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Sharper Bounds for the Chebyshev Functions $\theta(x)$ and $\psi(x)$

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Abstract. The authors demonstrate a wider zero-free region for the Riemann zeta function than has been given before. They give improved methods for using this and a recent determination that the first 3,502,500 zeros lie on the critical line to develop better bounds for functions of primes.

0. Introduction. As this paper is dedicated to D. H. Lehmer on the occasion of his 70th birthday, it is particularly appropriate to remark on Lehmer's long time interest in the application of numerical computation to problems in number theory. In particular, his papers [1956A, 1956B] reporting that the first 25,000 zeros of the Riemann function $\zeta(s)$ lie on the critical line led the way in the application of modern computing machinery to the study of the zeros of this function. In default of a proof of the Riemann hypothesis, the best estimates for $\psi(x)$ and $\theta(x)$, and hence of $\pi(x)$, p_n and other functions of the primes, depend on the current state of knowledge of the zeros of $\zeta(s)$.

The present paper is devoted to obtaining improved estimates for $\psi(x)$, the logarithm of the least common multiple of all integers not exceeding x, and $\theta(x)$, the logarithm of the product of all primes not exceeding x. We reserve for another paper the application of these results to $\pi(x)$ and p_n, simply remarking here that they permit the deduction of such inequalities as $\pi(2x) < 2\pi(x)$ for all $x \geqslant 11$ and $\theta(p_n) > n \log n$ for all $n \geqslant 13$. We are also able to show $(p_1 + p_2 + \cdots + p_n)/n < \frac{1}{2}p_n$ for $n \geqslant 9$, as conjectured by Robert Mandl.

To a considerable extent, this paper represents an up-to-date version of part of Rosser and Schoenfeld [1962], which will hereafter be cited as R–S. We also make considerable use of Rosser [1941]. We assume familiarity with these papers, and shall use notation and results from them freely.

Rosser, Yohe and Schoenfeld [1969]** announced that the first 3,500,000 zeros of $\zeta(s)$ lie on the critical line. By applying the stronger result contained in Theorem 4 of Lehman [1970], we are now able to show that the first 3,502,500 zeros are on the line. Our computations extended out to Gram No. 3,502,504; between here and the smaller Gram No. 3,502,483, $\zeta(s)$ behaves very regularly so that all of the Gram

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**We take the opportunity to correct a misprint on line 5, p. 71 of this paper. The coefficient of $\tau^{-7/4}$ given there should be 2.28 instead of 2.88.

numbers in this interval separate the zeros of $\zeta(s)$. Letting $N(T)$ be the number of zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ such that $0 < \gamma \leqslant T$, there is an approximation $F(T)$ to $N(T)$ given in Rosser [1941, p. 223]. We define A as the unique solution of $F(A) =$ 3,502,500; the calculations of Rosser, Yohe and Schoenfeld establish that $N(A) =$ 3,502,500 so that $N(A) = F(A)$. We note

$$\log A = 14.45443\ 30529\ 858 \cdots, \qquad A = 18\ 94438.51224 \cdots. \tag{0.1}$$

Throughout this paper, the inequality sign is used in the strict mathematical sense; if $A < B$ is written, where A and B contain approximations, then with the indicated approximations the inequality does indeed hold. We have not always given the very best bounding decimal approximation but have frequently given less strict (but correct) bounds which are easier to verify. We occasionally use the sign $\cong$ to indicate approximate equality with the approximations being accurate to 1 or 2 units in the least significant digit shown. Finally, we use $\bar{z}$ to denote the complex conjugate of z, $\Re z$ to denote the real part of z, and $\Im z$ to denote the imaginary part of z.

It is our pleasure to express our thanks to John W. Wrench, Jr. of the U.S. Navy Carderock Laboratory for the computations he performed for us. We also wish to thank Dianne Hollenbeck and Emerson Mitchell of the Mathematics Research Center for their help with calculations.

1. A Zero-Free Region for $\zeta(s)$. In this section we give such a region whose form is essentially that of the classical one of de la Vallée-Poussin. The result, stated in Theorem 1, is substantially better than the corresponding result, Theorem 26 of R–S. The improvement is due primarily to the work of Stechkin [1970B] with other improvements resulting from a better nonnegative cosine polynomial and from the knowledge that all zeros $\rho = \beta + i\gamma$ of $\zeta(s)$ for which $0 < |\gamma| \leqslant A$ lie on the critical line. Although better asymptotic zero-free regions are known from the work of Vinogradov and others, these regions only become wider at heights beyond the main interest of this paper.

We begin with the following result suggested by the work of Stechkin [1970B].

LEMMA 1. *Let* $s = \sigma + it$ *and* $s_0 = \sigma_0 + it$ *where* $\sigma_0 \geqslant \sigma > 1$. *Let*

$$\mu = \frac{\sigma_0(\sigma_0 - 1)}{(2\sigma_0 - 1)\sigma}, \qquad \lambda = (2\sigma - 1)\min\left\{\frac{\mu}{\sigma}, \frac{1}{2\sigma_0 - 1}\right\},$$

and $0 \leqslant \Re b \leqslant 1$. *Then*

$$\Re\left(\frac{1}{s - b} + \frac{1}{s - 1 + \bar{b}}\right) \geqslant \lambda \Re\left(\frac{1}{s_0 - b} + \frac{1}{s_0 - 1 + \bar{b}}\right). \tag{1.1}$$

If, in addition, $\Im b = t$, *then*

$$\min\left\{\Re\frac{1}{s - b}, \Re\frac{1}{s - 1 + \bar{b}}\right\} \geqslant \mu \Re\left(\frac{1}{s_0 - b} + \frac{1}{s_0 - 1 + \bar{b}}\right). \tag{1.2}$$

Proof. Let $\alpha = \Re b$. For (1.1), it suffices to deal with $0 \leqslant \alpha \leqslant \frac{1}{2}$, since otherwise we consider $b' = 1 - \bar{b}$. Let Q be the quotient of the left side of (1.1) by the real part on the right side of (1.1). Replacing τ in the proof of Lemma 2 of Stechkin [1970B] by $\sigma_0 \geqslant \sigma$, we find that

$$Q \geqslant \frac{2\sigma - 1}{F(\alpha, t^2)} \geqslant \frac{2\sigma - 1}{\max\{F(\alpha, 0), F(\alpha, \infty)\}} = \frac{2\sigma - 1}{\max\{\phi(\alpha), 2\sigma_0 - 1\}},$$

where $F(\alpha, u)$ and $\phi(\alpha)$ are as defined by Stechkin. Inasmuch as

$$\phi(\alpha) = (2\sigma_0 - 1) \cdot \frac{\sigma - \alpha}{\sigma_0 - \alpha} \cdot \frac{\sigma - \alpha}{\sigma_0 - 1 + \alpha} \leqslant \phi(0) = \frac{\sigma}{\mu},$$

we see that $Q \geqslant \lambda$ so that (1.1) holds.

To obtain (1.2), it suffices to prove it with the left side replaced by $R1/(s - b) = 1/(\sigma - \alpha)$. The quotient of this by the real part on the right side of (1.2) is $1/\phi_1(\alpha)$ where

$$\phi_1(\alpha) = \frac{\sigma - \alpha}{\sigma_0 - \alpha} + \frac{\sigma - \alpha}{\sigma_0 - 1 + \alpha} \leqslant \phi_1(0) = \frac{1}{\mu}.$$

This completes the proof of (1.2), which is essentially Remark 2 of Lemma 2 of Stechkin [1970B].

We define for $\sigma > 1$

$$\sigma_0 = \tfrac{1}{2}(\sqrt{8\sigma^2 - 4\sigma + 1} + 1), \tag{1.3}$$

$$\kappa_0 = \frac{2\sigma - 1}{2\sigma_0 - 1} = \left\{\frac{1}{2} - \frac{1}{4\sigma - 1 + 1/(4\sigma - 1)}\right\}^{1/2}. \tag{1.4}$$

Then

$$\lambda = \mu = \kappa_0 > 1/\sqrt{5}, \qquad \sigma_0 > \sigma. \tag{1.5}$$

For $0 < x \leqslant 0.03$ we easily verify that

$$\sqrt{5} < \sqrt{5 + 12x + 8x^2} < \sqrt{5} + 2.68847x;$$

putting $x = \sigma - 1$ and assuming $1 < \sigma \leqslant 1.03$, we get

$$\tau < \sigma_0 = \tfrac{1}{2}\sqrt{5 + 12x + 8x^2} + \tfrac{1}{2} < \tau + 1.34424(\sigma - 1) < 1.659, \tag{1.6}$$

where $\tau = \tfrac{1}{2}(\sqrt{5} + 1)$ is the golden ratio. Also

$$\kappa_0 < 0.458 \quad \text{if} \quad \sigma \leqslant 1.03. \tag{1.7}$$

If $0 < x \leqslant 1$, then

$$\begin{aligned}
&(5 + 12x + 8x^2)\left(1 + \frac{4}{5}x\right)^2\left(1 - \frac{26}{25}x^2\right)^2 \\
&= \left(5 + 20x + \frac{152}{5}x^2 + \frac{512}{25}x^3 + \frac{128}{25}x^4\right)\left(1 - \frac{26}{25}x^2\right)^2 \\
&\leqslant 5 + 20x + 20x^2 - 21x^3 - 52x^4 - 20x^5 + 23x^6 + 23x^7 + 6x^8 \\
&< 5 + 20x + 20x^2 = 5(1 + 2x)^2.
\end{aligned}$$

If $1 < \sigma \leqslant 1.03$ and $x = \sigma - 1$, then

$$\kappa_0 = \frac{1+2x}{\sqrt{5+12x+8x^2}} > \frac{1}{\sqrt{5}}\left(1+\frac{4}{5}x\right)\left(1-\frac{26}{25}x^2\right) \geqslant \frac{1}{\sqrt{5}}\left\{1+\frac{4}{5}(\sigma-1)-1.06496(\sigma-1)^2\right\}. \tag{1.8}$$

The following is the principal result needed for the proof of Theorem 1.

