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General Section

The mean square of the error term in the prime number theorem

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ABSTRACT

We show that, on the Riemann hypothesis, $\limsup_{X\to\infty} I(X)/X^2 \leqslant 0.8603$, where $I(X) = \int_X^{2X} (\psi(x) - x)^2\, dx$. This proves (and improves on) a claim by Pintz from 1982. We also show unconditionally that $1.86 \cdot 10^{-4} \leqslant I(X)/X^2$ for sufficiently large X, and that the $I(X)/X^2$ has no limit as $X \to \infty$.

1. Introduction

Let $\psi(x) = \sum_{n\leqslant x} \Lambda(n)$ where $\Lambda(n)$ is the von Mangoldt function. By the prime number theorem we have $\psi(x) \sim x$. Littlewood (see [8, Thm. 15.11]) showed that $\psi(x) - x = \Omega_{\pm}(x^{1/2} \log\log\log x)$ as $x \to \infty$. In view of Littlewood's result, it is of interest that,

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assuming the Riemann hypothesis (RH), the mean square of $(\psi(x)-x)/x^{1/2}$ is bounded. Under RH we have

$$\psi(x) - x \ll x^{1/2}\log^2 x, \quad \int_X^{2X} (\psi(x)-x)^2\, dx \ll X^2. \tag{1}$$

Note that using the first bound in (1) does not yield the second bound. Define

$$I(X) := \int_X^{2X} (\psi(x)-x)^2\, dx. \tag{2}$$

Unconditionally, it is known that $I(X) \gg X^2$. Indeed Popov and Stechkin [16, Thms. 6–7] showed that

$$\int_X^{2X} |\psi(x)-x|\, dx > \frac{X^{3/2}}{200}, \tag{3}$$

where X is sufficiently large. On using Cauchy–Schwarz, this shows that $I(X)/X^2 \geqslant 1/(40\,000)$.

Pintz wrote a series of papers giving bounds on the constant in (3): [10] has an ineffective constant, [12, Cor. 1] has $(22000)^{-1}$ and [11, Cor. 1] has 400^{-1}. Under RH, Cramér [3] proved that $I(X) \leqslant cX^2$ for sufficiently large X. Pintz [12,11] claims that one may take $c = 1$ for all X sufficiently large. We are unaware of a proof of this, or of any similar results in the literature.

It follows from the above discussion that there exist positive constants A_1 and A_2 for which $A_1 \leqslant I(X)X^{-2} \leqslant A_2$, for sufficiently large X. Actually the upper bound is conditional on RH whereas the lower bound is unconditional. The purpose of this article is to give what we believe to be the best known bounds on A_1 and A_2.

Theorem 1. *Assume the Riemann hypothesis and let $I(X)$ be defined in (2). Then, for X sufficiently large we have $1.86 \cdot 10^{-4} \leqslant I(X)X^{-2} \leqslant 0.8603$.*

Presumably, both bounds in Theorem 1 could be improved. We computed $I(X)$ for X at every integer $\in [1, 10^{11}]$ and include two plots showing its short term behaviour as Figs. 1 and 2. One can see by Fig. 1 that $I(X)/X^2$ exhibits erratic behaviour; Fig. 2 shows a large jump around $X = 5 \cdot 10^{10}$. We are not aware of any conjectured results on the limiting behaviour of $I(X)/X^2$. Hence we prove the following (possibly surprising) result.

Theorem 2. *With $I(X)$ defined by (2), we have that $\lim_{X\to\infty} I(X)/X^2$ does not exist.*

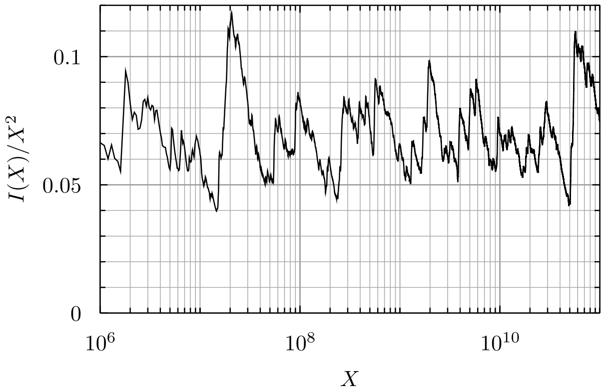

Fig. 1. Plot of $I(X)/X^2$ vs. X for $X \in [10^6, 10^{11}]$.

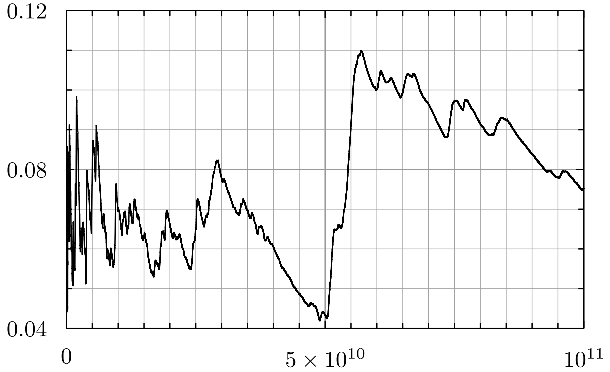

Fig. 2. Plot of $I(X)/X^2$ vs. X sampled every 10^5.

If RH is false, then $I(X)/X^2$ is unbounded. Hence, we assume RH except where noted (e.g. RH is not necessary in §2). Let

$$B := \sum_{\rho_1,\rho_2} \left| \frac{2^{2+i(\gamma_1-\gamma_2)} - 1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} \right| , \tag{4}$$

where $\rho_j = \frac{1}{2} + i\gamma_j$ denotes a nontrivial zero of $\zeta(s)$. Following along the lines of [8, Thm. 13.5], one can show that

$$\limsup_{X\to\infty} \frac{I(X)}{X^2} \leqslant B\,.$$

Corollary 2 shows that $B \leqslant 0.8603$. This proves the upper bound in Theorem 1, which proves Pintz's claim and provides a significant improvement.

A natural question arises as to the behaviour of higher moments of $\psi(x) - x$. For $k \geqslant 1$ define $I_k(X) = \int_X^{2X} (\psi(x) - x)^{2k}\, dx$ so that $I_1(X) = I(X)$. We have not investigated the existence of the limit $I_k(X)/X^{k+1}$ but suggest this as an avenue of future research.

The outline of this paper is as follows. In §2 we give some variations on a well-known lemma of Lehman that is useful for estimating bounds on sums over nontrivial zeros of $\zeta(s)$. We then give several such bounds that are used in the proof of Theorem 3. In §3 we prove Theorem 3, which bounds the tail of the sum in (4), and in Corollary 2 we deduce bounds on B. In §4 we prove the lower bound in Theorem 1. Finally, in §5 we prove Theorem 2.

Throughout this paper we write ϑ to denote a complex number with modulus at most unity. Also, expressions such as $T/2\pi$ should be interpreted as $T/(2\pi)$, and $\log^k x$ as $(\log x)^k$. The symbols $\gamma, \gamma_1, \gamma_2$ denote the ordinates of generic nontrivial zeros $\beta + i\gamma$ of $\zeta(s)$. If we wish to refer to the k-th such $\gamma > 0$ we denote it by $\widehat{\gamma_k}$. For example, $\widehat{\gamma_1} = 14.13472514\cdots$. Finally, we define $L = \log T$ and $\widehat{L} = \log(T/2\pi)$.

2. Preliminary results

The results in this section are unconditional.

We state a well-known result due to Backlund [1], with the constants[1] improved by several authors, most notably by Rosser [14, Thm. 19], Trudgian [19, Thm. 1, Cor. 1], and Platt and Trudgian [13, Cor. 1].

