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A NEW LEHMER PAIR OF ZEROS AND A NEW LOWER BOUND FOR THE DE BRUIJN-NEWMAN CONSTANT Λ*

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Dedicated to Wilhelm Niethammer on the occasion of his 60th birthday.

Abstract. The de Bruijn-Newman constant Λ has been investigated extensively because the truth of the Riemann Hypothesis is equivalent to the assertion that $\Lambda \leq 0$. On the other hand, C. M. Newman conjectured that $\Lambda \geq 0$. This paper improves previous lower bounds by showing that

$$-5.895 \cdot 10^{-9} < \Lambda.$$

This is done with the help of a spectacularly close pair of consecutive zeros of the Riemann zeta function.

Key words. Lehmer pairs of zeros, de Bruijn-Newman constant, Riemann Hypothesis.

AMS subject classifications. 30D10, 30D15, 65E05.

1. Introduction.

It is known (cf. Titchmarsh [9, p. 255]) that the Riemann ξ-function can be expressed in the form

$$\xi\left(\frac{x}{2}\right)/8 = \int_0^\infty \Phi(u)\cos(xu)du \qquad (x \in \mathbb{C}), \tag{1.1}$$

where

$$\Phi(u) := \sum_{n=1}^{\infty} \left(2\pi^2 n^4 e^{9u} - 3\pi n^2 e^{5u}\right)\exp\left(-\pi n^2 e^{4u}\right) \qquad (0 \leq u < \infty), \tag{1.2}$$

and the *Riemann Hypothesis is the statement that all zeros of ξ are real.* If we define

$$H_t(x) := \int_0^\infty e^{tu^2}\Phi(u)\cos(xu)du \qquad (t \in \mathbb{R}; x \in \mathbb{C}), \tag{1.3}$$

then H_0 and the Riemann ξ-function are related through

$$H_0(x) = \xi\left(\frac{x}{2}\right)/8, \tag{1.4}$$

so that the Riemann Hypothesis is also equivalent to the statement that all zeros of H_0 are real.

In 1950, De Bruijn [2] established that

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(*i*) H_t has only real zeros for $t \geq 1/2$;

(*ii*) if H_t has only real zeros for some real t, then $H_{t'}$ has only real zeros for any $t' \geq t$.

C.M. Newman showed further in [6] that there is a real constant Λ, which satisfies $-\infty < \Lambda \leq 1/2$, such that

$$H_t \text{ has only real zeros if and only if } t \geq \Lambda. \tag{1.5}$$

In the literature, this constant Λ is now called the **de Bruijn-Newman constant**. The Riemann Hypothesis is equivalent to the conjecture that $\Lambda \leq 0$. On the other hand, C. M. Newman conjectured that $\Lambda \geq 0$. The significance of Newman's conjecture is that if it is true, then the Riemann Hypothesis, even if it is true, is only barely so, as even slight perturbations of the zeta function give rise to zeros that are not on the critical line.

There has been extensive recent research activity in finding lower bounds for Λ, and these results have been summarized in Csordas, Smith, and Varga [4]. In particular, the best lower bound for Λ in that paper was

$$-4.379 \cdot 10^{-6} < \Lambda. \tag{1.6}$$

It is known (cf. Csordas, Norfolk, and Varga [3]) that H_t, defined in (1.3), is an *even* real entire function of order 1 and maximal type, for each real t. Thus, from the Hadamard factorization theorem, $H_t(x)$ can be represented as

$$H_t(x) = H_t(0)\prod_{j=1}^{\infty}\left(1 - \frac{x^2}{x_j^2(t)}\right) \qquad (t \in \mathbb{R}; x \in \mathbb{C}), \tag{1.7}$$

where from (1.3) and from the fact that $\Phi(u) > 0$ for all $u \geq 0$, it follows that $H_t(0) > 0$. It is also known that

$$\sum_{j=1}^{\infty} |x_j(t)|^{-2} < \infty. \tag{1.8}$$

It is convenient to order the zeros of H_0, $\{x_j(0)\}_{j=1}^{\infty}$, in Re $z > 0$ according to increasing modulus, and, from the evenness of H_0, we set

$$x_{-j}(0) := -x_j(0) \qquad (j = 1, 2, \cdots). \tag{1.9}$$

Following Csordas, Smith, and Varga [4], we make the following

DEFINITION 1.1. *With k a positive integer, let $x_k(0)$ and $x_{k+1}(0)$ (with $0 < x_k(0) < x_{k+1}(0)$) be two consecutive simple positive zeros of H_0, and set*

$$\Delta_k := x_{k+1}(0) - x_k(0). \tag{1.10}$$

Then, $\{x_k(0); x_{k+1}(0)\}$ is a **Lehmer pair of zeros** *of H_0 if*

$$\Delta_k^2 \cdot g_k(0) < 4/5, \tag{1.11}$$

where

$$g_k(0) := \sum_{j \neq k,k+1}{}' \left\{ \frac{1}{(x_k(0) - x_j(0))^2} + \frac{1}{(x_{k+1}(0) - x_j(0))^2} \right\}; \tag{1.12}$$

here (and in what follows), the prime in the above summation means that $j \neq 0$, so that the above summation extends over all positive and negative integers with $j \neq k, k+1, 0$.