LEMMA 2. *Let* $P(\theta) = \Sigma_{k=0}^{n} a_k \cos k\theta$ *be such that all* $a_k \geqslant 0$ *and* $P(\theta) \geqslant 0$ *for all real* θ. *If* $\beta + i\gamma$ *is a nontrivial zero of* $\zeta(s)$ *such that* $\beta \neq ½$ *and* $1 < \sigma \leqslant 1.03$, *then*

$$\frac{a_1}{\sigma-\beta} - \frac{a_0}{\sigma-1} < \frac{1-\kappa_0}{2} A_0 \log|\gamma| + B + 0.187\,6352\, a_0(\sigma-1) + \frac{17}{3\gamma^2}\sum_{k=1}^{n}\frac{a_k}{k^2}, \tag{1.9}$$

where C *is the Euler-Mascheroni constant, and*

$$A_0 = a_1 + a_2 + \cdots + a_n, \qquad B = a_0\left(\kappa_0 \frac{\zeta'(\sigma_0)}{\zeta(\sigma_0)} - C\right) - \frac{1-\kappa_0}{2}\sum_{k=1}^{n} a_k \log\frac{2\pi}{k}.$$

Proof. Using the series for $\zeta'(s)/\zeta(s)$ we get

$$\sum_{k=0}^{n} a_k R\left\{\kappa_0 \frac{\zeta'}{\zeta}(\sigma_0 + ikt) - \frac{\zeta'}{\zeta}(\sigma + ikt)\right\} = \sum_{m=2}^{\infty} \frac{\Lambda(m)}{m^\sigma}\left(1 - \frac{\kappa_0}{m^{\sigma_0 - \sigma}}\right) P(t\log m) \geqslant 0. \tag{1.10}$$

From Landau [1909, pp. 316–317], we get

$$\frac{\zeta'(s)}{\zeta(s)} = b - \frac{1}{s-1} - \frac{1}{2}\frac{\Gamma'}{\Gamma}\left(\frac{s}{2}+1\right) + T(s), \tag{1.11}$$

where

$$b = \log(2\pi) - 1 - ½C, \tag{1.12}$$

$$T(s) = \sum_\rho \left(\frac{1}{s-\rho} + \frac{1}{\rho}\right), \tag{1.13}$$

where ρ runs over the nontrivial zeros of $\zeta(s)$.

For real $s = \sigma$, we see from (1.11) that $T(\sigma)$ is real and hence is given by

$$T(\sigma) = \sum_\rho R\left(\frac{1}{\sigma-\rho} - \frac{1}{1-\rho}\right) + \sum_\rho R\frac{1}{1-\rho} + \sum_\rho R\frac{1}{\rho}. \tag{1.14}$$

As $1 - \bar{\rho}$ runs through all the nontrivial zeros of $\zeta(s)$ exactly once when $\rho = \beta + i\gamma$ does, we obtain from Rosser [1939, p. 29]

$$\sum_\rho R\frac{1}{1-\rho} = \sum_\rho R\frac{1}{1-(1-\bar{\rho})} = \sum_\rho R\frac{1}{\rho} = \sum_\rho \frac{\beta}{\beta^2+\gamma^2} = \frac{2+C-\log(4\pi)}{2} \tag{1.15}$$

Moreover, for $1 < \sigma \leqslant 1.03$, a typical term $G(\rho)$ of the first sum in (1.14) is

$$G(\rho) = \frac{\sigma - \beta}{(\sigma - \beta)^2 + \gamma^2} - \frac{1 - \beta}{(1 - \beta)^2 + \gamma^2} = \frac{(\sigma - 1)\{\gamma^2 - (\sigma - \beta)(1 - \beta)\}}{\{(\sigma - \beta)^2 + \gamma^2\}\{(1 - \beta)^2 + \gamma^2\}}$$
$$\geqslant \frac{\sigma - 1}{\gamma^2 + (1 - \beta)^2} \cdot \frac{\gamma^2 - (1.03 - \beta)(1 - \beta)}{\gamma^2 + (1.03 - \beta)^2}.$$

If $\beta = ½$, then since $|\gamma| > 14.13\,4725$ we easily get

$$G(\rho) > 0.997\,2714 \frac{\sigma - 1}{\gamma^2 + (1 - \beta)^2} = 0.997\,2714\,(\sigma - 1)\, R\left(\frac{1}{\rho} + \frac{1}{1 - \bar{\rho}}\right).$$

If $\beta \neq ½$, then $|\gamma| > A$; as $\gamma^2 R\{1/\rho + 1/(1 - \bar{\rho})\} < 1$ always holds, we have

$$G(\rho) > (\sigma - 1)\, R\left(\frac{1}{\rho} + \frac{1}{1 - \bar{\rho}}\right) \cdot \frac{\gamma^2(\gamma^2 - 1.03)}{(\gamma^2 + 1)(\gamma^2 + 1.03^2)}$$
$$> 0.9973\,(\sigma - 1) R\left(\frac{1}{\rho} + \frac{1}{1 - \bar{\rho}}\right).$$

Hence the first sum in (1.14) exceeds

$$0.997\,2714\,(\sigma - 1) \cdot 2 \sum_\rho R\, \frac{1}{\rho} > 0.0460\,6537\,(\sigma - 1)$$

by (1.15). Consequently, (1.11), (1.14), (1.15) and (1.12) yield

(1.16) $$-\frac{\zeta'(\sigma)}{\zeta(\sigma)} < \frac{1}{\sigma - 1} + \frac{1}{2}\,\psi\left(\frac{\sigma}{2} + 1\right) - 1 - \frac{1}{2}C + \log 2 - 0.0460\,6537(\sigma - 1),$$

where $\psi(s) = \Gamma'(s)/\Gamma(s)$. By the law of the mean, there is a $\xi \in (3/2, ½\sigma + 1)$ such that

$$\psi(½\sigma + 1) - \psi(3/2) = ½(\sigma - 1)\psi'(\xi) = ½(\sigma - 1) \sum_{n=1}^{\infty} (n + \xi - 1)^{-2}$$
$$< ½(\sigma - 1) \sum_{n=1}^{\infty} (n + ½)^{-2} = \{(\pi^2/4) - 2\}(\sigma - 1),$$

as a result of a standard formula for $\psi(s)$; cf. Whittaker and Watson [1940, p. 241]. Using $\psi(3/2) = 2 - C - \log 4$ from Rosser [1939, p. 29] and (1.16), we obtain

(1.17) $$-\zeta'(\sigma)/\zeta(\sigma) < 1/(\sigma - 1) - C + 0.187\,6352\,(\sigma - 1).$$

Next, putting $s_0 = \sigma_0 + it$ and $s = \sigma + it$, (1.11) yields

$$R\left\{\kappa_0 \frac{\zeta'}{\zeta}(\sigma_0 + it) - \frac{\zeta'}{\zeta}(\sigma + it)\right\}$$

(1.18) $$= (\kappa_0 - 1)b - R\left(\frac{\kappa_0}{s_0 - 1} - \frac{1}{s - 1}\right) - \frac{\kappa_0}{2}\, R\psi\left(\frac{s_0}{2} + 1\right)$$
$$+ \frac{1}{2}\, R\psi\left(\frac{s}{2} + 1\right) + \sum_\rho R\left(\frac{\kappa_0}{s_0 - \rho} - \frac{1}{s - \rho} + \frac{\kappa_0 - 1}{\rho}\right).$$

For $|t| \geqslant 1$, we have by (1.5) and (1.6)

(1.19)
$$\begin{aligned} R\left(\frac{\kappa_0}{s_0-1}-\frac{1}{s-1}\right) &> R\,\frac{1}{s_0-1}\left\{\frac{1}{\sqrt{5}}-\frac{\sigma-1}{\sigma_0-1}\cdot\frac{(\sigma_0-1)^2+t^2}{(\sigma-1)^2+t^2}\right\} \\ &\geqslant R\,\frac{1}{s_0-1}\left\{\frac{1}{\sqrt{5}}-\frac{0.03}{\tau-1}\cdot\frac{0.44+t^2}{t^2}\right\}>0. \end{aligned}$$

By (4) on p. 113 of Edwards [1974], we obtain for $\sigma \geqslant 0 \neq t$,

$$\left|\frac{\Gamma'(s)}{\Gamma(s)}-\log s+\frac{1}{2s}\right| \leqslant \frac{1}{12|s|^2}+\frac{1}{6}\int_0^\infty \frac{dx}{\{(\sigma+x)^2+t^2\}^{3/2}} \leqslant \frac{1}{4t^2}.$$

Hence, if $2 \geqslant \sigma \geqslant 0 \neq t$, there is a $\theta_0 \in (-5/9, 1)$ such that $R\psi(s) = \log|t| + 9\theta_0/(4t^2)$. As a result, if $1 < \sigma \leqslant 1.03$ and $t \neq 0$, then for suitable $\theta_1, \theta_2 \in (-5/9, 1)$

$$\begin{aligned} &-\frac{\kappa_0}{2}\,R\psi\left(\frac{s_0}{2}+1\right)+\frac{1}{2}R\psi\left(\frac{s}{2}+1\right) \\ &\qquad =\frac{1-\kappa_0}{2}\,\log\left|\frac{t}{2}\right|+\frac{9}{2t^2}\,(\theta_2-\theta_1\kappa_0) < \frac{1-\kappa_0}{2}\,\log\left|\frac{t}{2}\right|+\frac{5.65}{t^2} \end{aligned}$$

by (1.7). Using (1.18) and (1.19), we see that for $|t| \geqslant 1$

(1.20)
$$\begin{aligned} &R\left\{\kappa_0\frac{\zeta'}{\zeta}(\sigma_0+it)-\frac{\zeta'}{\zeta}(\sigma+it)\right\} \\ &\qquad < \frac{1-\kappa_0}{2}\log|t|-(1-\kappa_0)\left\{b+\sum_\rho R\frac{1}{\rho}+\frac{1}{2}\log 2\right\}+\frac{17}{3\gamma^2}+U, \end{aligned}$$

where

(1.21)
$$\begin{aligned} U &= \sum_\rho\left\{\kappa_0 R\,\frac{1}{s_0-\rho}-R\,\frac{1}{s-\rho}\right\} \equiv \sum_\rho H(\rho) = \frac{1}{2}\sum_\rho H(\rho)+\frac{1}{2}\sum_\rho H(1-\bar\rho) \\ &= \frac{1}{2}\sum_\rho\left\{\kappa_0 R\left(\frac{1}{s_0-\rho}+\frac{1}{s_0-1+\bar\rho}\right)-R\left(\frac{1}{s-\rho}+\frac{1}{s-1+\bar\rho}\right)\right\}. \end{aligned}$$

By (1.1), every term in the last sum is nonpositive. As a result of (1.12) and (1.15), (1.20) becomes for $|kt| \geqslant 1$

(1.22)
$$R\left\{\kappa_0\frac{\zeta'}{\zeta}(\sigma_0+ikt)-\frac{\zeta'}{\zeta}(\sigma+ikt)\right\} < \frac{1-\kappa_0}{2}\log|t|-\frac{1-\kappa_0}{2}\log\frac{2\pi}{k}+\frac{17}{3k^2t^2}.$$

Now let $\rho_0 = \beta_0 + i\gamma_0$ be a nontrivial zero of $\zeta(s)$ such that $\beta_0 \neq \tfrac{1}{2}$. In (1.21) set $t = \gamma_0$ and consider the two terms arising from the distinct values $\rho = \rho_0$, ρ_0' where $\rho_0' = 1 - \bar\rho_0$; in both cases $I\rho = \gamma_0$. By (1.2) the summand for ρ_0 does not exceed $-R1/(s-\rho_0)$, namely $-1/(\sigma-\beta_0)$; likewise, the summand for ρ_0' does not exceed $-R1/(s-1+\bar\rho_0')$, namely $-1/(\sigma-\beta_0)$ also. As a result, we get $U \leqslant -1/(\sigma-\beta_0)$. Consequently, (1.20) becomes

$$R\left\{\kappa_0 \frac{\zeta'}{\zeta}(\sigma_0 + i\gamma_0) - \frac{\zeta'}{\zeta}(\sigma + i\gamma_0)\right\} \tag{1.23}$$
$$< \frac{1-\kappa_0}{2}\log|\gamma_0| - \frac{1-\kappa_0}{2}\log(2\pi) + \frac{17}{3\gamma_0^2} - \frac{1}{\sigma - \beta_0}.$$

We now obtain (1.9) with β_0, γ_0 in place of β, γ by using (1.10) with $t = \gamma_0$, (1.17), (1.22) with $t = \gamma_0$ and $2 \leqslant k \leqslant n$, and finally (1.23). This completes the proof.

