1.00133.$$

By applying his theorem with $A = 170{,}000$ and $\eta = 0.034$, and by deriving small upper bounds for $|S_i|$, $i = 1, \ldots, 6$, he found that

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\}\,du > 0.00006. \tag{2.7}$$

He concluded that, because of the positivity of K (defined in (2.3)), there must be a value of u between $\omega - \eta$ and $\omega + \eta$ where $\pi(e^u) - \mathrm{li}(e^u) > 0$. Moreover, since $\int_{-\infty}^{\infty} K(u)\,du = 1$, it follows that

$$\int_{\omega-\eta}^{\omega+\eta} K(u-\omega)ue^{-u/2}\{e^{u/2}/u\}\,du < 1, \tag{2.8}$$

so that, by combination of (2.7) and (2.8), it follows that for some value of u between $\omega - \eta$ and $\omega + \eta$ we have

$$\pi(e^u) - \mathrm{li}(e^u) > 0.00006e^{u/2}/u > 10^{500}$$

(since $\omega = 2682.9768\ldots$ and $\eta = 0.034$). This implies that there are more than 10^{500} (in fact, probably many more than 2×10^{500}) successive integers x between 1.53×10^{1165} and 1.65×10^{1165} for which $\pi(x) > \mathrm{li}(x)$. Sherman Lehman suggested that one might prove a similar result in the neighborhood of $e^{853.853}$ if enough zeros of $\zeta(s)$ were calculated. We have followed this suggestion, and the results are described in the next section.

3. Applying Sherman Lehman's Theorem Near exp(853.853). In our attempt to show that $H(T, \alpha, \omega) > 1$, for ω close to 853.853, we have chosen, after several experiments,

$$\begin{aligned} &A = 450{,}000, \quad \alpha = 2 \times 10^8, \quad \eta = 0.0045, \\ &T = \gamma_{50{,}000} = 40433.6873854\ldots, \quad \omega = 853.852286. \end{aligned} \tag{3.1}$$

The truth of the Riemann hypothesis for all the complex zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ with $|\gamma| < 450{,}000$ follows already from [9]. In fact, one may choose for A any value not exceeding $545{,}439{,}823.215\ldots$ ($= \gamma_{1.5\times 10^9}$, cf. [7]), but this is much more than is actually needed for our purpose. The choice $T = \gamma_{50{,}000}$ implies the necessity to know γ_i for $i = 1, \ldots, 50{,}000$ to sufficient accuracy. The first 15,000 γ_i's were known already with an accuracy of about 28 digits from computations carried out in 1979 [8]. The next 35,000 γ_i's were computed with the help of the so-called Riemann-Siegel asymptotic formula for the function $Z(t)$ (whose real zeros coincide with the imaginary parts of the zeros $\beta + i\gamma$ of the Riemann zeta function $\zeta(s)$ which have $\beta = \frac{1}{2}$) truncated after four terms. According to Gabcke [2, p. 5], the absolute value of the error in the computation of $Z(t)$ caused by this truncation is bounded above by $0.031 \times t^{-2.25}$. The FORTRAN-function DZ(DT) on pp. 28–29 of [6] shows the details of our implementation of this Riemann-Siegel formula. Together with the γ_i, for $i = 15{,}001, \ldots, 50{,}000$, we also computed in the same way γ_i for $i = 10{,}001, \ldots, 15{,}000$, as a check.

The γ_i, $i = 10{,}001, \ldots, 50{,}000$, were computed in two steps. First, they were separated in the usual way (cf. [1]). This yielded numbers $\underline{\gamma}_i$ and $\bar{\gamma}_i$ such that

$$\underline{\gamma}_i < \gamma_i < \bar{\gamma}_i = \underline{\gamma}_{i+1} \quad \text{and} \quad Z(\underline{\gamma}_i) \times Z(\bar{\gamma}_i) < 0.$$

Next, with the aid of the zero-finding IMSL-routine ZBRENT, which uses a combination of linear interpolation, inverse quadratic interpolation and bisection, the approximations $\underline{\gamma}_i$ and $\bar{\gamma}_i$ to γ_i were improved until $\bar{\gamma}_i - \underline{\gamma}_i < 10^{-9}$ and $Z(\underline{\gamma}_i) \times Z(\bar{\gamma}_i) < 0$, thus yielding an approximation γ_i^* to γ_i for which

$$|\gamma_i^* - \gamma_i| < 10^{-9}. \tag{3.2}$$

The error due to the use of the truncated asymptotic formula for $Z(t)$ is bounded above by 3.2×10^{-11} (this number is obtained by substituting the smallest value of γ used, namely $\gamma_{10{,}001} = 9878.6\ldots$, in Gabcke's upper bound given above). All the computations were carried out in double precision on the CYBER 750 computer of SARA (with an accuracy of about 28 digits), so that the truncation and rounding errors are small compared with the accuracy (3.2) in γ_i. The "check" values γ_i, $i = 10{,}001, \ldots, 15{,}000$, were compared with the 28D approximations already computed in [8], and all the actual errors were bounded above by 10^{-12}. The time needed for the computations of γ_i^*, $i = 15{,}001, \ldots, 50{,}000$, was about one hour CPU-time.