We remark that the convergence of the sum in (1.12) is guaranteed by the convergence of the sum $\sum_{j=1}^{\infty} |x_j(0)|^{-2}$ (cf. (1.8)).

With Definition 1.1, we further have from Csordas, Smith, and Varga [4] the following result.

THEOREM 1.1. *Let $\{x_k(0); x_{k+1}(0)\}$ be a Lehmer pair of zeros of H_0. If (cf. (1.12)) $g_k(0) \leq 0$, then $\Lambda > 0$. If $g_k(0) > 0$, set*

$$\lambda_k := \frac{(1 - \frac{5}{4}\Delta_k^2 \cdot g_k(0))^{4/5} - 1}{8 g_k(0)}, \tag{1.13}$$

so that $-1/[8g_k(0)] < \lambda_k < 0$. Then, the de Bruijn-Newman constant Λ satisfies

$$\lambda_k \leq \Lambda. \tag{1.14}$$

2. Application of Theorem 1.1. For our applications below, let $N(T)$ denote the number of zeros of the Riemann zeta function $\zeta(s)$, with $s = \sigma + it$, in the rectangle $0 \leq \sigma \leq 1$ and $0 \leq t \leq T$. The following result was proved by Backlund [1].

THEOREM 2.1. *$N(T)$ satisfies*

$$N(T) = \frac{T}{2\pi} \log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} + e(T), \tag{2.1}$$

where

$$|e(T)| < 0.137 \log T + 0.443 \log\log T + 4.35 \qquad (T \geq 2). \tag{2.2}$$

A straightforward calculation, based on (2.1) and (2.2), gives the following result, whose proof is given (for completeness) in the Appendix.

LEMMA 2.1. *$N(T)$ satisfies*

$$N(T+1) - N(T) \leq \log T \qquad (T \geq 3 \cdot 10^8). \tag{2.3}$$

This brings us to

LEMMA 2.2. . *Suppose $\Lambda < 0$, so that all zeros, $x_j := x_j(0)$, of H_0 are real (cf. (1.5)) and recall that $x_j = 2\gamma_j$, where $\frac{1}{2} + i\gamma_j$ is the associated zero of $\zeta(s)$. Then,*

$$\sum_{j=m}^{\infty} \frac{1}{x_j^2} \leq \frac{\log([\gamma_m] - 1) + 1}{4([\gamma_m] - 1)} \qquad ([\gamma_m] \geq 3 \cdot 10^8), \tag{2.4}$$

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where, for each real u, $[u]$ denotes the greatest integer $\leq u$.
Proof: We have

$$\begin{aligned}\sum_{j=m}^{\infty} \frac{1}{x_j^2} &= \frac{1}{4}\sum_{j=m}^{\infty} \frac{1}{\gamma_j^2} \leq \frac{1}{4}\sum_{j=[\gamma_m]}^{\infty} \sum_{j\leq \gamma_\ell < j+1} \frac{1}{\gamma_\ell^2} \\ &\leq \frac{1}{4}\sum_{j=[\gamma_m]}^{\infty} \left(\frac{N(j+1)-N(j)}{j^2}\right) \leq \frac{1}{4}\sum_{j=[\gamma_m]}^{\infty} \frac{\log j}{j^2},\end{aligned}$$

the last inequality following from (2.3) of Lemma 2.1. But, this last sum is bounded above by

$$\frac{1}{4}\int_{[\gamma_m]-1}^{\infty} \frac{\log u \; du}{u^2} = \frac{\log([\gamma_m]-1)+1}{4([\gamma_m]-1)},$$

which is the desired result of (2.4). □

In their important numerical study of the zeros of the Riemann ζ-function on the critical line, van de Lune, te Riele, and Winter [5] found a *spectacularly* close pair of consecutive simple zeros, namely, $\frac{1}{2}+i\gamma_K$ and $\frac{1}{2}+i\gamma_{K+1}$, for which (cf. (2.8))

$$\gamma_{K+1}-\gamma_K = 0.000\ 108\ 569\ 6 \qquad (K := 1,048,449,114).$$

Then, $2\gamma_K$ and $2\gamma_{K+1}$ are zeros of the function H_0, so that (cf. (1.4))