We note that by the law of the mean there is a $\xi \in (\tau, \sigma_0)$ such that for $1 \leqslant \sigma \leqslant 1.03$.

$$\frac{\zeta'}{\zeta}(\sigma_0) - \frac{\zeta'}{\zeta}(\tau) = (\sigma_0 - \tau)\left\{\frac{d}{ds}\frac{\zeta'}{\zeta}(s)\right\}_{s=\xi} \tag{1.24}$$
$$\leqslant (\sigma_0 - \tau)\left\{\frac{d}{ds}\frac{\zeta'}{\zeta}(s)\right\}_{s=\tau} < 3.33493(\sigma - 1),$$

as a result of (1.6) and the value

$$\left\{\frac{d}{ds}\frac{\zeta'}{\zeta}(s)\right\}_{s=\tau} = 2.48089\ 75061 \cdots$$

supplied to us by John W. Wrench, Jr., who has computed this quantity to more than 40 decimals. Wrench has also given more than 40 decimals for

$$\zeta'(\tau)/\zeta(\tau) = -1.13991\ 58683 \cdots,$$

which, taken in conjunction with (1.24), yields for $1 < \sigma \leqslant 1.03$

$$\zeta'(\sigma_0)/\zeta(\sigma_0) < -1.139\ 9158 + 3.33493(\sigma - 1). \tag{1.25}$$

Wrench computed these values by using the power series expansions about $s = 1$ of $(s-1)\zeta(s)$ and its first two derivatives. His values have been confirmed by an independent calculation by Herman Robinson. In addition, the values appearing in (1.25) have been again confirmed by a less extensive, and independent, calculation by Emerson Mitchell of the Mathematics Research Center, based on a table of values of $\zeta(\sigma)$ supplied by Livermore Laboratories.

In Theorem 1 below, we apply these results and Lemma 2 to establish a zero-free region for $\zeta(s)$, which is of the kind $\beta \geqslant 1 - 1/(R_1 \log|\gamma|)$, by choosing the σ of Lemma 2 to be about $1 + \nu/\log|\gamma|$ where

$$\nu = \frac{2\sqrt{a_0}(\sqrt{a_1} - \sqrt{a_0})}{(1 - 1/\sqrt{5})A_0}, \quad R_0 = \frac{A_0}{2(\sqrt{a_1} - \sqrt{a_0})^2}, \quad R_1 = \left(1 - \frac{1}{\sqrt{5}}\right)R_0 \tag{1.26}$$

provided $a_1 > a_0 > 0$. It can be shown that this value of ν is optimal, and it is therefore important to select $P(\theta)$ so that R_0 is minimal. For fourth-degree polynomials, R_0 appears to be minimal for $P(\theta) = 8(a + \cos\theta)^2\,(b + \cos\theta)^2$ where (according to calculations by Dianne Hollenbeck of the Mathematics Research Center)

$$a \cong 0.9126\ 08743, \qquad b \cong 0.2766\ 14921.$$

For the choices

$$a = 0.9126\ 0875, \qquad b = 0.2766\ 1490,$$

we obtained a value $R_0 = 17.449\ 61294\ 38363 \cdots$. An extensive computer search by Emerson Mitchell of the Mathematics Research Center failed to find a fifth-or sixth-degree cosine polynomial giving a smaller value for R_0. Further, the work of French [1966] shows that, regardless of the degree of $P(\theta)$, $R_0 > 16.2568$; for other results concerning $P(\theta)$ see also Stechkin [1970A], who essentially shows, for example, that for fourth-degree polynomials $R_0 > 17.174\ 8395$.

To simplify the calculations, we choose $a = 0.9126$ and $b = 0.2766$, which yield

$$a_0 = 11.185\ 93553\ 12082\ 048, \qquad a_1 = 19.073\ 34400\ 4352,$$
$$a_2 = 11.676\ 18784, \qquad a_3 = 4.7568, \qquad a_4 = 1,$$
$$A_0 = 36.506\ 33184\ 4352, \qquad R_0 = 17.449\ 61294\ 58 \cdots,$$
$$\sum_{k=1}^{4} a_k \log(2\pi/k) > 52.38865, \qquad \sum_{k=1}^{4} a_k/k^2 < 22.584.$$

The preceding value of R_0 is smaller by about 0.00014 than a value given by Stechkin [1970B]. Prior to this work of Stechkin, zero-free regions of the present kind had R_1 replaced by the larger R_0. The result below improves Stechkin's Theorem 2 not only by having a smaller value for R but also by the presence of the denominator 17.

THEOREM 1. *There are no zeros of* $\zeta(s)$ *in the region*

$$\sigma \geqslant 1 - 1/(R \log|t/17|), \qquad |t| \geqslant 21, \tag{1.27}$$

where $R = 9.6459\ 08801$.

Proof. First, suppose $\beta + i\gamma$ is a nontrivial zero of $\zeta(s)$ such that $\beta \neq ½$; then $|\gamma| > A$. We assume that $1 < \sigma \leqslant 1.03$ so that by (1.7) the coefficient of $\Sigma_{k=1}^{4} a_k \log(2\pi/k)$ in the expression for B is negative; hence this sum can be replaced by its lower bound 52.38865. We also replace $\zeta'(\sigma_0)/\zeta(\sigma_0)$ by its upper bound given in (1.25). As the resulting total coefficient of κ_0 in (1.9) is negative, we may replace κ_0 by the right side of (1.8). With ν defined by (1.26), we set

$$x = \sigma - 1 = \nu/\log|\gamma/17|$$

and observe that $0 < x < 0.029172$ since $|\gamma| > A$; hence $1 < \sigma < 1.03$. On noting that $(\sigma - 1)\log|\gamma| = \nu + x\log 17$, a calculation shows that (1.9) yields

$$\frac{a_1}{\sigma - \beta} - \frac{a_0}{\sigma - 1} < \frac{1}{2}\left(1 - \frac{1}{\sqrt{5}}\right)A_0 \log|\gamma| - 28.85290 + 8.0365x + 31.574x^2 - 17.76x^3$$
$$< \frac{1}{2}\left(1 - \frac{1}{\sqrt{5}}\right)A_0 \log|\gamma/17|.$$

Hence

$$\frac{a_1}{\sigma - \beta} < \frac{a_0}{\nu}\log\left|\frac{\gamma}{17}\right| + \frac{1}{2}\left(1 - \frac{1}{\sqrt{5}}\right)A_0 \log\left|\frac{\gamma}{17}\right| = R_1(\sqrt{a_1} - \sqrt{a_0})\sqrt{a_1}\,\log\left|\frac{\gamma}{17}\right|.$$

From this we easily get

$$\beta < 1 - 1/(R_1 \log|\gamma/17|). \tag{1.28}$$

Second, if $\beta = ½$ and $|\gamma| \geqslant 21$, then (1.28) clearly holds. Finally, as $R_1 < R$, the proof is complete.

2. Estimates for Certain Integrals Related to the Bessel Functions. In subsequent sections, there appear integrals of the form

$$K_\nu(z, x) = \frac{1}{2}\int_x^\infty t^{\nu-1} H^z(t)\, dt \tag{2.1}$$

where $z > 0, x \geqslant 0$ and

$$H^z(t) = \{H(t)\}^z = \exp\{-½ z\,(t + 1/t)\}. \tag{2.2}$$

The substitution $t = e^w$ shows that

$$K_\nu(z, 0) = K_\nu(z) \tag{2.3}$$

in accordance with a standard notation for the modified Bessel functions of the second kind; see [NBS #55, p. 376, 9.6.24]. Tabulations for some values of ν and other means of calculation for $K_\nu(z)$ are given in Chapter 9 of NBS #55.

Note that $K_\nu(z, x)$ has the form of (24) on p. 600 of Rosser [1955]. The techniques of that paper can be used to derive estimates for $K_\nu(z, x)$ for large z.

LEMMA 3. $K_\nu(z, x) + K_{-\nu}(z, 1/x) = K_\nu(z)$.

Proof. Put $t = 1/u$ in the definition of $K_{-\nu}(z, 1/x)$.

LEMMA 4. *If* $1 \geqslant \nu, 0 < z,$ *and* $1 < x,$ *we have*

$$\left(1 + 2\frac{(\nu+1)x - (\nu-1)x^3}{z(x^2-1)^2}\right)^{-1} Q_\nu(z, x) < K_\nu(z, x) < Q_\nu(z, x), \tag{2.4}$$

where

$$Q_\nu(z, x) = x^{\nu+1} H^z(x)/\{z(x^2-1)\}. \tag{2.5}$$

Proof. Integration by parts yields

$$K_\nu(z, x) = Q_\nu(z, x) - \frac{1}{z}\int_x^\infty \frac{(\nu+1)t^\nu - (\nu-1)t^{\nu+2}}{(t^2-1)^2} H^z(t)\, dt. \tag{2.6}$$

We have

$$\frac{(\nu+1)t - (\nu-1)t^3}{(t^2-1)^2} = \frac{2t}{(t^2-1)^2} - \frac{(\nu-1)t}{t^2-1},$$

which is positive and decreasing, since $1 \geqslant \nu$ and $1 < x \leqslant t$. By referring to (2.1) we establish our lemma.

If $|(x-1)^2 z/x(\nu-1)|$ is large, this gives quite satisfactory bounds for $K_\nu(z, x)$. When $\nu = 1$, we get satisfactory bounds if $|(x-1)^2 xz/4|$ is large.