Lemma 1. *For all $T \geqslant 2\pi e$,*

$$N(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} + Q(T),$$

where

$$|Q(T)| \leqslant 0.137\log T + 0.443\log\log T + 1.588 + 0.2/T\,.$$

On RH we have $Q(T) = O(\log T/\log\log T)$, see [8, Cor. 14.4], and indeed, this has been made explicit in recent work by Simonič [15]. Since the bound on $Q(T)$ in [15] only improves on that in Lemma 1 for very large T, we do not use this result in what follows.

Corollary 1. *For all $T \geqslant 2\pi$,*

$$N(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} + (0.28\vartheta)\log T.$$

Proof. By Lemma 1, the result holds for all $T \geqslant T_1 := 7.7\cdot 10^8$. For $T \in [2\pi, T_1)$, it has been verified by an interval-arithmetic computation, using the nontrivial zeros $\beta + i\gamma$ of $\zeta(s)$ with $\gamma \in (0, T_1)$. $\square$

[1] Of the results mentioned here, the sharpest are from [19] and [13]. However, as pointed out by Patel [9], these results rely on an incorrect lemma by Cheng and Graham. This was corrected in [9]; new constants have been worked out by Hasanalizade, Shen, and Wong [5]. We have used the constants from Rosser's work [14] in Lemma 1 since these have been checked independently by Trudgian in [18].

Let A be a constant such that

$$N(T) = \frac{T}{2\pi}\log\frac{T}{2\pi} - \frac{T}{2\pi} + \frac{7}{8} + (\vartheta A)\log T$$

holds for all $T \geqslant 2\pi$. By Corollary 1, we can assume that $A \leqslant 0.28$. We remark here that there is only a little room for improvement in the bound for A. Indeed, the function $Q(T)/\log T$ appears to take its maximum just after $T = \widehat{\gamma}_1$, whence one has $A \geqslant 0.208$. It is possible that the results of [5], and a further interval-arithmetic computation, could improve very slightly on A and hence on the subsequent results in this article.

We state a lemma of Lehman [7, Lem. 1]. We have generalised Lehman's wording, but the original proof still applies.

Lemma 2 *(Lehman-decreasing). If $2\pi e \leqslant T_1 \leqslant T_2$ and $\phi : [T_1, T_2] \mapsto [0, \infty)$ is monotone non-increasing on $[T_1, T_2]$, then*

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

In Lemma 2, we can let $T_2 \to \infty$ if the first integral converges. Lemma 2 does not apply if $\phi(t)$ is *increasing*. In this case, Lemma 3 provides an alternative.

Lemma 3 *(Lehman-increasing). If $2\pi e \leqslant T_1 \leqslant T_2$ and $\phi : [T_1, T_2] \mapsto [0, \infty)$ is monotone non-decreasing on $[T_1, T_2]$, then*

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

Proof. We follow the proof of [7, Lem. 1] with appropriate modifications. □

We need to apply a Lehman-like lemma to a function $\phi(t)$ which decreases and then increases. Hence we state the following lemma.

Lemma 4 *(Lehman-unimodal). Suppose that $2\pi e \leqslant T_1 \leqslant T_2$, and that $\phi : [T_1, T_2] \mapsto [0, \infty)$. If there exists $\theta \in [T_1, T_2]$ such that ϕ is non-increasing on $[T_1, \theta]$ and non-decreasing on $[\theta, T_2]$, then*

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

Proof. Apply Lemma 2 on $[T_1, \theta]$ and Lemma 3 on $[\theta, T_2]$. □

We need some elementary integrals. For $k \geqslant 0$, $T \geqslant 1$ let

$$I_k := T \int_T^\infty \frac{\log^k t}{t^2}\, dt.$$

Then $I_0 = 1$ and I_k satisfies the recurrence $I_k = L^k + kI_{k-1}$ for $k \geqslant 1$. Thus $I_1 = L + 1$, $I_2 = L^2 + 2L + 2$, $I_3 = L^3 + 3L^2 + 6L + 6$, etc.

We also need

$$T^2 \int_T^\infty \frac{\log t}{t^3}\, dt = \frac{2L+1}{4} \tag{5}$$

and

$$T^2 \int_T^\infty \frac{\log^2 t}{t^3}\, dt = \frac{2L^2+2L+1}{4}\,, \tag{6}$$

which may be found in a similar fashion to I_1 and I_2 respectively.

We now state some lemmas that will be used in §3. Lemmas 5–8 are applications of Lemma 2.

Lemma 5. *If $T \geqslant 2\pi e$, then*

$$\sum_{\gamma > T} \frac{1}{\gamma^2} \leqslant \frac{L}{2\pi T}.$$

Proof. We apply Lemma 2 with $\phi(t) = 1/t^2$, $T_1 = T$, and let the upper limit $T_2 \to \infty$. Using the integral I_1 above, this gives

$$\begin{aligned}
\sum_{\gamma > T} \frac{1}{\gamma^2} &= \frac{1}{2\pi} \int_T^\infty \frac{\log(t/2\pi)}{t^2}\, dt + A\vartheta \left(\frac{2L}{T^2} + \int_T^\infty \frac{dt}{t^3} \right) \\
&= \frac{L + 1 - \log(2\pi)}{2\pi T} + A\vartheta \left(\frac{4L+1}{2T^2} \right) \\
&\leqslant \frac{L}{2\pi T}\,,
\end{aligned}$$

where the final inequality uses $T \geqslant 2\pi e$ and $A \leqslant 0.28$. □

Lemma 6. *If $T \geqslant 4\pi e$, then*

$$\sum_{\gamma>T} \frac{\log(\gamma/2\pi)}{\gamma^2} \leqslant \frac{L^2 - L}{2\pi T}.$$

Proof. We apply Lemma 2 with $\phi(t) = \log(t/2\pi)/t^2$, $T_1 = T$, and let the upper limit $T_2 \to \infty$. Since $\log(t/2\pi)/t^2$ is decreasing on $[4\pi e, \infty)$, Lemma 2 is applicable. Making use of the integrals I_2 and (5) above, we obtain

$$\begin{aligned}\sum_{\gamma>T} \frac{\log(\gamma/2\pi)}{\gamma^2} &= \frac{1}{2\pi}\int_T^\infty \frac{\log^2(t/2\pi)}{t^2}\,dt \\ &\quad + A\vartheta\left(\frac{2\log(T/2\pi)\log T}{T^2} + \int_T^\infty \frac{\log(t/2\pi)}{t^3}\,dt\right) \\ &= \frac{\widehat{L}^2 + 2\widehat{L} + 2}{2\pi T} + A\vartheta\left(\frac{2L\widehat{L}}{T^2} + \frac{2\widehat{L}+1}{4T^2}\right) \leqslant \frac{L^2 - L}{2\pi T},\end{aligned}$$

where the final inequality uses $T \geqslant 4\pi e$ and $A \leqslant 0.28$. $\square$

Lemma 7. *If $T \geqslant 100$, then*

$$\sum_{\gamma>T} \frac{\log^2(\gamma/2\pi)}{\gamma^2} \leqslant \frac{L^3 - 1.39L^2}{2\pi T}.$$

Proof. We apply Lemma 2 with $\phi(t) = \log^2(t/2\pi)/t^2$, $T_1 = T$, and $T_2 \to \infty$. Since $\phi(t)$ is monotonic decreasing on $[100, \infty)$, Lemma 2 is applicable. Using the integrals I_3 and (6) above, we obtain

$$\begin{aligned}\sum_{\gamma>T} \frac{\log^2(\gamma/2\pi)}{\gamma^2} &= \frac{1}{2\pi}\int_T^\infty \frac{\log^3(t/2\pi)}{t^2}\,dt \\ &\quad + A\vartheta\left(\frac{2\log^2(T/2\pi)\log T}{T^2} + \int_T^\infty \frac{\log^2(t/2\pi)}{t^3}\,dt\right) \\ &= \frac{\widehat{L}^3 + 3\widehat{L}^2 + 6\widehat{L} + 6}{2\pi T} + A\vartheta\left(\frac{8L\widehat{L}^2 + 2\widehat{L}^2 + 2\widehat{L} + 1}{4T^2}\right) \\ &\leqslant \frac{L^3 - 1.39L^2}{2\pi T},\end{aligned}$$

where the final inequality uses $T \geqslant 100$ and $A \leqslant 0.28$. $\square$

The following lemma improves on the upper bound of [4, Lem. 2.10].

