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# On the Sign of the Difference $\pi(x) - li(x)$

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Following a method of Sherman Lehman we show that between  $6.62 \times 10^{370}$  and  $6.69 \times 10^{370}$  there are more than  $10^{180}$  successive integers  $x$  for which  $\pi(x) - li(x) > 0$ . This brings down Sherman Lehman's bound on the smallest number  $x$  for which  $\pi(x) - li(x) > 0$ , namely from  $1.65 \times 10^{1165}$  to  $6.69 \times 10^{370}$ . 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.

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## 1. INTRODUCTION

The prime number theorem, proved by Hadamard and de la Vallée Poussin in 1896, states that  $\pi(x) \sim li(x)$ , as  $x \rightarrow \infty$ , where  $\pi(x)$  is the number of primes  $\leq x$  and  $li(x) = \int_0^x dt / \log t$ . This result tells us that the ratio  $\pi(x) / li(x)$  tends to 1 as  $x \rightarrow \infty$ , but it does not say anything about the difference  $\pi(x) - li(x)$ . 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  $\pi(x) - li(x)$  changes sign infinitely often. More precisely, he proved the existence of a number  $K > 0$  such that

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

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  $\pi(x) > li(x)$ , namely  $\exp(\exp(\exp(\exp(7.705))))$ . In 1966, SHERMAN LEHMAN ([ 10 ]) brought down this bound considerably by proving that between  $1.53 \times 10^{1165}$  and  $1.65 \times 10^{1165}$  there are more than  $10^{500}$  successive integers for which  $\pi(x) > li(x)$ . 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  $1/2 + i\gamma$  of the Riemann zeta function for which  $0 < \gamma < 12,000$  to about 7 decimal places.

In Section 3 we will bring down Sherman Lehman's bound by showing that there are more than  $10^{180}$  successive integers  $x$  between  $6.62 \times 10^{370}$  and  $6.69 \times 10^{370}$  for which  $\pi(x) > li(x)$ . 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.

## 2. SHERMAN LEHMAN'S METHOD

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

THEOREM. ([ 10 ])

Let  $A$  be a positive number such that  $\beta = 1/2$  for all the zeros  $\rho = \beta + i\gamma$  of the Riemann zeta function  $\zeta(s)$  with  $0 < \gamma \leq A$ . Let  $\alpha, \eta$  and  $\omega$  be positive numbers such that  $\omega - \eta > 1$  and the conditions

$$4A / \omega \leq \alpha \leq A^2 \quad (2.1)$$

and

$$2A / \alpha \leq \eta < \omega / 2 \quad (2.2)$$

hold. Let

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

Then for  $2\pi\epsilon < T < A$

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

where

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

and

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

with

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

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  $li(x)$ , namely, in the neighbourhood of values of  $u$  for which the sum

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

— which is the sum in (2.5) with the  $\exp$  — factor omitted — is somewhat larger than 1. He found three values of  $u$ , namely

$$727.952, \quad 853.853 \quad \text{and} \quad 2682.977$$

for which  $S_{1000}(u)$  is approximately 0.96. Next, after experiments with values of  $T$  larger 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  $6.8 \times 10^{-4}$ , so that

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

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

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

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  $\pi(e^u) - li(e^u) > 0$ . Moreover, since  $\int_{-\infty}^{\infty} K(u)du = 1$ , it follows that

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

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

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

( since  $\omega = 2682.9768\dots$  and  $\eta = 0.034$  ). This implies that there are more than  $10^{500}$  ( in fact, probably many more than  $2 \times 10^{500}$  ) successive integers  $x$  between  $1.53 \times 10^{1165}$  and  $1.65 \times 10^{1165}$  for which  $\pi(x) > li(x)$ . Sherman Lehman suggested that one might prove a similar result in the neighbourhood 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  $\omega$  close to  $853.853$ , we have chosen, after several experiments:

$$A = 450,000, \quad \alpha = 2 \times 10^8, \quad \eta = 0.0045, \quad (3.1)$$

$$T = \gamma_{50,000} = 40433.6873854\dots, \quad \omega = 853.852286.$$

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  $545,439,823.215\dots$  ( =  $\gamma_{1.5 \times 10^9}$ , 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  $\gamma_i$  for  $i = 1, \dots, 50,000$  to sufficient accuracy. The first 15,000  $\gamma_i$ 's were known already with an accuracy of about 28 digits from computations carried out in 1979 ( [ 8 ] ). The next 35,000  $\gamma_i$ 's were computed with help of the so-called Riemann-Siegel asymptotic formula for the function  $Z(t)$  ( whose real zeros coincide with the ordinates of the zeros  $\beta + i\gamma$  of the Riemann zeta function  $\zeta(s)$  which have  $\beta = 1/2$  ) 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  $\gamma_i$ , for  $i = 15,001, \dots, 50,000$ , we also computed in the same way  $\bar{\gamma}_i$  for  $i = 10,001, \dots, 15,000$ , as a check.

The  $\gamma_i$ ,  $i = 10,001, \dots, 50,000$ , 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  $\gamma_i$  and  $\bar{\gamma}_i$  to  $\gamma_i$  where improved until  $\bar{\gamma}_i - \gamma_i < 10^{-9}$  and  $Z(\gamma_i) \times Z(\bar{\gamma}_i) < 0$ , thus yielding an approximation  $\gamma_i^*$  to  $\gamma_i$  for which

$$|\gamma_i^* - \gamma_i| < 10^{-9}. \quad (3.2)$$

The error due to the use of the truncated asymptotic formula for  $Z(t)$  is bounded above by  $3.2 \times 10^{-11}$  (this number is obtained by substituting the smallest value of  $\gamma$ , namely  $\gamma_{10,001} = 9878.6\dots$ , 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  $\gamma_i$ . The "check" values  $\gamma_i$ ,  $i = 10,001, \dots, 15,000$  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  $\gamma_i^*$ ,  $i = 15,001, \dots, 50,000$  was about one hour CPU-time.

With these  $\gamma_i^*$  we computed the following approximation  $H^*$  to  $H$ :

$$H^*(\gamma_{50,000}, 2 \times 10^8, 853.852286) = 1.0240109\dots \quad (3.3)$$

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

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

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

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

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

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

it follows that

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

From ( 3.1), (3.5), (3.7) and the errors in  $\gamma_i^*$  we deduce

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

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  $S_i$ ,  $i = 1, \dots, 6$ , 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

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

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

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

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

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