LEMMA 5. *If* $0 < z$ *and* $0 < x,$ *then*

$$(x-1)Q_1(z,x) + (1 + 2/z - 2/z(1+x)^2)K_1(z,x) < K_2(z,x) < (x-1)Q_1(z,x) + (1+2/z)K_1(z,x). \tag{2.7}$$

Proof. By (2.1)

$$K_2(z,x) - K_1(z,x) = \frac{1}{2}\int_x^\infty (t-1)H^z(t)\,dt.$$

Integrating by parts gives

$$K_2(z,x) - K_1(z,x) = (x-1)Q_1(z,x) + \frac{1}{z}\int_x^\infty \left(1 - \frac{1}{(t+1)^2}\right)H^z(t)\,dt.$$

Then our lemma follows.

COROLLARY. *If* $0 < z$ *and* $1 < x$, *then*

$$K_2(z,x) < (x + 2/z)Q_1(z,x). \tag{2.8}$$

Proof. Combine Lemmas 4 and 5.

LEMMA 6. *If* $1 \geqslant \nu, 0 < z,$ *and* $1 < x$, *we have*

$$\left(1 + 2\,\frac{(3-\nu)x^2 + \nu - 1}{zx(x^2-1)^2}\right)^{-1}\left(Q_\nu(z,x) + \frac{2(\nu-1)}{z}K_{\nu-1}(z,x)\right) < K_\nu(z,x) < Q_\nu(z,x) + \frac{2(\nu-1)}{z}K_{\nu-1}(z,x). \tag{2.9}$$

Proof. By (2.6) and (2.1)

$$K_\nu(z,x) = Q_\nu(z,x) + \frac{2(\nu-1)}{z}K_{\nu-1}(x,z) - \frac{1}{z}\int_x^\infty \frac{(3-\nu)t^{\nu+1} + (\nu-1)t^{\nu-1}}{t(t^2-1)^2}H^z(t)\,dt.$$

We have

$$\frac{(3-\nu)t^2 + \nu - 1}{t(t^2-1)^2} = \frac{2t}{(t^2-1)^2} - \frac{\nu-1}{t(t^2-1)},$$

which is positive and decreasing. So our lemma follows.

COROLLARY. *If* $1 \geqslant \nu, 0 < z,$ *and* $1 < x$, *then*

$$\left(1 + 2\,\frac{(3-\nu)x^2 + \nu - 1}{zx(x^2-1)^2}\right)^{-1}\left(1 + \frac{2(\nu-1)}{xz}\right)Q_\nu(z,x) < K_\nu(z,x) < \left\{1 + \frac{2(\nu-1)}{xz}\left(1 + 2\,\frac{\nu x - (\nu-2)x^3}{z(x^2-1)^2}\right)^{-1}\right\}Q_\nu(z,x). \tag{2.10}$$

Proof. Combine Lemmas 4 and 6, and use (2.5).

We will be mainly interested in the cases $\nu = 1$ and $\nu = 2$. If x is appreciably greater than unity, Lemma 4 with $\nu = 1$ and Lemma 5 will serve nicely. If $1/x$ is appreciably greater than unity, we can use Lemma 3 to write

$$K_1(z,x) = K_1(z) - K_{-1}(z, 1/x),$$

and similarly for K_2. By use of NBS #55, we can evaluate $K_1(z)$. The term $K_{-1}(z, 1/x)$ will be small compared to $K_1(z)$ if z is of appreciable size. So a rough approximation for $K_{-1}(z, 1/x)$ will suffice, and this is available by (2.10).

We still have the matter of dealing with $K_1(z, x)$ and $K_2(z, x)$ when x is near unity. We first consider the case where z is small or of moderate size. For this, with the computing facilities now widely available, numerical quadrature seems the best procedure. In the present situation, it suffices to use the trapezoid rule and the midpoint formula, which are (A2) and (A3), respectively, on p. 446 of Rosser [1967].

We observe that by (2.1)

$$K_\nu(z, x) = K_\nu(z, y) + \frac{1}{2}\int_x^y t^{\nu-1}H^z(t)\, dt.$$

We take y large enough so that $K_\nu(z, y)$ can be estimated with adequate accuracy by Lemmas 4 and 5; note that a high order of accuracy for $K_\nu(z, y)$ itself is not needed, since it is usually much smaller than the other term on the right. So we desire to estimate

$$\frac{1}{2}\int_x^y f(t)\, dt \tag{2.11}$$

by numerical quadrature. When $\nu = 1$, we have

$$f(t) = H^z(t), \tag{2.12}$$

$$f'(t) = -\frac{z}{2t^2}(t^2 - 1)H^z(t), \tag{2.13}$$

$$f''(t) = \frac{z}{4t^4}\{z(t^2 - 1)^2 - 4t\}H^z(t). \tag{2.14}$$

By Descartes' rule of signs, the polynomial on the right of (2.14) has at most two positive roots. As the polynomial is positive at $t = 0$, negative at $t = 1$, and positive for large t, it must have exactly two positive roots, t_1 and t_2, with $t_1 < 1 < t_2$. For z not too small, the values of t_1 and t_2 are approximately

$$1 \pm \frac{1}{\sqrt{z}}\left(1 - \frac{1}{8z}\right). \tag{2.15}$$

If we take $1 + q$ to be t_1 or t_2, then the recursion

$$q_{n+1} = \pm\, 2\sqrt{1 + q_n}/\{\sqrt{z}(2 + q_n)\} \tag{2.16}$$

will converge fairly rapidly to q.

To get an upper bound for (2.11), we use the midpoint formula for $t_1 \leqslant t \leqslant t_2$, and the trapezoid rule for the rest of the range of integration. For a lower bound, we interchange the midpoint formula and trapezoid rule. If the bounds are not as close together as desired, use shorter intervals in the quadrature formula.

When $\nu = 2$, we have

$$f(t) = tH^z(t), \tag{2.17}$$

$$f'(t) = -\frac{1}{2t}\{z(t^2 - 1) - 2t\}H^z(t), \tag{2.18}$$

$$f''(t) = \frac{z}{4t^3}\{z(t^2 - 1)^2 - 4t^3\}H^z(t). \tag{2.19}$$

Clearly we proceed in exact analogy with the case $\nu = 1$. Note that the two positive zeros of $f''(t)$ are the reciprocals of the t_1 and t_2 obtained above.

We now consider the case for large z. Define

$$w = (\sqrt{t} - 1/\sqrt{t})/\sqrt{2}. \tag{2.20}$$

Then

$$t = 1 + w^2 + w\sqrt{2 + w^2}, \tag{2.21}$$

$$dt/dw = 2w + 2(1 + w^2)/\sqrt{2 + w^2}, \tag{2.22}$$

$$\begin{aligned} tdt/dw &= 4w(1 + w^2) + 2(1 + 4w^2 + 2w^4)/\sqrt{2 + w^2} \\ &= 4w^2\sqrt{2 + w^2} + 4w(1 + w^2) + 2/\sqrt{2 + w^2}. \end{aligned} \tag{2.23}$$

We have of course

$$K_1(z, x) = \frac{e^{-z}}{2}\int_y^\infty e^{-zw^2}\,\frac{dt}{dw}\,dw, \tag{2.24}$$

$$K_2(z, x) = \frac{e^{-z}}{2}\int_y^\infty e^{-zw^2}\,t\frac{dt}{dw}dw, \tag{2.25}$$

where

$$y = (\sqrt{x} - 1/\sqrt{x})/\sqrt{2}. \tag{2.26}$$

By squaring both sides, we verify that for $w^2 > 0$

$$\frac{1 + w^2}{\sqrt{2 + w^2}} < \left(1 + \frac{3w^2}{4}\right)\Big/\sqrt{2}, \tag{2.27}$$

$$\frac{1 + 4w^2 + 2w^4}{\sqrt{2 + w^2}} < \left(1 + \frac{15w^2}{4} + \frac{35w^4}{32}\right)\Big/\sqrt{2}. \tag{2.28}$$

Integration by parts gives

$$\int_y^\infty w^n e^{-zw^2}\,dw = \frac{y^{n-1}}{2z}\,e^{-zy^2} + \frac{n-1}{2z}\int_y^\infty w^{n-2}e^{-zw^2}\,dw. \tag{2.29}$$

Using the relations above gives

$$K_1(z, x) < \frac{e^{-z}}{2z}\left\{\left(1 + \frac{3\sqrt{2}y}{8}\right)e^{-zy^2} + \left(\frac{3}{8} + z\right)\sqrt{2}\int_y^\infty e^{-zw^2}\,dw\right\}, \tag{2.30}$$

$$\begin{aligned} K_2(z, x) < \frac{e^{-z}}{2z}\Bigg\{&\left[\frac{35\sqrt{2}}{64}y^3 + 2y^2 + \left(\frac{105}{128z} + \frac{15}{8}\right)\sqrt{2}y + 2 + \frac{2}{z}\right]e^{-zy^2} \\ &+ \left(\frac{105}{128z} + \frac{15}{8} + z\right)\sqrt{2}\int_y^\infty e^{-zw^2}\,dw\Bigg\}. \end{aligned} \tag{2.31}$$

The integrals appearing in the formulas above are the complementary error function. Means for calculating or bounding it are well known; see particularly 7.1.5, 7.1.6, 7.1.13, and 7.1.23 of NBS #55.

To get lower bounds, we first verify that for $w^2 > 0$

$$\frac{1}{\sqrt{2+w^2}} > \left(1 - \frac{w^2}{4}\right)\Big/\sqrt{2}, \tag{2.32}$$

whence

$$\frac{1+w^2}{\sqrt{2+w^2}} > \left(1 + \frac{3w^2}{4} - \frac{w^4}{4}\right)\Big/\sqrt{2}. \tag{2.33}$$

With this and (2.22), we can get a lower bound for $K_1(z, x)$. Integration by parts gives

$$\int_y^\infty w^2\sqrt{2+w^2}\, e^{-zw^2}\, dw = \frac{y\sqrt{2+y^2}}{2z}\, e^{-zy^2} + \frac{1}{z}\int_y^\infty \frac{1+w^2}{\sqrt{2+w^2}}\, e^{-zw^2}\, dw. \tag{2.34}$$

With this, (2.23), (2.32), and (2.33), we can get a lower bound for $K_2(z, x)$.