Lemma 8. *If $T \geqslant 4\pi e$, then*

$$\sum_{0<\gamma\leqslant T} \frac{1}{\gamma} \leqslant \frac{\widehat{L}^2}{4\pi}. \tag{7}$$

Proof. Suppose that $T \geqslant T_1$, where $T_1 \geqslant 4\pi e$ will be determined later. Using Lemma 2 with $\phi(t) = 1/t$, we obtain

$$\begin{aligned}\sum_{T_1<\gamma\leqslant T} \frac{1}{\gamma} &= \frac{1}{2\pi}\int_{T_1}^{T} \frac{\log(t/2\pi)}{t}\,dt + A\vartheta\left(\frac{2\log T_1}{T_1} + \int_{T_1}^{T}\frac{dt}{t^2}\right)\\ &= \frac{1}{4\pi}\left(\widehat{L}^2 - \log^2(T_1/2\pi)\right) + A\vartheta\left(\frac{2\log T_1 + 1}{T_1}\right). \end{aligned} \tag{8}$$

Thus, including a sum over $\gamma \leqslant T_1$, we have

$$\sum_{0<\gamma\leqslant T} \frac{1}{\gamma} \leqslant \frac{\widehat{L}^2}{4\pi} + \varepsilon(T_1),$$

where

$$\varepsilon(T_1) = \sum_{0<\gamma\leqslant T_1} \frac{1}{\gamma} - \frac{\log^2(T_1/2\pi)}{4\pi} + A\left(\frac{2\log T_1 + 1}{T_1}\right).$$

Using $A \leqslant 0.28$, and summing over the first 80 nontrivial zeros of $\zeta(s)$, shows that $\varepsilon(202) < 0$. Thus, we take $T_1 = 202$, whence (7) holds for $T \geqslant T_1 = 202$. We can verify numerically that (7) also holds for $T \in [4\pi e, T_1)$. □

Remark 1. The motivation for our proof of Lemma 8 is as follows. Define

$$H := \lim_{T\to\infty}\left(\sum_{0<\gamma\leqslant T} \frac{1}{\gamma} - \frac{\log^2(T/2\pi)}{4\pi}\right).$$

It is easy to show, using (8), that the limit defining H exists. A computation shows that $H \approx -0.0171594$. Since H is negative, we expect that $\varepsilon(T_1)$ should be negative for all sufficiently large T_1. See also [6], and [2].

3. Bounding the tail in the series for B

We are now ready to bound the tail of the series (4). Our main result is stated in Theorem 3. Bounds on B are deduced in Corollary 2.

Theorem 3. *Assume RH. If $T \geqslant 100$, $L = \log T$, and B is defined by (4), then*

$$B \leqslant \sum_{|\gamma_1|\leqslant T, |\gamma_2|\leqslant T} \left| \frac{2^{2+i(\gamma_1-\gamma_2)} - 1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} \right| + \frac{10L^3 + 11L^2}{\pi^2 T}.$$

Proof. Initially, we ignore the numerators $|2^{2+i(\gamma_1-\gamma_2)} - 1|$ in (4), since they are easily bounded. Define

$$S(T) := \sum_{|\gamma_1|\leqslant T, |\gamma_2|\leqslant T} \left| \frac{1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} \right|, \tag{9}$$

and $S_\infty := \lim_{T\to\infty} S(T)$, with $S_\infty \approx 0.217$. We refer to $E(T) := S_\infty - S(T)$ as the *tail* of the series with parameter T. Thus, the tail is the sum of terms with $\max(|\gamma_1|, |\gamma_2|) > T$. Comparing with (4), and using $|2^{2+i(\gamma_1-\gamma_2)} - 1| \leqslant 5$, we see that the error caused by summing (4) with $\max(|\gamma_1|, |\gamma_2) \leqslant T$ is at most $5E(T)$.

We consider bounding sums of the tail terms. By using the symmetry $(\gamma_1, \gamma_2) \to (-\gamma_1, -\gamma_2)$, i.e. complex conjugation, we can assume that $\gamma_1 > 0$ (but we must multiply the resulting bound by 2). We can also use the symmetry $(\gamma_1, \gamma_2) \to (\gamma_2, \gamma_1)$ if $\gamma_2 > 0$, and $(\gamma_1, \gamma_2) \to (-\gamma_2, -\gamma_1)$ if $\gamma_2 < 0$, to reduce to the case that $|\gamma_2| \leqslant \gamma_1$ (again doubling the resulting bound). Terms on the diagonal $\gamma_1 = \gamma_2$ and anti-diagonal $\gamma_1 = -\gamma_2$ are given double the necessary weight, but this does not affect the validity of the bound.

For each $\gamma_1 > 0$, possible γ_2 satisfy $\gamma_2 \in [-\gamma_1, \gamma_1]$. Since γ_2 is the ordinate of a nontrivial zero of $\zeta(s)$, it is never zero, in fact $|\gamma_2| > 14$.

We now bound the terms $1/|\rho_1\overline{\rho_2}(2 + i(\gamma_1 - \gamma_2))|$ and various sums. Our strategy is to fix γ_1 and sum over all possible γ_2, then allow γ_1 to vary and sum over all $\gamma_1 > T$. Since $|\gamma_1| < |\rho_1|$ and $|\gamma_2| < |\rho_2|$, we actually bound

$$t(\gamma_1, \gamma_2) := \frac{1}{|\gamma_1\gamma_2(2 + i(\gamma_1 - \gamma_2))|},$$

which is only slightly larger, since $1 \leqslant |\rho_j/\gamma_j| \leqslant 1 + 1/8\gamma_j^2 \leqslant 1.001$.

It is useful to define $D := 1/t(\gamma_1, \gamma_2)$. We assume that $T \geqslant T_0 = 100$. Since we eventually sum over $\gamma_1 > T$, we also assume that $\gamma_1 \geqslant T_0$.

First suppose that γ_2 is positive. In this case, we have $0 < \gamma_2 \leqslant \gamma_1$ and $D \geqslant \gamma_1\gamma_2 \max(2, \gamma_1 - \gamma_2)$. Thus the terms $t(\gamma_1, \gamma_2)$ are bounded by $\phi(\gamma_2)/\gamma_1^2$, where, writing $T = \gamma_1$,

$$\phi(t) := \begin{cases} \dfrac{T}{t(T-t)} = \dfrac{1}{t} + \dfrac{1}{T-t} & \text{if } t \in (0, T-2]; \\ \dfrac{T/2}{T-2} = \dfrac{1}{2} + \dfrac{1}{T-2} & \text{if } t \in (T-2, T]. \end{cases}$$

Note that $\phi(t)$ is positive, decreasing on the interval $(0, T/2]$, increasing on the interval $(T/2, T-2]$, and constant on the interval $[T-2, T]$. Thus, for summing $\phi(\gamma_2)$ over $\gamma_2 \in (2\pi e, T]$, Lemma 4 applies with $T_1 = 2\pi e$, $T_2 = T \geqslant 2T_1$, and $\theta = T/2$.