$$\text{(2.5)}\quad \begin{cases} x_K := x_K(0) = 2\gamma_K &= 7.777\ 177\ 720\ 045\ 702\ 406 \cdot 10^8, \text{ and} \\ x_{K+1} := x_{K+1}(0) = 2\gamma_{K+1} &= 7.777\ 177\ 720\ 047\ 873\ 798 \cdot 10^8, \end{cases}$$

is similarly a spectacularly close pair of consecutive simple positive zeros of H_0. The calculations of van de Lune, te Riele, and Winter [5] established that the first $1.5\cdot 10^9$ zeros are real, but they did not compute accurate values for them. Therefore, we have used a CRAY-YMP and techniques from Odlyzko [7] to determine, to high precision, a large number of zeros of H_0 on either side of the zeros of (2.5), in order to facilitate the estimation of $g_K(0)$ of (1.12). As we shall see below, only a surprisingly small number of these nearby zeros is actually needed to estimate $g_K(0)$.

The general expectation is that there are other Lehmer pairs that produce bounds for Λ that are even closer to 0 (see the discussion in Csordas, Smith, and Varga [4] and Odlyzko [8]). However, at this time we do not know of another pair that is likely to produce a better bound. The computations of van de Lune, te Riele, and Winter [5] do not prove conclusively that there is no closer pair among the first $1.5\cdot 10^9$ zeros of the zeta function. However, given the search method used, it seems unlikely that such a pair was missed. The computations of Odlyzko [8] near the zero $\frac{1}{2}+i\gamma_m$ of the ζ-function, with $m = 10^{20}$, as well as in some other high intervals, did find some close Lehmer pairs, but none of them seem to lead to results as good as we obtain here.

The proof of the next lemma is patterned after Lemma 5.1 of Csordas, Smith, and Varga [4].

LEMMA 2.3. *Suppose $\Lambda < 0$. Then, the pair of consecutive simple positive zeros $\{x_K(0); x_{K+1}(0)\}$ in (2.5) is a Lehmer pair of zeros of H_0.*
Proof. We first establish an upper bound for $g_K(0)$ of (1.12) for $K := 1,048,449,114$. Writing for convenience $x_j := x_j(0)$, $g_K(0)$ can be expressed as the sum of the following three terms:

$$\text{(2.6)}\qquad g_K(0) = M_{K,n} + I_{K,n+1} + R_{K,K+n+2}, \text{ where } n := 9,998,$$

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and where

$$M_{K,n} := \sum_{\substack{j=K-n \\ j\neq K,K+1}}^{K+n+1} \left\{ \frac{1}{(x_K - x_j)^2} + \frac{1}{(x_{K+1} - x_j)^2} \right\},$$

$$I_{K,n+1} := {\sum_{j=-K-n-1}^{K-n-1}}' \left\{ \frac{1}{(x_K - x_j)^2} + \frac{1}{(x_{K+1} - x_j)^2} \right\},$$

and

$$R_{K,K+n+2} := \sum_{|j|\geq K+n+2} \left\{ \frac{1}{(x_K - x_j)^2} + \frac{1}{(x_{K+1} - x_j)^2} \right\}.$$

We separately bound the sums $M_{K,n}, I_{K,n+1}$, and $R_{K,K+n+2}$.

Consider first $M_{K,n}$. Since $\Lambda < 0$ by hypothesis, it follows that all the zeros of H_0 are real and simple (cf. Lemma 2.2 of Csordas, Smith, and Varga [4]). Hence, from the definition of $M_{K,n}$,

$$\begin{aligned} M_{K,n} &< \sum_{\substack{j=K-n \\ j\neq K,K+1}}^{K+n+1} \left\{ \frac{1}{(x_K - x_{K-1})^2} + \frac{1}{(x_{K+1} - x_{K+2})^2} \right\} \\ &= 2n \left\{ \frac{1}{(x_K - x_{K-1})^2} + \frac{1}{(x_{K+1} - x_{K+2})^2} \right\}, \end{aligned}$$

so that

$$M_{K,n} < \frac{n}{2} \left\{ \frac{1}{(\gamma_K - \gamma_{K-1})^2} + \frac{1}{(\gamma_{K+2} - \gamma_{K+1})^2} \right\}. \tag{2.7}$$

Now, the newly computed zeros, γ_{K-1} and γ_{K+2}, along with γ_K and γ_{K+1}, are

$$\left\{ \begin{aligned} \gamma_{K-1} &= 3.888\ 588\ 853\ 843\ 374\ 083 \cdot 10^8, \\ \gamma_K &= 3.888\ 588\ 860\ 022\ 851\ 203 \cdot 10^8, \\ \gamma_{K+1} &= 3.888\ 588\ 860\ 023\ 936\ 899 \cdot 10^8, \\ \gamma_{K+2} &= 3.888\ 588\ 866\ 907\ 450\ 543 \cdot 10^8. \end{aligned} \right. \tag{2.8}$$