If we let x go to 0 in (2.30) and (2.31), we get the known results

$$K_1(z) \leqslant \sqrt{\frac{\pi}{2z}}\, e^{-z}\left(1 + \frac{3}{8z}\right), \qquad K_2(z) \leqslant \sqrt{\frac{\pi}{2z}}\, e^{-z}\left(1 + \frac{15}{8z} + \frac{105}{128z^2}\right). \tag{2.35}$$

3. Bounds for $\psi(x) - x$ for Large Values of x.

LEMMA 7. *Let $1 < U \leqslant V$, and let $\Phi(y)$ be nonnegative and differentiable for $U < y < V$. Let $(W - y)\Phi'(y) \geqslant 0$ for $U < y < V$, where W need not lie in $[U, V]$. Let Y be one of U, V, W which is neither greater than both the others nor less than both the others. Choose $j = 0$ or 1 so that $(-1)^j(V - W) \geqslant 0$. Then*

$$\begin{aligned} \sum_{U<\gamma\leqslant V} \Phi(\gamma) \leqslant{}& \frac{1}{2\pi}\int_U^V \Phi(y)\log\frac{y}{2\pi}\, dy \\ &+ (-1)^j\left\{0.137 + \frac{0.443}{\log Y}\right\}\int_U^V \frac{\Phi(y)}{y}\, dy + E_j(U, V), \end{aligned} \tag{3.1}$$

where the error term $E_j(U, V)$ is given by

$$\begin{aligned} E_j(U, V) ={}& \{1 + (-1)^j\}R(Y)\Phi(Y) \\ &+ \{N(V) - F(V) - (-1)^j R(V)\}\Phi(V) - \{N(U) - F(U) + R(U)\}\Phi(U). \end{aligned} \tag{3.2}$$

Proof. By the result of Ingham [1932, p. 18], we have

$$\sum_{U<\gamma\leqslant V} \Phi(\gamma) = -\int_U^V N(y)\Phi'(y)\, dy + N(V)\Phi(V) - N(U)\Phi(U). \tag{3.3}$$

Case 1. $j = 1$. We take $Y = \min(V, W)$. On the right of (3.3), we replace $N(y)$ by $F(y) - R(y)$, and integrate by parts, deducing (3.1) by the observation that

$$-\int_U^V R'(y)\Phi(y)\, dy \leqslant (-1)^j\left\{0.137 + \frac{0.443}{\log V}\right\}\int_U^V \frac{\Phi(y)}{y}\, dy,$$

since $yR'(y) \geqslant 0.137 + 0.443/\log V$ for $1 < y \leqslant V$.

Case 2. $j = 0$. We take $Y = \max(U, W)$. In (3.3), we split the integral at Y. In the first part, we replace $N(y)$ by $F(y) - R(y)$, and in the second part we replace

$N(y)$ by $F(y) + R(y)$. Integration by parts gives

$$\sum_{U<\gamma\leqslant V} \Phi(\gamma) \leqslant \frac{1}{2\pi}\int_U^V \Phi(y)\log\frac{y}{2\pi}\,dy + \int_Y^V R'(y)\Phi(y)\,dy - \int_U^Y R'(y)\Phi(y)\,dy + E_0(U, V).$$

We discard the third integral, and use the result

$$\int_Y^V R'(y)\Phi(y)\,dy \leqslant (-1)^j\left\{0.137 + \frac{0.443}{\log Y}\right\}\int_Y^V \frac{\Phi(y)}{y}\,dy \leqslant (-1)^j\left\{0.137 + \frac{0.443}{\log Y}\right\}\int_U^V \frac{\Phi(y)}{y}\,dy.$$

COROLLARY. *If, in addition,* $2\pi < U$, *then*

$$\sum_{U<\gamma\leqslant V} \Phi(\gamma) \leqslant \left\{\frac{1}{2\pi} + (-1)^j q(Y)\right\}\int_U^V \Phi(y)\log\frac{y}{2\pi}\,dy + E_j(U, V), \tag{3.4}$$

where

$$q(y) = \frac{0.137\log y + 0.443}{y\log y\log(y/2\pi)}.$$

Proof. Proceed as in the proof of the lemma, using

$$(-1)^j R'(y)/\log(y/2\pi) \leqslant (-1)^j q(Y)$$

for y in the range of integration.

Define, for $x \geqslant 1$,

$$X = \sqrt{(\log x)/R}, \tag{3.5}$$

where $R = 9.6459\ 08801$, as in Theorem 1. Also, for positive v, positive integer m, and nonnegative real T_1 and T_2, define

$$R_m(v) = \{(1+v)^{m+1} + 1\}^m, \tag{3.6}$$

$$S_1(m, v) = 2\sum_{\beta\leqslant 1/2;\,0<\gamma\leqslant T_1} \frac{2+mv}{2|\rho|}, \tag{3.7}$$

$$S_2(m, v) = 2\sum_{\beta\leqslant 1/2;\,T_1<\gamma} \frac{R_m(v)}{v^m|\rho(\rho+1)\cdots(\rho+m)|}, \tag{3.8}$$

$$S_3(m, v) = 2\sum_{1/2<\beta;\,0<\gamma\leqslant T_2} \frac{(2+mv)\exp\{-X^2/\log(\gamma/17)\}}{2|\rho|}, \tag{3.9}$$

$$S_4(m, v) = 2\sum_{1/2<\beta;\,T_2<\gamma} \frac{R_m(v)\exp\{-X^2/\log(\gamma/17)\}}{v^m|\rho(\rho+1)\cdots(\rho+m)|}. \tag{3.10}$$

LEMMA 8. *Let* T_1 *and* T_2 *be nonnegative real numbers. Let* m *be a positive integer. Let* $x > 1$ *and* $0 < \delta < (x-1)/(xm)$. *Then*

$$\frac{1}{x}\left|\psi(x) - \{x - \log(2\pi) - \tfrac{1}{2}\log(1 - x^{-2})\}\right| \leqslant \{S_1(m, \delta) + S_2(m, \delta)\}/\sqrt{x} + S_3(m, \delta) + S_4(m, \delta) + m\delta/2. \tag{3.11}$$

Proof. Split the sum on the right of Theorem 13 of Rosser [1941] into four sums over the regions: I, $\beta \leqslant \frac{1}{2}$, $0 < |\gamma| \leqslant T_1$; II, $\beta \leqslant \frac{1}{2}$, $T_1 < |\gamma|$; III, $\frac{1}{2} < \beta$, $0 < |\gamma| \leqslant T_2$; IV, $\frac{1}{2} < \beta$, $T_2 < |\gamma|$. In regions I and III, write the summand in the equivalent form

$$-\frac{1}{\rho}\int_0^h (x + z)^\rho \, dz. \tag{3.12}$$

If we now integrate term-by-term $m - 1$ times, we will get a result similar to Theorem 14 of Rosser [1941], except that the sum is split into four sums over the four regions. (Note that the quantity on the left of Theorem 14 of Rosser [1941] is NOT the function of our Section 2.) In regions I and III, as we integrated (3.12) $m - 1$ times, we see that an alternative form for the summand is

$$-\frac{x^{\rho+m}}{\rho}\int_0^{\pm\delta} dy_1 \int_0^{\pm\delta} dy_2 \cdots \int_0^{\pm\delta} (1 + y_1 + y_2 + \cdots + y_m)^\rho \, dy_m, \tag{3.13}$$

If we use $+\delta$ as the upper limit, we can bound the absolute value of (3.13) by

$$\frac{x^{\beta+m}}{|\rho|}\int_0^{\delta} dy_1 \int_0^{\delta} dy_2 \cdots \int_0^{\delta} (1 + y_1 + y_2 + \cdots + y_m) \, dy_m,$$

which equals

$$\frac{x^{\beta+m}\delta^m}{|\rho|}\,\frac{2 + m\delta}{2}. \tag{3.14}$$

If we use $-\delta$ as the upper limit, the integrand of (3.13) is bounded in absolute value by unity, so that in this case also (3.14) is an absolute bound for (3.13).

In regions II and IV, we get bounds by the reasoning for Theorem 15 of Rosser [1941]. By symmetry, we replace sums over all ρ by twice the sums for positive γ. If $\beta \leqslant \frac{1}{2}$, we have $x^{\beta+m} \leqslant x^{m+1}/\sqrt{x}$, while if $\frac{1}{2} < \beta$ we can use Theorem 1 to conclude that

$$x^{\beta+m} \leqslant x^{m+1} \exp\{-X^2/\log(\gamma/17)\}.$$

Finally, we use the reasoning for the proof of Theorem 12 of Rosser [1941].

As $1/|\rho(\rho + 1) \cdots (\rho + m)| \leqslant \gamma^{-m-1}$ for positive γ, we can use Lemma 7 to write bounds for $S_j(m, \delta)$ in terms of integrals for suitable $\Phi(y)$. We note that for $m \neq 0$

$$\int_U^V y^{-m-1} \log\frac{y}{2\pi}\, dy = \frac{1 + m\log(U/2\pi)}{m^2 U^m} - \frac{1 + m\log(V/2\pi)}{m^2 V^m}, \tag{3.15}$$

$$\int_U^V y^{-m-1} \exp\{-X^2/\log(y/17)\}\log\frac{y}{2\pi}\, dy = \frac{z^2}{2m^2 17^m}\{K_2(z, U') - K_2(z, V')\} + \frac{z\log(17/2\pi)}{m17^m}\{K_1(z, U') - K_1(z, V')\}, \tag{3.16}$$

where $z = 2X\sqrt{m}$, $U' = (2m/z)\log(U/17)$, $V' = (2m/z)\log(V/17)$; we get (3.16) by putting $y = 17\exp(zt/2m)$. Also we get

$$\int_U^V y^{-1}\exp\{-X^2/\log(y/17)\}\log\frac{y}{2\pi}\,dy \tag{3.17}$$
$$= X^4\{\Gamma(-2, V'') - \Gamma(-2, U'')\} + X^2(\log 17/2\pi)\{\Gamma(-1, V'') - \Gamma(-1, U'')\}$$

with $U'' = X^2/\log(U/17)$, $V'' = X^2/\log(V/17)$ by putting $y = 17\exp(X^2/t)$.