To apply Lemma 4, we need to bound $(1/2\pi) \int_{T_1}^{T} \phi(t) \log(t/2\pi)\, dt$ (the main term), and also the error terms $A \int_{T_1}^{T} (\phi(t)/t)\, dt$ and $2A\phi(T_j) \log(T_j)$ $(j = 1, 2)$. We consider these in turn.

First consider the main term:

$$\begin{aligned} &\frac{1}{2\pi} \int_{T_1}^{T} \phi(t) \log(t/2\pi)\, dt \\ &= \frac{1}{2\pi} \left(\int_{T_1}^{T-2} \left(\frac{1}{t} + \frac{1}{T-t} \right) \log(t/2\pi)\, dt + \phi(T) \int_{T-2}^{T} \log(t/2\pi)\, dt \right) \\ &\leqslant \frac{1}{2\pi} \left(\int_{T_1}^{T} \frac{\log(t/2\pi)}{t}\, dt + \widehat{L} \int_{0}^{T-2} \frac{dt}{T-t} + \widehat{L} \left(1 + \frac{2}{T-2} \right) \right) \\ &\leqslant \frac{1}{4\pi} \left(\widehat{L}^2 - 1 + 2\widehat{L} \log(T/2) + 2\widehat{L} + \frac{4\widehat{L}}{T-2} \right) \\ &\leqslant \frac{1}{4\pi} \left(3\widehat{L}^2 + 2\widehat{L}(2 + \log \pi) - 0.88 \right). \end{aligned}$$

Now consider the error terms. We have

$$\begin{aligned} \int_{T_1}^{T} \frac{\phi(t)}{t}\, dt &= \int_{T_1}^{T-2} \frac{\phi(t)}{t}\, dt + \phi(T) \int_{T-2}^{T} \frac{dt}{t} \\ &= \int_{T_1}^{T-2} \left(\frac{1}{t^2} + \frac{1}{T} \left(\frac{1}{t} + \frac{1}{T-t} \right) \right) dt + \phi(T) \int_{T-2}^{T} \frac{dt}{t} \\ &\leqslant \frac{1}{T_1} - \frac{1}{T} + \frac{\log(T/T_1) + \log(T/2)}{T} + \frac{T}{(T-2)^2} \leqslant 0.12\,. \end{aligned}$$

Also,

$$2\phi(T_1) \log T_1 = \frac{2 \log T_1}{T_1} \left(\frac{T}{T - T_1} \right) \leqslant 0.41,$$

and

$$2\phi(T_2)\log T_2 \leqslant \left(1+\frac{2}{T-2}\right)\log T \leqslant \widehat{L}+\log(2\pi)+\frac{2\log T}{T-2} \leqslant \widehat{L}+1.94\,.$$

Thus, Lemma 4 gives

$$\begin{aligned}\sum_{T_1<\gamma\leqslant T}\phi(\gamma) &\leqslant \frac{3\widehat{L}^2+2\widehat{L}(2+\log\pi)-0.88}{4\pi}+A\vartheta\left(0.41+\widehat{L}+1.94+0.12\right)\\ &\leqslant \frac{3\widehat{L}^2+9.81\widehat{L}+7.82}{4\pi}\,.\end{aligned}$$

Since $\widehat{\gamma_1}<T_1<\widehat{\gamma_2}$, we have to treat $\phi(\widehat{\gamma_1})$ separately. We have

$$\phi(\widehat{\gamma_1})=\frac{T}{\widehat{\gamma_1}(T-\widehat{\gamma_1})}<0.083\,,$$

and thus

$$\sum_{0\leqslant\gamma\leqslant T}\phi(\gamma)\leqslant\frac{3\widehat{L}^2+9.81\widehat{L}+8.87}{4\pi}\,.$$

Hence, we have shown that

$$\sum_{0<\gamma_2\leqslant\gamma_1} t(\gamma_1,\gamma_2)\leqslant\frac{3\log^2(\gamma_1/2\pi)+9.81\log(\gamma_1/2\pi)+8.87}{4\pi\gamma_1^2}\,. \tag{10}$$

We now consider the case that γ_2 is negative, whence $0<-\gamma_2\leqslant\gamma_1$. We could use Lemma 2, but we adopt a simpler approach that gives the same leading term.[2]

Assuming that $\gamma_2<0$, we have $D\geqslant\gamma_1|\gamma_2|(\gamma_1+|\gamma_2|)\geqslant\gamma_1^2|\gamma_2|$, and the terms are bounded by

$$t(\gamma_1,\gamma_2)\leqslant\frac{1}{\gamma_1^2|\gamma_2|}\,.$$

Summing over γ_2 satisfying $0<-\gamma_2\leqslant\gamma_1$, using Lemma 8, gives the bound

$$\sum_{-\gamma_1\leqslant\gamma_2<0} t(\gamma_1,\gamma_2)\leqslant\frac{\log^2(\gamma_1/2\pi)}{4\pi\gamma_1^2}\,. \tag{11}$$

We now combine the results for positive and negative γ_2. Adding the bounds (10) and (11) gives

[2] This is not surprising, since we use Lemma 8, whose proof depends on Lemma 2.

$$\sum_{-\gamma_1 \leqslant \gamma_2 \leqslant \gamma_1} t(\gamma_1, \gamma_2) \leqslant \frac{\log^2(\gamma_1/2\pi) + 2.46\log(\gamma_1/2\pi) + 2.22}{\pi\gamma_1^2}. \tag{12}$$

Finally, we sum (12) over all $\gamma_1 > T$ and use Lemmas 5–7, giving

$$\begin{aligned}\sum_{\gamma_1 > T,\ |\gamma_2| \leqslant \gamma_1} t(\gamma_1, \gamma_2) &\leqslant \frac{(L^3 - 1.39L^2) + 2.46(L^2 - L) + 2.22L}{2\pi^2 T} \\ &\leqslant \frac{L^3 + 1.1L^2}{2\pi^2 T}. \end{aligned} \tag{13}$$

Allowing a factor of 4 for symmetry, and a factor of 5 to allow for the numerator in (4), the tail bound $5E(T)$ is 20 times the bound (13), so

$$5E(T) \leqslant \frac{10L^3 + 11L^2}{\pi^2 T}, \tag{14}$$

which proves the theorem. □

It is possible to avoid the use of Lemma 4 in the proof of Theorem 3, by summing the tail terms in a different order, so that the terms in the inner sums are monotonic decreasing and Lemma 2 applies. However, the resulting integrals are more difficult to bound than those occurring in our proof of Theorem 3. Both methods give the same leading term.

Corollary 2. *The constant B defined by (4) satisfies* $0.8520 \leqslant B \leqslant 0.8603$.

Proof. The bounds on B follow from Theorem 3 by taking $T = 260877$ and evaluating the finite double sum, which requires the first $4 \cdot 10^5$ nontrivial zeros of $\zeta(s)$. The evaluation, using interval arithmetic, shows that the finite sum is in the interval $[0.852089, 0.852098]$, so the lower bound 0.8520 stated in the corollary is correct. The tail bound (14) is $\leqslant 0.008199$, and $0.852098 + 0.008199 = 0.860297$. This proves the stated upper bound. □

Remark 2. Since the proof of Corollary 2 uses $T = 260877$, but Theorem 3 and Lemma 7 assume only that $T \geqslant 100$, it is natural to ask if the bounds can be improved if we assume that T is sufficiently large. This is indeed the case. For $T \geqslant 80000$, the bound (13) can be improved to $(L^3 + 0.4L^2)/(2\pi^2 T)$, and it follows that the upper bound in Corollary 2 can be improved to $B \leqslant 0.8599$. The coefficient of L^2 in the bound (13) can be replaced by $c(T) = 4 - 3\log 2 - \frac{5}{2}\log\pi + \pi A + O(1/L) \leqslant -0.06 + O(1/L)$, and a bound on the $O(1/L)$ term shows that $c(T) \leqslant 0$ for $T \geqslant 10^{42}$. The coefficient of L^3 is, however, the best that can be attained by our method.