With these γ_i^* we computed the following approximation H^* to H:

$$H^*\left(\gamma_{50{,}000}, 2 \times 10^8, 853.852286\right) = 1.0240109\ldots. \tag{3.3}$$

The error $|H - H^*|$ may be bounded from above as follows. Since the complex zeros of the Riemann zeta function appear in complex conjugate pairs, it follows from (2.5) that

$$H(T, \alpha, \omega) = -\sum_{0 < \gamma \leqslant T} t(\gamma) \tag{3.4}$$

where

$$t(\gamma) = e^{-\gamma^2/2\alpha} \frac{\cos(\omega\gamma) + 2\gamma \sin(\omega\gamma)}{0.25 + \gamma^2}.$$

By the mean-value theorem, we have

$$|t(\gamma^*) - t(\gamma)| = |\gamma^* - \gamma| \cdot |t'(\bar{\gamma})| \quad \text{with } |\bar{\gamma} - \gamma| < |\gamma^* - \gamma|. \tag{3.5}$$

For $t'(\gamma)$ we have

$$t'(\gamma) = e^{-\gamma^2/2\alpha}\left[\frac{\cos(\omega\gamma)(2\omega\gamma - \gamma/\alpha) - \sin(\omega\gamma)(\omega + 2\gamma^2/\alpha)}{0.25 + \gamma^2} - \frac{2\gamma\{\cos(\omega\gamma) + 2\gamma\sin(\omega\gamma)\}}{(0.25 + \gamma^2)^2}\right],$$

so that, since $\gamma < \alpha$ (cf. (3.1), and (3.6) below),

$$\begin{aligned}|t'(\gamma)| &< e^{-\gamma^2/2\alpha}\left[\frac{2\omega\gamma + \omega + 2\gamma^2/\alpha}{0.25 + \gamma^2} + \frac{2\gamma(1 + 2\gamma)}{(0.25 + \gamma^2)^2}\right]\\ &< e^{-\gamma^2/2\alpha}\left[\frac{2\omega}{\gamma} + \frac{\omega}{\gamma^2} + \frac{2}{\alpha} + \frac{2}{\gamma^3} + \frac{4}{\gamma^2}\right].\end{aligned}$$

From the (in)equalities

$$(3.6) \qquad 14 < \gamma_1 \leqslant \gamma \leqslant \gamma_{50,000} < 40434, \quad \omega < 854, \quad \alpha = 2 \times 10^8,$$

it follows that

$$(3.7) \qquad |t'(\gamma)| < \frac{1770}{\gamma}.$$

From (3.1), (3.5), (3.7) and the errors in γ_i^*, we deduce

$$\begin{aligned}|H - H^*| &\leqslant \sum_{i=1}^{15,000} |t(\gamma_i) - t(\gamma_i^*)| + \sum_{i=15,001}^{50,000} |t(\gamma_i) - t(\gamma_i^*)|\\ &= \sum_{i=1}^{15,000} |\gamma_i - \gamma_i^*|\,|t'(\bar\gamma_i)| + \sum_{i=15,001}^{50,000} |\gamma_i - \gamma_i^*|\,|t'(\bar\gamma_i)|\\ &< 10^{-22}\sum_{i=1}^{15,000}\frac{1770}{\gamma_i} + 10^{-9}\sum_{i=15,001}^{50,000}\frac{1770}{\gamma_i}\\ &< 10^{-22} \times 15,000 \times \frac{1770}{14} + 10^{-9} \times 35,000 \times \frac{1770}{14040}\\ &< 5 \times 10^{-6}.\end{aligned}$$

The many computations of H^* needed to find (3.1) and (3.3) were carried out on the CYBER 205 vector computer of SARA, which is very suitable for such very long sums. One H^*-computation consumed about one second CPU-time on this CYBER.

For the numbers S_i, $i = 1, \ldots, 6$, in Sherman Lehman's theorem, we found

$$\begin{aligned}&|S_1| < 0.0036, \quad |S_2| < 10^{-58}, \quad |S_3| < 10^{-100},\\ &|S_4| < 10^{-100}, \quad |S_5| < 0.0058, \quad |S_6| < 10^{-28}.\end{aligned}$$

With these inequalities and (3.3), we conclude from Sherman Lehman's theorem that, for $\omega = 853.852286$ and $\eta = 0.0045$, we have

$$\begin{aligned}&\int_{\omega-\eta}^{\omega+\eta} K(u - \omega)ue^{-u/2}\{\pi(e^u) - \mathrm{li}(e^u)\}\,du\\ &\qquad > -1 + 1.024010 - 5 \times 10^{-6} - 0.0036 - 0.0058 > 0.0146.\end{aligned}$$

Proceeding in the same way as Sherman Lehman did (cf. Section 2), we find that between $\omega - \eta$ and $\omega + \eta$ there is a u such that

$$\pi(e^u) - \mathrm{li}(e^u) > 0.0146 \times e^{u/2}/u > 10^{180}.$$

This implies that there are more than 10^{180} successive integers x between $e^{\omega-\eta} = 6.627\ldots \times 10^{370}$ and $e^{\omega+\eta} = 6.687\ldots \times 10^{370}$ for which $\pi(x) > \mathrm{li}(x)$. This proves the result announced in Section 1.

Remark. We have done some experiments in the neighborhood of $e^{727.952}$, the smallest of the three candidates given by Sherman Lehman. These experiments indicate that for the choice of the parameters: $T = 4.10^5$, $\alpha = 10^{10}$, and $A = 3.10^6$, it might be possible to prove the existence of another interval for which $\pi(x) - \mathrm{li}(x) > 0$. This would require computing all the zeros of the Riemann zeta function with imaginary part below 4.10^5 to sufficient accuracy: about ten times as many zeros as we used.

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