THEOREM 2. *If* $\log x \geq 105$, *then*

$$|\psi(x) - x|,\ |\theta(x) - x| < x\epsilon(x), \tag{3.18}$$

where one may take either

$$\epsilon(x) = 0.257\,634\left\{1 + \frac{0.96642}{X}\right\}X^{3/4}e^{-X} \tag{3.19}$$

or, with $R = 9.6459\,08801$,

$$\epsilon(x) = 0.110\,123\left\{1 + \frac{3.0015}{\sqrt{\log x}}\right\}(\log x)^{3/8}\exp\{-\sqrt{(\log x)/R}\}. \tag{3.20}$$

Proof. Take $m = 1$ and $T_1 = T_2 = 0$ in (3.6) through (3.11). By Lemma 17 of Rosser [1941],

$$S_1(1, \delta) + S_2(1, \delta) < (0.0463)\,(2 + 2\delta + \delta^2)/\delta. \tag{3.21}$$

Also, as $\beta = \frac{1}{2}$ for $|\gamma| \leq A$, and the zeros off the critical line occur in pairs which are symmetrical with respect to this line, we have

$$S_3(1, \delta) + S_4(1, \delta) \leq \frac{2 + 2\delta + \delta^2}{\delta}\sum_{A<\gamma}\phi_1(\gamma), \tag{3.22}$$

where

$$\phi_m(y) = y^{-m-1}\exp\{-X^2/\log(y/17)\}. \tag{3.23}$$

We appeal to Lemma 7, Corollary with $\Phi(y) = \phi_1(y)$, $j = 0$, $U = A$, $V = \infty$, and $W = W_1$, where for $m > -1$

$$W_m = 17\exp(X/\sqrt{m+1}). \tag{3.24}$$

Note that $q(Y) \leq q(A)$. Also, as $N(A) = F(A)$, we have

$$E_0 = 2R(Y)\phi_1(Y) - R(A)\phi_1(A). \tag{3.25}$$

Further, by Lemma 3 and (3.16), we have

$$\int_A^\infty \phi_1(y)\log\frac{y}{2\pi}\,dy \leq \frac{2X}{17}\{XK_2(2X) + \log(17/2\pi)K_1(2X)\}.$$

Then, by (2.35), we conclude

$$\sum_{A<\gamma}\phi_1(\gamma) < 0.01659\,38121\left\{1 + \frac{1.93284}{X} + \frac{0.3918}{X^2}\right\}X^{3/2}e^{-2X} + E_0. \tag{3.26}$$

If $W_1 \leq A$, then $Y = A$. Then by (3.25)

$$E_0 = R(A)\phi_1(A) = \frac{R(A)}{A^2}\{\exp\{-X^2/\log(A/17)\}X^{1/2}e^{2X}\}X^{-1/2}e^{-2X}.$$

As the expression in the large braces takes its maximum at

$$X = \frac{1}{2}\log\frac{A}{17} + \frac{1}{2}\left\{\log^2\frac{A}{17} + \log\frac{A}{17}\right\}^{1/2},$$

we conclude

$$E_0 < 10^{-6}X^{-1/2}e^{-2X}. \tag{3.27}$$

If $W_1 > A$, then $Y = W_1$ and $X > 16$. As $R(y)/\log y$ is decreasing for $y > e^e$, (3.25) gives

$$\begin{aligned} E_0 < 2R(Y)\phi_1(Y) &< \frac{2R(A)}{\log A}\phi_1(W_1)\log W_1 \\ &= \frac{2R(A)}{17^2\log A}\left\{\frac{X}{\sqrt{2}} + \log 17\right\} e^{-2\sqrt{2}X}, \end{aligned}$$

so that we conclude (3.27) for this case also. Then by (3.26)

$$\sum_{A<\gamma}\phi_1(\gamma) < 0.01659\,38121\left\{1 + \frac{1.93284}{X} + \frac{0.3919}{X^2}\right\}X^{3/2}e^{-2X}. \tag{3.28}$$

As $\log x \geqslant 105$,

$$0.0463/\sqrt{x} = 0.0463\exp(-RX^2/2) < 10^{-21}X^{-1/2}e^{-2X}. \tag{3.29}$$

Choose

$$\delta = 2(0.01659\,38121)^{1/2}\left\{1 + \frac{0.96642}{X}\right\}X^{3/4}e^{-X}. \tag{3.30}$$

As $\log x \geqslant 105$, we see that δX^2 is a decreasing function of X; hence $\delta X^2 < 0.3277$ and $0 < \delta < 1 - 1/x$. Hence

$$2 + 2\delta + \delta^2 < 2\left\{1 + \frac{0.333}{X^2}\right\}. \tag{3.31}$$

Combining (3.21), (3.22), (3.28), (3.29), and (3.31) gives

$$\begin{aligned} &\{S_1(1,\delta) + S_2(1,\delta)\}/\sqrt{x} + S_3(1,\delta) + S_4(1,\delta) \\ &\quad < \delta^{-1}2(0.01659\,38121)\left\{1 + \frac{0.96642}{X}\right\}^2 X^{3/2}e^{-2X}. \end{aligned}$$

Using the value of δ from (3.30) with Lemma 8 substantiates (3.19). From it, we can get (3.20) by (3.5).

This establishes the stated inequality for $\psi(x)$. By Theorem 13 of R–S,

$$|\psi(x) - \theta(x)| < 1.43\sqrt{x}.$$

Thus, it would appear that for $\theta(x)$ we should increase $\epsilon(x)$ by $1.43/\sqrt{x}$. However, we can treat it as in (3.29) to show it is absorbed when we round up some of the coefficients.

THEOREM 3. *If* $\log x \geqslant 105$, *then*

(3.32) $$|\psi(x) - x|, |\theta(x) - x| < x\epsilon^*(x),$$

where

(3.33) $$\epsilon^*(x) = \frac{\epsilon(x)}{\sqrt{2}}\left\{1 + \frac{3 \log X}{2\sqrt{\pi(4X - 3\log X)}} + \frac{1.43813}{r(x)\sqrt{X}}\right\};$$

here we take $\epsilon(x)$ *as in* (3.19) *or* (3.20), *and*

(3.34) $$r(x) = 1 + 0.96642/X.$$

Proof. Take

(3.35) $$\delta = \frac{1}{\sqrt{2}}(0.2576\ 33942)r(x)X^{3/4}e^{-X}.$$

We may assume $X > 59$, since otherwise $\epsilon^*(x) > \epsilon(x)$ and we can appeal to Theorem 2. In (3.6) through (3.11), we take $m = 1$, $T_1 = 0$, and

(3.36) $$T_2 = 17X^{-3/4}e^X.$$

As $X > 59$, we have $A < T_2 < W_0$ and $W_1 < T_2$.

We can treat $\{S_1(1, \delta) + S_2(1, \delta)\}/\sqrt{x}$ and the error terms $E_j(U, V)$ arising from the use of Lemma 7, Corollary, as we did in the proof of Theorem 2. Thus, we can proceed as though

(3.37) $$S_3(1, \delta) < \frac{2 + \delta}{2}\left\{\frac{1}{2\pi} - q(T_2)\right\}\int_A^{T_2} \phi_0(y) \log \frac{y}{2\pi}\, dy.$$

If $\nu \leqslant 1$ and $x > 0$, then

$$\Gamma(\nu, x) \leqslant x^{\nu - 1}\int_x^\infty e^{-t}\,dt = x^{\nu-1}e^{-x}.$$

Hence, by (3.17), we have in effect

(3.38) $$S_3(1, \delta) < \frac{2 + \delta}{4\pi}e^{-V''}\{X^4(V'')^{-3} + X^2 d(V'')^{-2}\},$$

where $d = \log(17/2\pi)$ and

(3.39) $$V'' = \frac{X^2}{\log(T_2/17)} = \frac{4X^2}{4X - 3\log X}.$$

Then

(3.40) $$V'' > X + (3/4)\log X, \qquad e^{-V''} < X^{-3/4}e^{-X}.$$

Also

$$X^4(V'')^{-3} + X^2 d(V'')^{-2} = \left(1 - \frac{3\log X}{4X}\right)^2\left(X - \frac{3\log X}{4} + d\right) < X.$$

So, effectively,

(3.41) $$S_3(1, \delta) < \frac{2 + \delta}{4\pi}X^{1/4}e^{-X}.$$

Similarly, we can proceed as though

(3.42) $$S_4(1, \delta) < \frac{2 + 2\delta + \delta^2}{\delta}\left\{\frac{1}{2\pi} + q(T_2)\right\}\int_{T_2}^\infty \phi_1(y)\log\frac{y}{2\pi}\,dy.$$

By (3.16)

$$\int_{T_2}^{\infty} \phi_1(y) \log \frac{y}{2\pi}\, dy = \frac{2}{17}\{X^2K_2(2X, U') + XdK_1(2X, U')\}, \tag{3.43}$$

where

$$U' = \frac{1}{X} \log \frac{T_2}{17} = 1 - \frac{3 \log X}{4X}. \tag{3.44}$$

Write temporarily

$$q = \frac{3 \log X}{4X}, \qquad y = (\sqrt{U'} - 1/\sqrt{U'})/\sqrt{2}. \tag{3.45}$$

Then y is negative, and $y^2 = \tfrac{1}{2}(U' + 1/U') - 1 = q^2/\{2(1-q)\}$. So, by splitting the integral at $w = 0$, we get

$$\sqrt{2}\int_{y}^{\infty} e^{-2Xw^2}\, dw < \frac{\sqrt{\pi}}{2\sqrt{X}} + \frac{q}{\sqrt{1-q}}. \tag{3.46}$$

Hence, by (2.30) we get

$$XdK_1(2X, U') < \frac{\sqrt{\pi}}{4} X^{3/2}e^{-2X}\left\{\frac{d}{\sqrt{\pi}X^{3/2}} + \left(1 + \frac{2q\sqrt{X}}{\sqrt{\pi(1-q)}}\right)\left(\frac{d}{X} + \frac{3d}{16X^2}\right)\right\}. \tag{3.47}$$

As $1 + zy^2 < e^{zy^2}$, we have $(2y^2 + 2/z)e^{-zy^2} < 2/z = 1/X$. Hence, by (2.31) we get

$$X^2K_2(2X, U') < \frac{\sqrt{\pi}}{4} X^{3/2}e^{-2X} \cdot\left\{\frac{2}{\sqrt{\pi}\sqrt{X}} + \frac{1}{\sqrt{\pi}X^{3/2}} + \left(1 + \frac{2q\sqrt{X}}{\sqrt{\pi(1-q)}}\right)\left(1 + \frac{15}{16X} + \frac{105}{512X^2}\right)\right\}. \tag{3.48}$$

Combining with (3.43) and (3.47) gives

$$\int_{T_2}^{\infty} \phi_1(y) \log \frac{y}{2\pi}\, dy < \frac{\sqrt{\pi}}{34} X^{3/2} e^{-2X}Q_1,$$

where

$$Q_1 = \frac{2}{\sqrt{\pi}\sqrt{X}} + \frac{1+d}{\sqrt{\pi}X^{3/2}} + \left\{1 + \frac{2q\sqrt{X}}{\sqrt{\pi(1-q)}}\right\}\left\{1 + \frac{1.93284}{X} + \frac{0.3918}{X^2}\right\}.$$

So finally by (3.42) and (3.35)

$$S_4(1, \delta) < \frac{1}{\sqrt{8}}(0.2576\ 33942)r(x)X^{3/4}e^{-X}Q_2, \tag{3.49}$$

where

$$Q_2 = 1 + \frac{2q\sqrt{X}}{\sqrt{\pi(1-q)}} + \frac{2 + 2\delta + \delta^2}{\{r(x)\}^2}\left\{\frac{0.56419}{\sqrt{X}} + \frac{0.5629}{X^{3/2}}\right\}. \tag{3.50}$$

As $X > 59$, δ is extremely small, so that our theorem follows by (3.11) and (3.41).