4. Lower bound on $I(X)$

Stechkin and Popov [16, Thm. 7] showed that, if RH were false, then $\liminf_{X\to\infty} I(X)/X^2 = \infty$. Given this, we may as well assume RH in this section. Stechkin and Popov [16, Thm. 6] showed that we have for X large enough

$$\int_X^{2X} |\psi(u) - u| \, du > \frac{X^{\frac{3}{2}}}{200}, \tag{15}$$

which by Cauchy–Schwarz leads immediately to $I(X)/X^2 \geqslant (40\,000)^{-1}$. The bound in (15) follows from showing under the same assumptions that

$$H(X) := \int_{X-\frac{\log 2}{2}}^{X+\frac{\log 2}{2}} \left| \sum_{n\neq 0} \frac{\exp(i\gamma_n t)}{\rho_n} \right| dt > \frac{X^{\frac{3}{2}}}{200}, \tag{16}$$

where, throughout this section only, for $k \geqslant 1$ we define γ_k (resp. γ_{-k}) to be the ordinate of the kth non-trivial zero of $\zeta(s)$, above (resp. below) the real axis. We interpret the sum in (16), which is not absolutely convergent, as

$$\lim_{N\to\infty} \sum_{n=1}^{N} \left(\frac{\exp(i\gamma_n t)}{\rho_n} + \frac{\exp(i\gamma_{-n} t)}{\rho_{-n}} \right).$$

The key result we need is the following.

Lemma 9. *Let $g(z)$ be such that $g(0) = 1$ and*

$$\delta = \frac{1}{\rho_1} - \sum_{n\geqslant 2} \left| \frac{g(\gamma_n - \gamma_1)}{\rho_n} \right| - \sum_{n\geqslant 1} \left| \frac{g(-\gamma_n - \gamma_1)}{\rho_n} \right|$$

exists and is finite. Additionally, assume that

$$\widehat{g}(y) = \frac{1}{2\pi} \int_{\mathbb{R}} g(z) \exp(-izy) \, dz$$

exists and is supported on $[-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$. Then we have

$$|H(X)| \geqslant \frac{\delta}{\max\limits_{y\in\mathbb{R}} \widehat{g}(y)}.$$

Proof. This follows from displays (15.4) to (17.4) of [16, Sec. 4]. □

Lemma 10. *Let* $\alpha = \frac{\log 2}{6}$ *and* $\lambda > 0$. *Define*

$$g(z) = \left(\frac{\sin(\alpha z)}{\alpha z}\right)^3 \left(1 - \frac{z}{\lambda}\right)$$

and

$$\widehat{g}(y) = \frac{1}{2\pi} \int_{\mathbb{R}} g(z) \exp(-izy)\, dz.$$

Then $g(0) = 1$ *and* $\widehat{g}(y)$ *is supported on* $[-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$. *Furthermore, for real* y, $|\widehat{g}(y)|$ *attains its maximum of* $\frac{9}{4\log 2}$ *at* $y = 0$.

We note that Stechkin and Popov used the fourth power of the sinc function in place of our cube. Almost certainly better choices of the function $g(z)$ are possible: we leave this to future researchers, in the hope that they can thereby improve the lower bound in Theorem 1.

Lemma 11. *Let* g *be as defined in Lemma 10. For* $T > \max(\gamma_1 + \lambda, 2\pi e)$ *not the ordinate of a zero of* ζ *set*

$$\delta_{T,\lambda} = \sum_{\gamma > T} \frac{|g(\gamma - \gamma_1)| + |g(-\gamma - \gamma_1)|}{\rho}.$$

Then

$$\delta_{T,\lambda} \leqslant \int_T^\infty h_\lambda(t) \log \frac{t}{2\pi}\, dt + 0.56 h_\lambda(T) \log T + 0.28 \int_T^\infty \frac{h_\lambda(t)}{t}\, dt$$

where

$$h_\lambda(t) = \frac{t - \lambda - \gamma_1}{t(\alpha(t - \gamma_1))^3} + \frac{t + \lambda + \gamma_1}{t(\alpha(t + \gamma_1))^3}.$$

Proof. This is a straightforward application of Corollary 1 and Lemma 2. □

Corollary 3. *Let* $\delta_{T,\lambda}$ *be as in Lemma 11, with* $T = 446\,000$ *and* $\lambda = 10.876$. *Then*

$$\delta_{T,\lambda} \leqslant 3.5 \cdot 10^{-9}.$$

We can now compute the contribution to δ from the 721 913 nontrivial zeros with imaginary part less than 446 000, using $\lambda = 10.876$. We find

$$\frac{1}{|\rho_1|} - \sum_{n=2}^{721\,913} \frac{g(\gamma_n - \gamma_1)}{\rho_n} - \sum_{n=1}^{721\,913} \frac{g(-\gamma_n - \gamma_1)}{\rho_n} \geqslant 4.428\,225\,55 \cdot 10^{-2},$$

so we have $\delta \geqslant 0.044\,282\,252$.

Appealing to Lemmas 9 and 10 we can now claim

$$|H(X)| \geqslant 0.044\,282\,252 \frac{4\log 2}{9} \geqslant 0.013\,641\,83,$$

and the lower bound of Theorem 1 results.

5. Non-convergence of $I(X)/X^2$

Our aim now is to show that $I(X)/X^2$ does not tend to a limit as $X \to \infty$. It is more convenient to work with

$$J(X) := \int_0^X (\psi(x) - x)^2 \, dx, \tag{17}$$

and deduce results for $I(X)$. In Theorems 4 and 5 we show that there exist effectively computable constants c_1 and c_2, satisfying $c_1 < c_2$, such that

$$\limsup_{X\to\infty} \frac{2}{X^2} J(X) \geqslant c_2, \quad \liminf_{X\to\infty} \frac{2}{X^2} J(X) \leqslant c_1.$$

Hence $J(X)/X^2$ cannot tend to a limit as $X \to \infty$. In Theorem 2 we deduce that $I(X)/X^2$ cannot tend to a limit $X \to \infty$.

5.1. Some constants

In sums over zeros, each zero ρ is counted according to its multiplicity m_ρ. More precisely, a term involving ρ is given a weight m_ρ. In double sums, a term involving ρ_1 and ρ_2 is given a weight $m_{\rho_1} m_{\rho_2}$.

We now define three real constants that are needed later. First, a constant that appears in [8, Thm. 13.6 and Ex. 13.1.1.3] and our Theorem 5:

$$c_1 := \sum_\rho \frac{m_\rho}{|\rho|^2} \approx 0.046. \tag{18}$$

Second, we define a constant that occurs in Theorem 4:

$$c_2 := \sum_{\rho_1,\rho_2} \frac{2}{\rho_1 \overline{\rho_2}(1 + \rho_1 + \overline{\rho_2})} \approx 0.104\,. \tag{19}$$

Observe that, assuming RH, the "diagonal terms" (i.e. those with $\rho_1 = \rho_2$) in (19) sum to c_1.

Third, a constant that will be used in §5.3:

$$c_3 := \sum_{\gamma>0} \frac{1}{\gamma^2} \leqslant 0.023\,105, \tag{20}$$

where this estimate has been computed to high accuracy previously (see, e.g. [4]). We can replicate this result by summing numerically over zeros below $3.72146 \cdot 10^8$ and using Lemma 5 for the tail.

5.2. The limsup result

We use the explicit formula for $\psi(x)$ (see, e.g., [8, Thm. 12.5]) in the form

$$\psi(x) - x = -\sum_{|\gamma|\leqslant T} \frac{x^\rho}{\rho} + O\left(\frac{x\log^2 x}{T}\right)$$

for $T \geqslant T_0$, $x \geqslant X_0$, and $x \geqslant T$.

Theorem 4. *With $J(X)$ as in (17) and c_2 as in (19),*

$$\limsup_{X\to\infty} \frac{2J(X)}{X^2} \geqslant c_2.$$

Proof. Fix some small $\varepsilon > 0$. We can assume RH, since otherwise $J(X)/X^2$ is unbounded. Proceeding as in the proof of [8, Thm. 13.5], but with the integral over $[T, X]$ instead of $[X, 2X]$, and using the Cauchy–Schwartz inequality for the error term, we obtain

$$\int_T^X (\psi(x) - x)^2\,dx = \int_T^X \sum_{|\gamma_1|\leqslant T,\,|\gamma_2|\leqslant T} \frac{x^{1+i(\gamma_1-\gamma_2)}}{\rho_1\overline{\rho_2}}\,dx + O\left(\frac{X^{5/2}\log^2 X}{T}\right),$$

provided $X \geqslant T \geqslant \max(T_0, X_0)$. We also have, from [8, Thm. 13.5],

$$\int_0^T (\psi(x) - x)^2\,dx \ll T^2.$$

Thus

$$\int_0^X (\psi(x) - x)^2\,dx = \int_T^X \sum_{|\gamma_1|\leqslant T,\,|\gamma_2|\leqslant T} \frac{x^{1+i(\gamma_1-\gamma_2)}}{\rho_1\overline{\rho_2}}\,dx$$
$$+ O\left(T^2 + X^{5/2}(\log X)^2/T\right).$$

Now, from [8, (13.16)], $\sum_{\rho_1,\rho_2} \left| \frac{1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2)} \right| \ll 1.$

Thus, if we exchange the order of integration and summation (valid since the sum is finite), and normalise by X^2, we obtain

$$\frac{J(X)}{X^2} = \sum_{|\gamma_1|\leqslant T,\, |\gamma_2|\leqslant T} \frac{X^{i(\gamma_1-\gamma_2)}}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} + O\left(\frac{T^2}{X^2} + \frac{X^{1/2}\log^2 X}{T}\right).$$

Choosing $T = X^{5/6}$, and assuming that $X \geqslant X_0^{6/5}$ so $T \geqslant X_0$, the error term becomes $O(X^{-1/3}(\log X)^2)$. Now, choosing $X \geqslant \log^6(1/\varepsilon)/\varepsilon^3$, the error term is $O(\varepsilon)$. To summarise, we obtain error $O(\varepsilon)$ provided that $T = X^{5/6}$ and $X \geqslant X_1$, where $X_1 = \max(X_0^{6/5}, T_0^{6/5}, \log^6(1/\varepsilon)/\varepsilon^3)$.

We shall need another parameter $Y = \log^3(1/\varepsilon)/\varepsilon$. Note that, by the conditions on T and X, we necessarily have $Y \leqslant T$ for $\varepsilon \in (0, 1/e)$, since $T = X^{5/6} \geqslant \log(1/\varepsilon)^5/\varepsilon^{5/2} \geqslant \log^3(1/\varepsilon)/\varepsilon = Y$.

It remains to consider the main sum over pairs $(1/2 + i\gamma_1, 1/2 - i\gamma_2)$ of zeros with $|\gamma_1|, |\gamma_2| \leqslant T$. Observe that the sum is real, as we can see by grouping the term for $(1/2 + i\gamma_1, 1/2 - i\gamma_2)$ with the conjugate term for $(1/2 - i\gamma_1, 1/2 + i\gamma_2)$. Using Dirichlet's theorem [17, §8.2], we can find some $t \geqslant \log X_1$, such that $|\{t\gamma/(2\pi)\}| \leqslant \varepsilon$ for all zeros $1/2 + i\gamma$ with $0 < \gamma \leqslant Y$, where $Y \leqslant T$ is as above.[3] Set $X = \exp(t)$. Then, for all the (γ_1, γ_2) occurring in the main sum with $\max(|\gamma_1|, |\gamma_2|) \leqslant Y$, we have $X^{i(\gamma_1-\gamma_2)} = 1 + O(\varepsilon)$. Hence, for this choice of X, we have

$$\frac{J(X)}{X^2} = \sum_{|\gamma_1|\leqslant Y,\, |\gamma_2|\leqslant Y} \frac{1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} + R(Y) + O(\varepsilon),$$

where

$$|R(Y)| \leqslant \sum_{\max(|\gamma_1|,|\gamma_2|)>Y} \left| \frac{1}{\rho_1\overline{\rho_2}(2+i(\gamma_1-\gamma_2))} \right| \ll \frac{\log^3 Y}{Y}$$

is the tail of an absolutely convergent double sum, see (9) and [8, p. 424]. Thus, with our choice $Y = \log^3(1/\varepsilon)/\varepsilon$, we have $R(Y) = O(\varepsilon)$.

Recalling the definition of the constant c_2 in (19), we have shown that, for any sufficiently small $\varepsilon > 0$, there exists $X = X(\varepsilon)$ such that

$$\frac{2J(X)}{X^2} \geqslant c_2 - O(\varepsilon). \tag{21}$$

Since ε can be arbitrarily small, this proves the result. □

[3] Here $\{x\}$ denotes the fractional part of x.

Remark 3. The least X satisfying (21) may be bounded using [17, (8.2.1)]. The result is doubly exponential in $1/\varepsilon$. More precisely,

$$X(\varepsilon) \leqslant \exp(\exp((1/\varepsilon)^{1+o(1)})) \text{ as } \varepsilon \to 0.$$

5.3. A lower bound on c_2

The constants c_1 and c_2 are of little interest, so far as the theory of $\psi(x)$ goes, if RH is false. Hence, we assume RH. In Corollary 5 we show that $c_1 < c_2$. Although computations of c_2 suggest this, they do not provide a proof unless they come with a (possibly one-sided) error bound. Here we show how rigorous lower bounds on c_2 can be computed. This provides a way of proving rigorously, without extensive computation, that $c_1 < c_2$.

First we extract the real part of the expression (19). This leads to sharper bounds on the terms than if we included the imaginary parts, which must ultimately cancel.

Lemma 12. *Assume RH. If c_2 is defined by (19), then*

$$c_2 = \sum_{\gamma_1 > 0,\ \gamma_2} T(\gamma_1, \gamma_2),$$

where

$$T(\gamma_1, \gamma_2) = \frac{2(1 + 6\gamma_1\gamma_2 - \gamma_1^2 - \gamma_2^2)}{(\frac{1}{4} + \gamma_1^2)(\frac{1}{4} + \gamma_2^2)(4 + (\gamma_1 - \gamma_2)^2)}\,. \tag{22}$$

Proof. We expand (19), using $\rho_j = \frac{1}{2} + i\gamma_j$ (this is where RH is required), omit the imaginary parts since the final result is real, and use symmetry to reduce to the case $\gamma_1 > 0$ (so in the resulting sum, γ_1 is positive but γ_2 may have either sign). □

Lemma 13 gives a region in which the terms occurring in (22) are positive.