4. Numerical Bounds for $\psi(x) - x$ for Moderate Values of x. In our main table (at the end of the paper) we tabulate values of ϵ against b. These have been determined so that if $x \geqslant e^b$, then

$$|\psi(x) - x| < \epsilon x. \tag{4.1}$$

If a value of b is chosen, it is clear from (3.5) through (3.11) that a value can be determined for ϵ, so as to satisfy (4.1), which will depend not only on b but on the four parameters δ, m, T_1, and T_2, as well as a parameter D which will be introduced. It was not practical in the majority of cases to minimize ϵ by determining the optimum values of all five of δ, m, T_1, T_2, and D. An effort was made, especially in crucial regions for b, to make reasonably good choices for δ, m, T_1, T_2, and D; the values chosen for δ and m are listed in the table, and the choices for T_1, T_2, and D will be described in the text. For the chosen δ, m, T_1, T_2, and D, computations were made which ensured that the values listed in the table for ϵ are upper bounds for what would be given by (3.11). To keep the computations reasonable in extent, they were usually terminated before the best possible upper bound for ϵ had been determined. Thus, for most entries in the table, (3.11) would give a slightly smaller value of ϵ than that listed. However, great pains were taken to ensure that the values listed for ϵ are indeed upper bounds. The two authors made quite independent calculations, on different computers, with different programs, and commonly with different schemes of computation, one of which was that described in Section 2. Each scheme of computation provided both upper and lower bounds. When these had been brought fairly close together, and were consistent as between the two independent calculations, the larger of the two computed ϵ's was rounded up and entered in the table.

In the main, T_2 was taken to be 0. Uniformly we took

$$T_1 = \frac{1}{\delta}\left(\frac{2R_m(\delta)}{2 + m\delta}\right)^{1/m}, \tag{4.2}$$

since an analysis showed that for a given m and δ this was reasonably close to its optimum. We chose also

$$D = 158.8\,4998. \tag{4.3}$$

The zeros for which $0 < \gamma \leqslant D$ are exactly 57 in number, and have been calculated to high accuracy by Lehman as stated in his paper [1966, p. 408]. Using Lehman's values, two independent calculations verified

$$S \equiv \sum_{0<\gamma\leqslant D} |\rho|^{-1} = \sum_{0<\gamma\leqslant D} (\gamma^2 + 1/4)^{-1/2} < 0.811\,3925. \tag{4.4}$$

LEMMA 9. *With* T_1 *and* D *given by* (4.2) *and* (4.3), *if* $T_1 \geqslant D$, $\delta > 0$, *and* m *is a positive integer, then*

$$S_1(m, \delta) + S_2(m, \delta) < \frac{2 + m\delta}{4\pi}\left\{\left(\log \frac{T_1}{2\pi} + \frac{1}{m}\right)^2 + 0.038207 + \frac{1}{m^2} - \frac{2.82m}{(m+1)T_1}\right\}. \tag{4.5}$$

Proof. By (3.7) and (4.4)

$$S_1(m, \delta) < (2 + m\delta) \left\{ S + \sum_{D<\gamma\leq T_1} \gamma^{-1} \right\}.$$

Taking $\Phi(y) = y^{-1}, j = 0, U = D, V = T_1$, and $W = 0$ in Lemma 7 gives

$$\sum_{D<\gamma\leq T_1} \gamma^{-1} \leq \frac{1}{4\pi} \left\{ \log^2 \frac{T_1}{2\pi} - \log^2 \frac{D}{2\pi} \right\} - \left(0.137 + \frac{0.443}{\log D}\right) \left\{ \frac{1}{T_1} - \frac{1}{D} \right\} + E_0.$$

Then (4.4) together with $N(D) = 57$ gives

$$\begin{aligned} \frac{S_1(m, \delta)}{2 + m\delta} &< \frac{1}{4\pi} \log^2 \frac{T_1}{2\pi} + 0.003\,0404 \\ &\quad - \frac{1}{T_1} \left\{ F(T_1) - N(T_1) + R(T_1) + 0.137 + \frac{0.443}{\log D} \right\}. \end{aligned} \tag{4.6}$$

Taking $\Phi(y) = y^{-m-1}, j = 0, U = T_1, V = \infty$, and $W = 0$ in Lemma 7, and using (3.15) gives

$$\begin{aligned} \frac{\delta^m S_2(m, \delta)}{2R_m(\delta)} &\leq \frac{1}{T_1^m} \left\{ \frac{1}{2\pi m} \log \frac{T_1}{2\pi} + \frac{1}{2\pi m^2} \right. \\ &\quad \left. + \left(0.137 + \frac{0.443}{\log T_1}\right) \frac{1}{(m+1)T_1} \right\} + E_0^*. \end{aligned}$$

Using (4.2) and combining with (4.6) gives

$$S_1(m, \delta) + S_2(m, \delta) \leq \frac{2 + m\delta}{4\pi} \left\{ \left(\log \frac{T_1}{2\pi} + \frac{1}{m} \right)^2 + \frac{1}{m^2} + J \right\},$$

where

$$\begin{aligned} J &= 4\pi(0.003\,0404) + \frac{4\pi}{(m+1)T_1} \left(0.137 + \frac{0.443}{\log T_1}\right) - \frac{4\pi}{T_1}\left(0.137 + \frac{0.443}{\log D}\right) \\ &< 4\pi(0.003\,0404) - \frac{4\pi}{T_1}\left(0.137 + \frac{0.443}{\log D}\right) \left(1 - \frac{1}{m+1}\right). \end{aligned}$$

Our lemma follows from this.

THEOREM 4. *Let $T_1 \geq D$. Let m be a positive integer, let Ω_1 denote the right side of* (4.5) *and let*

$$\begin{aligned} \Omega_2 &= \frac{(0.159155)R_m(\delta)z}{2m^2 17^m} \left\{ zK_2(z, A') + 2m\left(\log \frac{17}{2\pi}\right)K_1(z, A') \right\} \\ &\quad + R_m(\delta) \left\{ 2R(Y)\phi_m(Y) - R(A)\phi_m(A) \right\}, \end{aligned} \tag{4.7}$$

where $z = 2X\sqrt{m} = 2\sqrt{mb/R}$, $A' = (2m/z)\log(A/17)$, $Y = \max\{A, 17\exp\sqrt{b/(m+1)R}\}$. If $b > 1/2$ and $0 < \delta < (1 - e^{-b})/m$, then (4.1) *holds for all $x \geq e^b$, where*

$$\epsilon = \Omega_1 e^{-b/2} + \Omega_2 \delta^{-m} + m\delta/2 + e^{-b} \log 2\pi. \tag{4.8}$$

Proof. Take $T_2 = 0$. Then by Lemma 7, Corollary and (3.16),

$$S_3(m, \delta) + S_4(m, \delta) \leqslant \Omega_2 \delta^{-m}.$$

So we use Lemmas 8 and 9.

THEOREM 5. *Let* $T_1 \geqslant D$ *and* $A \leqslant T_2 \leqslant 17 \exp \sqrt{b/R}$. *Let* m *be a positive integer and let*

$$\Omega_3 = \frac{2 + m\delta}{4\pi}\left[X^4\left\{\Gamma(-2, T'') - \Gamma(-2, A'')\right\} + X^2\left(\log\frac{17}{2\pi}\right)\left\{\Gamma(-1, T'') - \Gamma(-1, A'')\right\}\right] + \frac{2 + m\delta}{2}\left[2R(T_2)\phi_0(T_2) - R(A)\phi_0(A)\right] + \Omega_2^*\delta^{-m}, \tag{4.9}$$

where $A'' = b/\{R \log (A/17)\}$, $T'' = b/\{R \log(T_2/17)\}$, *and* Ω_2^* *is obtained from* Ω_2 *by deleting the term* $-R(A)\phi_m(A)$ *in* (4.7) *and then replacing* A *by* T_2 *in the definitions of* A' *and* Y. *If* $b > ½$ *and* $0 < \delta < (1 - e^{-b})/m$, *then* (4.1) *holds for all* $x \geqslant e^b$, *where*

$$\epsilon = \Omega_1 e^{-b/2} + \Omega_3 + m\delta/2 + e^{-b} \log 2\pi. \tag{4.10}$$

Proof. Like those of Theorems 3 and 4.

We note that, with a slightly different notation, tabulations and other means of calculation for $\Gamma(\nu, x)$ with nonpositive integer ν are given in Chapter 5 of NBS #55. For many values of x, one can get quite accurate approximations by means of Airey's converging factor; see Rosser [1955, pp. 603–611]. Actually, integration by parts gives for $x > 0$

$$\Gamma(\nu, x) = x^{\nu-1} e^{-x} + (\nu - 1)\Gamma(\nu - 1, x), \tag{4.11}$$

whence for $\nu < 1$ we get

$$\Gamma(\nu, x) < x^{\nu-3} e^{-x} \{x^2 + (\nu - 1)x + (\nu - 1)(\nu - 2)\}. \tag{4.12}$$

We note also for $x > 0$ and $\nu < 1$

$$\Gamma(\nu, x) = x^\nu e^{-x} \int_0^\infty \frac{e^{-xw}\, dw}{(1 + w)^{1-\nu}} > x^\nu e^{-x} \int_0^\infty \frac{e^{-xw}\, dw}{e^{(1-\nu)w}} = \frac{x^\nu e^{-x}}{x + 1 - \nu}. \tag{4.13}$$

Using these bounds, the entries in the table for $b \geqslant 3000$ were calculated by (4.10), using T_2 given by (3.36). For large b it appears that (4.10), with $m = 1$ and T_2 given by (3.36), gives a better bound than those given by any of Theorems 2, 3, or 4; and a similar statement can be made for $T_2 = T_1$ where T_1 is given by (4.2).

ADDENDUM

By Lowell Schoenfeld

5. Some Inequalities for $\psi(x)$ and $\theta(x)$. In this section I give a few applications of the results of the preceding sections, with a more complete treatment reserved for another paper. In particular, I have not yet determined the exact point at which some inequalities, like (5.2), become false.

THEOREM 6. *We have*

$$\theta(x) < 1.001\ 102x \quad \text{if } 0 < x, \tag{5.1}$$

$$0.998\ 684x < \theta(x) \quad \text{if } 1{,}319{,}007 \leqslant x, \tag{5.2}$$

$$\psi(x) - \theta(x) < 1.001\ 102\sqrt{x} + 3x^{1/3} \quad \text{if } 0 < x, \tag{5.3}$$

$$0.998\ 684\sqrt{x} < \psi(x) - \theta(x) \quad \text{if } 121 \leqslant x. \tag{5.4}$$

Proof. If $10^8 \leqslant x < e^{18.43}$, then (4.11) of R–S and the first entry of our table give

$$\theta(x) < \psi(x) - \sqrt{x} < 1.001\ 2015x - \sqrt{x}$$
$$< 1.001\ 2015x - e^{-18.43/2}x < 1.001\ 102x.$$

By handling the intervals $[e^{18.43}, e^{18.44})$, etc., similarly, we derive the same inequality. And for $x \geqslant e^{18.7}$ we use the table and $\theta(x) \leqslant \psi(x)$. This proves (5.1) for all $x \geqslant 10^8$; for $x < 10^8$, it follows from (4.5) of R–S. Then (5.3) is an immediate consequence of (3.38) of R–S.

If $10^8 \leqslant x < 10^{16}$, then (4.12) of R–S and the first entry of the table yield

$$\theta(x) > \psi(x) - \sqrt{x} - 3x^{1/3}$$
$$> (1 - 0.001\ 2015)x - 10^{-4}x - 3 \cdot 10^{-16/3}x > 0.998\ 684x.$$

If $x \geqslant 10^{16}$, then we use (5.3) and the table. If $2{,}309{,}661 \leqslant x < 10^8$, then (4.6) of R–S gives

$$\theta(x) > x - 2\sqrt{x} > x - 0.001\ 316x,$$

so that (5.2) follows. By using the Appel-Rosser tables [1961] and D. N. Lehmer's well-known table of primes, we then verify (5.2) for $1{,}319{,}007 \leqslant x$. We also discover that (5.2) fails for x slightly below 1,090,697. This leaves a region in which I have not yet resolved the status of (5.2).

From (2.24) and (4.11) of R–S and (5.2), we deduce (5.4).

COROLLARY. *We have* $\theta(x) > 0.998x$ *if* $x \geqslant 487{,}381$; $\theta(x) > 0.995x$ *if* $x \geqslant 89{,}387$; $\theta(x) > 0.990x$ *if* $x \geqslant 32{,}057$; $\theta(x) > 0.985x$ *if* $x \geqslant 11{,}927$.

Proof. These follow from (5.2) above, from (4.6) of R–S and from the Appel-Rosser tables [1961].

This corollary supplements Theorem 10 of R–S, and the lower bounds given for x cannot be replaced by smaller ones.

THEOREM 7. *If* $x \geqslant 10^8$, *then*

$$|\theta(x) - x|,\ |\psi(x) - x| < 0.024\ 2269x/\log x. \tag{5.5}$$

Proof. If $10^8 \leqslant x < e^{18.43}$, then (4.12) of R–S and our table give

$$\theta(x) - x > \{\psi(x) - x\} - \sqrt{x} - 3x^{1/3}$$
$$> -\left\{0.0012\ 0116 \log x + \frac{\log x}{x^{1/2}} + \frac{3 \log x}{x^{2/3}}\right\} \frac{x}{\log x}.$$

As the material in the braces increases for the x specified, it does not exceed its value at $x = e^{18.43}$ which value is less than 0.024 2269. We continue to use the table in this way until we have dealt with the range $e^{29} \leqslant x < e^{30}$. In place of (4.12) of R–S, we then use the slightly weaker (5.3) above and continue to use the table up to $x = e^{1300}$. For $x \geqslant e^{1300}$, we apply Theorem 2 and note that $\epsilon(x)\log x < 0.021$ so that

$$\theta(x) - x > -\{\epsilon(x)\log x\}x/\log x > -0.021x/\log x.$$

This completes the proof of the lower bound for $\theta(x)$ and hence for $\psi(x)$. The proof for the upper bound for $\psi(x)$ is easier since the extra terms $\sqrt{x}$ and $3x^{1/3}$ do not appear.

COROLLARY 1. *If* $x \geqslant 525{,}752$, *then*

$$\theta(x) - x \leqslant \psi(x) - x < 0.024\ 2334x/\log x.$$

Proof. We apply (4.12) and (4.5) of R–S.

This result may hold for smaller values of x as well. However, in the next corollary, the bounds for x cannot be lowered.

COROLLARY 2. *We have*

$$(5.6) \qquad |\theta(x) - x| < 0.024\ 2334x/\log x \quad \text{if } 758{,}699 \leqslant x,$$

$$(5.7) \qquad |\theta(x) - x| < x/(40\log x) \quad \text{if } 678{,}407 \leqslant x.$$

Proof. The previous corollary takes care of the upper bounds for $\theta(x)$. The lower bounds are handled by using (4.6) of R–S as well as the Appel-Rosser tables [1961].

THEOREM 8. *If* $x > 1$, *then*

$$(5.8) \qquad |\theta(x) - x|,\ |\psi(x) - x| < \eta_k x/\log^k x,$$

where

$$(5.9) \qquad \eta_2 = 8.6853, \quad \eta_3 = 11762, \quad \eta_4 = 1.8559 \cdot 10^7.$$

Proof. We proceed as in the proof of the previous theorem. For $k = 2$, we use the table up to $x = e^{1750}$ and then apply Theorem 2. For $k = 3$ and 4, the table is used up to $x = e^{2000}$. This establishes the results for $x \geqslant 10^8$. For $1 < x < 10^8$ we use (4.12) and (4.5) of R–S to get

$$\psi(x) - x < \theta(x) - x + \sqrt{x} + 3x^{1/3} < \left\{\frac{\log^k x}{\sqrt{x}} + 3\frac{\log^k x}{x^{2/3}}\right\}\frac{x}{\log^k x}$$
$$\leqslant \left\{\frac{(2k)^k}{e^k} + 3\frac{(3k/2)^k}{e^k}\right\}\frac{x}{\log^k x} < \eta_k \frac{x}{\log^k x}$$

for $k = 2, 3, 4$. Also, (4.5) of R–S gives for $1 < x < 10^8$

b	m	δ	ϵ	b	m	δ	ϵ
18.42	2	2.69(-4)	1.2015(-3)	450	9	2.59(-6)	1.2968(-5)
18.43	2	2.68(-4)	1.1969(-3)	500	9	2.48(-6)	1.2407(-5)
18.44	2	2.67(-4)	1.1924(-3)	600	8	2.51(-6)	1.1288(-5)
18.45	2	2.66(-4)	1.1878(-3)	700	7	2.55(-6)	1.0196(-5)
18.5	2	2.61(-4)	1.1653(-3)	800	7	2.28(-6)	9.1330(-6)
18.7	2	2.45(-4)	1.0800(-3)	900	6	2.30(-6)	8.0657(-6)
19.0	2	2.24(-4)	9.6459(-4)	1000	5	2.35(-6)	7.0482(-6)
19.5	2	1.97(-4)	8.0243(-4)	1100	5	2.03(-6)	6.0924(-6)
20	3	8.47(-5)	6.5941(-4)	1150	4	2.24(-6)	5.6057(-6)
21	3	5.88(-5)	4.4170(-4)	1200	4	2.06(-6)	5.1392(-6)
22	3	4.61(-5)	3.0007(-4)	1300	3	2.16(-6)	4.3179(-6)
23	4	2.11(-5)	2.0211(-4)	1350	3	1.94(-6)	3.8791(-6)
24	5	1.18(-5)	1.3730(-4)	1400	3	1.74(-6)	3.4850(-6)
25	6	7.75(-6)	9.4081(-5)	1500	3	1.41(-6)	2.8135(-6)
26	8	4.69(-6)	6.5642(-5)	1600	2	1.48(-6)	2.2220(-6)
27	9	3.90(-6)	4.7407(-5)	1700	2	1.13(-6)	1.6887(-6)
28	11	3.05(-6)	3.5960(-5)	1750	2	9.82(-7)	1.4727(-6)
29	11	3.02(-6)	2.8876(-5)	1800	2	8.56(-7)	1.2847(-6)
30	12	2.76(-6)	2.4539(-5)	1850	2	7.47(-7)	1.1210(-6)
35	12	2.73(-6)	1.8315(-5)	1900	2	6.52(-7)	9.7837(-7)
40	12	2.72(-6)	1.7748(-5)	2000	2	4.97(-7)	7.4600(-7)
50	12	2.70(-6)	1.7583(-5)	2100	2	3.80(-7)	5.6958(-7)
75	12	2.66(-6)	1.7285(-5)	2200	2	2.90(-7)	4.3542(-7)
100	12	2.61(-6)	1.6993(-5)	2300	2	2.22(-7)	3.3333(-7)
150	12	2.53(-6)	1.6424(-5)	2400	2	1.70(-7)	2.5556(-7)
200	11	2.64(-6)	1.5830(-5)	2500	2	1.31(-7)	1.9624(-7)
250	11	2.54(-6)	1.5257(-5)	2700	2	7.75(-8)	1.1629(-7)
300	10	2.67(-6)	1.4682(-5)	3000	1	4.77(-8)	5.1018(-8)
350	10	2.56(-6)	1.4104(-5)	3500	1	1.22(-8)	1.3069(-8)
400	10	2.46(-6)	1.3548(-5)	4000	1	3.42(-9)	3.6668(-9)

With $b = 18.42068, m = 2$, and $\delta = 2.6855(-4)$, one gets $\epsilon < 1.20116(-3)$. Most entries were calculated by (4.8). The last three were calculated by (4.10).

$$\theta(x) - x > -2.06\sqrt{x} = -2.06\frac{\log^k x}{\sqrt{x}} \cdot \frac{x}{\log^k x}$$

$$\geqslant -2.06\frac{(2k)^k}{e^k} \cdot \frac{x}{\log^k x} > -\eta_k \frac{x}{\log^k x}$$

for $k = 2, 3, 4$.

THEOREM 9. *If* $\epsilon(x)$ *is defined by* (3.19) *or* (3.20), *then*

(5.10) $$\theta(x) - x \leqslant \psi(x) - x < x\epsilon(x) \quad \textit{for} \quad 0 < x,$$

(5.11) $$\psi(x) - x \geqslant \theta(x) - x > -x\epsilon(x) \quad \textit{for} \quad 39.4 \leqslant x.$$

Proof. As a result of Theorem 2, we need only verify (5.10) and (5.11) for

$x < e^{105}$. As $\epsilon(x)$ decreases for $x > 1$, we have $\epsilon(x) > 0.03$ if $x < e^{105}$. From the table and (5.2), we deduce (5.10) and (5.11) for $10^8 \leqslant x < e^{105}$. For $1 < x < 10^8$, we have $\epsilon(x) > 0.14$. Hence (3.35) of R–S gives for $0 < x < 10^8$

$$\psi(x) < 1.04x < x + x\epsilon(x).$$

And Theorem 10 of R–S implies that for $149 \leqslant x < 10^8$

$$\theta(x) > 0.86x > x - x\epsilon(x).$$

For $1 < x < 149$, $\epsilon(x) > 0.23$ so that Theorem 10 of R–S yields $\theta(x) > x - x\epsilon(x)$ for $101 \leqslant x < 149$. We readily complete the proof of (5.11) for $39.4 \leqslant x < 101$.

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