Lemma 13. *If $T(\gamma_1, \gamma_2)$ is as in (22), and $\gamma_2/\gamma_1 \in [3 - \sqrt{8}, 3 + \sqrt{8}]$, then $T(\gamma_1, \gamma_2) > 0$.*

Proof. Since the denominator of $T(\gamma_1, \gamma_2)$ is positive, it is sufficient to consider the numerator, which we write as $2P(\gamma_1, \gamma_2)$, where

$$P(x, y) = 1 + 6xy - x^2 - y^2.$$

Let $r = y/x$, so $P(x, y) = 1 - (r^2 - 6r + 1)x^2$. Now $r^2 - 6r + 1 = (r - 3)^2 - 8$ vanishes at $r = 3 \pm \sqrt{8}$, and is negative iff $r \in (3 - \sqrt{8}, 3 + \sqrt{8})$. Thus $P(x, y)$ is positive for $r \in [3 - \sqrt{8}, 3 + \sqrt{8}]$. Taking $x = \gamma_1, y = \gamma_2$ proves the lemma. □

Define

$$S(Y) = \sum_{\substack{0<\gamma_1\leqslant Y\\ -Y\leqslant\gamma_2\leqslant Y}} T(\gamma_1,\gamma_2).$$

Then $c_2 = \lim_{Y\to\infty} S(Y)$. Clearly $S(Y)$ is constant between ordinates of nontrivial zeros of $\zeta(s)$, and has jumps

$$J(\gamma) = \lim_{\varepsilon\to 0}(S(\gamma+\varepsilon) - S(\gamma-\varepsilon))$$

at positive ordinates γ of zeros of $\zeta(s)$. We shall show that all these jumps are positive, so $S(Y)$ is monotonic non-decreasing, and $c_2 > S(Y)$ for all $Y > 0$. This allows us to prove that $c_2 > c_1$ by computing $S(Y)$ for sufficiently large Y (see Corollary 5).

If $\gamma > 0$ is the ordinate of a simple zero[4] of $\zeta(s)$, then

$$\begin{aligned} J(\gamma) &= \sum_{0<\gamma_1\leqslant\gamma} T(\gamma_1,\gamma) + \sum_{0<\gamma_1\leqslant\gamma} T(\gamma_1,-\gamma) + \sum_{-\gamma<\gamma_2<\gamma} T(\gamma,\gamma_2) \\ &= T(\gamma,\gamma) + T(\gamma,-\gamma) + 2\sum_{-\gamma<\gamma_2<\gamma} T(\gamma,\gamma_2)\,. \end{aligned} \tag{23}$$

This may be seen by drawing a rectangle with vertices at $(0,\gamma)$, (γ,γ), $(\gamma,-\gamma)$, $(0,-\gamma)$, following the north, east and south edges, and using the symmetry $T(x,y) = T(y,x)$.

To show that $J(\gamma) > 0$, we split the last sum in (23) into three pieces, $A := (-\gamma, 0]$, $B := (0,(3-\sqrt{8})\gamma)$, and $C := [(3-\sqrt{8})\gamma,\gamma)$. This gives

$$\begin{aligned} J(\gamma) = {} & T(\gamma,\gamma) + T(\gamma,-\gamma) \\ & + 2\sum_{\gamma_2\in A} T(\gamma,\gamma_2) + 2\sum_{\gamma_2\in B} T(\gamma,\gamma_2) + 2\sum_{\gamma_2\in C} T(\gamma,\gamma_2). \end{aligned}$$

By Lemma 13, the sum with $\gamma_2 \in C$ consists only of positive terms, so

$$J(\gamma) \geqslant T(\gamma,\gamma) + T(\gamma,-\gamma) + 2\sum_{\gamma_2\in A} T(\gamma,\gamma_2) + 2\sum_{\gamma_2\in B} T(\gamma,\gamma_2). \tag{24}$$

We now show that the diagonal term $T(\gamma,\gamma)$ in (24) is positive, and sufficiently large to dominate the anti-diagonal term $T(\gamma,-\gamma)$ and the sums over A and B.

Lemma 14 *(Diagonal term). We have $T(\gamma,\gamma) \geqslant 1.99/\gamma^2$.*

Proof. Since $\gamma > 0$ is the ordinate of a nontrivial zero of $\zeta(s)$, we have $\gamma > 14$. Thus, using (22), we have $T(\gamma,\gamma) = 2/(\frac{1}{4}+\gamma^2) > 1.99/\gamma^2$. □

[4] For simplicity we assume here that all zeros of $\zeta(s)$ are simple, but one can modify the proofs in an obvious way to account for multiple zeros, if they exist.

Lemma 15 *(Anti-diagonal term and interval A). If c_3 is as in (20), then*

$$\frac{|T(\gamma,-\gamma)|}{2}+\sum_{-\gamma<\gamma_2<0}|T(\gamma,\gamma_2)|\leqslant\frac{16c_3}{\gamma^2}<\frac{0.37}{\gamma^2}\,.$$

Proof. Write (22) as $T(\gamma,\gamma_2)=N/D$, where the numerator is

$$N=2(1+6\gamma\gamma_2-\gamma^2-\gamma_2^2),\tag{25}$$

and the denominator is

$$D=(\tfrac{1}{4}+\gamma^2)(\tfrac{1}{4}+\gamma_2^2)(4+(\gamma-\gamma_2)^2)>\gamma^2\gamma_2^2(\gamma-\gamma_2)^2.\tag{26}$$

Thus, $N/2=1-(r^2-6r+1)\gamma^2$, where $r=\gamma_2/\gamma$. Now $r^2-6r+1\in[1,8]$ for $r\in[-1,0]$. Thus $N/2\in[1-8\gamma^2,1-\gamma^2]$, and $|N|<16\gamma^2$.

For the denominator, we have $D>\gamma^4\gamma_2^2(1-r)^2\in[\gamma^4\gamma_2^2,4\gamma^4\gamma_2^2]$, so $D>\gamma^4\gamma_2^2$. Combining the inequalities for N and D gives

$$|T(\gamma,\gamma_2)|<\frac{16}{\gamma^2\gamma_2^2}\,.$$

Now, summing over $\gamma_2<0$, and recalling the definition of c_3 in (20), gives the result. □

Lemma 16 *(Interval B). We have*

$$\sum_{0<\gamma_2<(3-\sqrt{8})\gamma}|T(\gamma,\gamma_2)|\leqslant\frac{(3+\sqrt{8})c_3}{2\gamma^2}<\frac{0.068}{\gamma^2}\,.$$

Proof. As in the proof of Lemma 15, write (22) as $T(\gamma,\gamma_2)=N/D$, where N and D are as in (25)–(26). Now $\gamma_2/\gamma<3-\sqrt{8}$, so $1-\gamma_2/\gamma>\sqrt{8}-2$, and $(\gamma-\gamma_2)^2>4(3-\sqrt{8})\gamma^2$. This gives

$$D>4(3-\sqrt{8})\gamma^4\gamma_2^2.$$

Also, $N/2=1-(r^2-6r+1)\gamma^2$, where $r=\gamma_2/\gamma\in[0,3-\sqrt{8}]$. Thus $0\leqslant r^2-6r+1\leqslant 1$ and $|N|\leqslant 2\gamma^2$. The inequalities for D and N give

$$|T(\gamma,\gamma_2)|<\frac{2\gamma^2}{4(3-\sqrt{8})\gamma^4\gamma_2^2}=\frac{3+\sqrt{8}}{2\gamma^2\gamma_2^2}\,.$$

Now, summing over $\gamma_2>0$ gives the result. □

Lemma 17. *$S(Y)$ is monotonic non-decreasing for $Y\in[0,\infty)$, with jumps of at least $1.11/\gamma^2$ at ordinates $\gamma>0$ of $\zeta(s)$.*

Proof. Using the inequality (24) and Lemmas 14–16, we have

$$J(\gamma) \geqslant \frac{1.99 - 2 \cdot 0.37 - 2 \cdot 0.068}{\gamma^2} > \frac{1.11}{\gamma^2} .$$

Thus, $S(Y)$ has positive jumps at ordinates $\gamma > 0$ of zeros of $\zeta(s)$, and is constant between these ordinates. □

Corollary 4. *Assume RH. For all $Y > 0$, we have $c_2 > S(Y)$.*

Proof. This follows as $S(Y)$ is monotonic non-decreasing with limit c_2, and has positive jumps at arbitrarily large Y. □

Corollary 5. *Assume RH. Then $c_1 < c_2$.*

Proof. Take $Y = 70$ in Corollary 4. Computing $S(70)$, which involves a double sum over first 17 nontrivial zeros in the upper half-plane, gives a lower bound $c_2 > S(70) > 0.0466$. Since $c_1 < 0.0462$, the result follows. □

Remark 4. RH is probably not necessary for Corollary 5. Any exceptional zeros off the critical line must have large height, and consequently they would make little difference to the numerical values of c_1 and c_2.

Remark 5. Taking $Y = 74\,920.83$ in Corollary 4, and using the first 10^5 zeros of $\zeta(s)$, we obtain

$$c_2 > S(Y) > 0.104004 \text{ and } c_2 - c_1 > 0.0578 .$$

This is much stronger than the bound used in the proof of Corollary 5, though at the expense of more computation. Our best estimate, using an integral approximation for the higher zeros, is $c_2 \approx 0.10446$.

5.4. Non-existence of a limit

First we prove a result analogous to Theorem 4, but with lim sup replaced by lim inf. Then we deduce that neither $I(X)/X^2$ nor $J(X)/X^2$ has a limit as $X \to \infty$.

Theorem 5. *Assume RH. With $J(X)$ as in (17) and c_1 as in (18),*

$$\liminf_{X\to\infty} \frac{2J(X)}{X^2} \leqslant c_1.$$

Proof. Define

$$F(X) := \int_1^X (\psi(x) - x)^2 \, dx = J(X) - J(1), \text{ and}$$

$$G(X) := \int_1^X (\psi(x) - x)^2 \, \frac{dx}{x^2} \sim c_1 \log X.$$

Here the asymptotic result is given in [8, Ex. 13.1.1.3], which follows from [8, Thm. 13.6] after a change of variables $x = \exp(u)$. Using integration by parts, we obtain

$$G(X) = \frac{F(X)}{X^2} + 2 \int_1^X F(x) \, \frac{dx}{x^3} \, .$$

Now $F(X) \ll X^2$, so

$$2 \int_1^X F(x) \, \frac{dx}{x^3} \sim G(X) \sim c_1 \log X \text{ as } X \to \infty.$$

Dividing by $2 \log X$ gives

$$\int_1^X \frac{F(x)}{x^2} \, \frac{dx}{x} \Big/ \int_1^X \frac{dx}{x} \sim \frac{c_1}{2} \text{ as } X \to \infty. \tag{27}$$

Now, if $F(x)/x^2 \geqslant c_1/2 + \varepsilon$ for some positive ε and all sufficiently large x, we get a contradiction to (27). Thus, letting $\varepsilon \to 0$, we obtain the result. $\square$

Corollary 6. *With $J(X)$ as in (17), $\lim_{X\to\infty} \dfrac{J(X)}{X^2}$ does not exist.*

Proof. The result holds if RH is false. Hence, assume RH. From Corollary 5, $c_1 < c_2$, so the result is implied by Theorems 4 and 5. $\square$

We conclude by showing the non-existence of $\lim_{X\to\infty} I(X)X^{-2}$, thereby proving Theorem 2. Suppose, on the contrary, that the limit exists. Now, from the definitions (2) and (17), we have

$$\frac{J(X)}{X^2} = \sum_{k=1}^{\infty} \frac{I(X/2^k)}{X^2} = \sum_{k=1}^{\infty} 4^{-k} \frac{I(X/2^k)}{(X/2^k)^2} \, ,$$

and the series converge since the k-th terms are $O(4^{-k})$. Hence there exists $\lim_{X\to\infty} J(X)/X^2$, but this contradicts Corollary 6. Thus, our original assumption is false, and the result follows.

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References

[1] R.J. Backlund, Über die Nullstellen der Riemannschen Zetafunktion, Acta Math. 41 (1918) 345–375.
[2] R.P. Brent, D.J. Platt, T.S. Trudgian, A harmonic sum over the ordinates of nontrivial zeros of the Riemann zeta-function, Bull. Aust. Math. Soc. 104 (1) (2021) 59–65.
[3] H. Cramér, Ein Mittelwertsatz in der Primzahltheorie, Math. Z. 12 (1922) 147–153.
[4] P. Demichel, Y. Saouter, T. Trudgian, A still sharper region where $\pi(x) - \mathrm{li}(x)$ is positive, Math. Comput. 84 (295) (2015) 2433–2446.
[5] E. Hasanalizade, Q. Shen, P.-J. Wong, Counting zeros of the Riemann zeta function, J. Number Theory 235 (2022) 219–241.
[6] M. Hassani, Explicit approximation of the sums over the imaginary part of the non-trivial zeros of the Riemann zeta function, Appl. Math. E-Notes 16 (2016) 109–116.
[7] R.S. Lehman, On the difference $\pi(x) - \mathrm{li}(x)$, Acta Arith. 11 (1966) 397–410.
[8] H. Montgomery, R.C. Vaughan, Multiplicative Number Theory. I. Classical Theory, Cambridge Studies in Advanced Mathematics, vol. 97, Cambridge University Press, Cambridge, 2007.
[9] D. Patel, An explicit upper bound for $|\zeta(1 + it)|$, submitted for publication, preprint available at arXiv:2009.00769v1.
[10] J. Pintz, On the remainder term of the prime number formula VI. Ineffective mean value theorems, Studia Sci. Math. Hung. 15 (1980) 225–230.
[11] J. Pintz, On the remainder term of the prime number formula and the zeros of Riemann's zeta-function, in: Number Theory, Noordwijkerhout, 1983, in: Lecture Notes in Mathematics, vol. 1068, Springer-Verlag, Berlin, 1984.
[12] J. Pintz, On the mean value of the remainder term of the prime number formula, in: Elementary and Analytic Theory of Numbers, Warsaw, 1982, in: Banach Center Publ., vol. 17, PWN, Warsaw, 1985, pp. 411–417.
[13] D.J. Platt, T.S. Trudgian, An improved explicit bound on $|\zeta(\frac{1}{2} + it)|$, J. Number Theory 147 (2015) 842–851.
[14] J.B. Rosser, Explicit bounds for some functions of prime numbers, Am. J. Math. 63 (1941) 211–232.
[15] A. Simonič, On explicit estimates for $S(t)$, $S_1(t)$, and $\zeta(1/2 + it)$ under the Riemann hypothesis, J. Number Theory 231 (2022) 464–491.
[16] S.B. Stechkin, A.Yu. Popov, The asymptotic distribution of prime numbers on the average, Russ. Math. Surv. 51 (6) (1996) 1025–1092.
[17] E.C. Titchmarsh, The Theory of the Riemann Zeta-Function, 2nd edition, Oxford Univ. Press, New York, 1986, edited and with a preface by D. R. Heath-Brown.
[18] T. Trudgian, An improved upper bound for the argument of the Riemann zeta-function on the critical line, Math. Comput. 81 (278) (2012) 1053–1061.
[19] T.S. Trudgian, An improved upper bound for the argument of the Riemann zeta-function on the critical line, II, J. Number Theory 134 (2014) 280–292.