Thus, with the above numbers and with $n := 9,998$, the upper bound of (2.7), when rounded upward to the next integer, becomes

$$M_{K,n} < 23,642. \tag{2.9}$$

We next bound above $I_{K,n+1}$ by

$$\begin{aligned} I_{K,n+1} &< 2 {\sum_{j=-K-n-1}^{K-n-1}}' \frac{1}{(x_K - x_{K-n-1})^2} \\ &= \frac{4K}{(x_K - x_{K-n-1})^2} \\ &= \frac{K}{(\gamma_K - \gamma_{K-n-1})^2}. \end{aligned} \tag{2.10}$$

With the value of γ_K from (2.8) and with our calculated value of

$$\gamma_{K-n-1} = \gamma_{K-9999} = 3.888\ 553\ 840\ 902\ 274\ 209 \cdot 10^8,$$

the upper bound of (2.10), when rounded upward to the next integer, is

$$I_{K,n+1} < 86. \tag{2.11}$$

Finally, we bound above $R_{K,K+n+2}$. Since H_0 is an even function, we have (cf. (1.9)) $x_{-j}(0) = -x_j(0)$, so that $R_{K,K+n+2}$ can be expressed as

$$R_{K,K+n+2} = \sum_{j=K+n+2}^{\infty} \left\{ \frac{1}{(x_K - x_j)^2} + \frac{1}{(x_{K+1} - x_j)^2} + \frac{1}{(x_K + x_j)^2} + \frac{1}{(x_{K+1} + x_j)^2} \right\}. \tag{2.12}$$

Since $\frac{1}{(x_K - x_j)^2} = \frac{x_j^2}{(x_K - x_j)^2} \cdot \frac{1}{x_j^2}$, where $\frac{x_j^2}{(x_K - x_j)^2}$ is monotone decreasing for $j \geq K+n+2$, the sum of the first term from the bracketed quantity in (2.12) is bounded above by $\frac{x_{K+n+2}^2}{(x_K - x_{K+n+2})^2} \cdot \sum_{j=K+n+2}^{\infty} \frac{1}{x_j^2}$, and the sum of the third term from the bracketed quantity in (2.12) is bounded above simply by $\sum_{j=K+n+2}^{\infty} \frac{1}{x_j^2}$. With an analogous treatment for the remaining terms from the bracketed quantity in (2.12), we thus have

$$R_{K,K+n+2} < \left\{ \frac{x_{K+n+2}^2}{(x_K - x_{K+n+2})^2} + \frac{x_{K+n+2}^2}{(x_{K+1} - x_{K+n+2})^2} + 2 \right\} \cdot \sum_{j=K+n+2}^{\infty} \frac{1}{x_j^2}. \tag{2.13}$$

With the values of γ_K and γ_{K+1} from (2.8), and with the calculated value of

$$\gamma_{K+n+2} = \gamma_{K+10,000} = 3.888\ 623\ 880\ 181\ 523\ 962 \cdot 10^8, \tag{2.14}$$

we find that

$$\left\{ \frac{x_{K+n+2}^2}{(x_K - x_{K+n+2})^2} + \frac{x_{K+n+2}^2}{(x_{K+1} - x_{K+n+2})^2} + 2 \right\} = 2.465\ 957 \ldots \cdot 10^{10}.$$

Also, since $\gamma_{K+10,000}$ from (2.14) satisfies $[\gamma_{K+10,000}] > 3 \cdot 10^8$, applying Lemma 2.2 gives

$$\sum_{j=K+n+2}^{\infty} \frac{1}{x_j^2} \leq \frac{\log([\gamma_{K+n+2}] - 1) + 1}{4([\gamma_{K+n+2}] - 1)} = 1.335\ 866\ 927 \ldots \cdot 10^{-8}.$$

Substituting in the right side of (2.13) then gives, on rounding upward to the next integer,

$$R_{K,K+n+2} < 330. \tag{2.15}$$

Combining the upper estimates of (2.9), (2.11), and (2.15) gives

$$g_K(0) < 24,058. \tag{2.16}$$

But $\Delta_K := x_{K+1} - x_K = 2\,(\gamma_{K+1} - \gamma_K)$, so (2.8) gives

$$\Delta_K = 2.171\ 392\ldots\ \cdot 10^{-4}, \tag{2.17}$$

and with (2.16), we then have

$$\Delta_K^2 \cdot g_K(0) < 1.134\ 321\ldots \cdot 10^{-3} < 4/5.$$

Thus from (1.11) of Definition 1.1, $\{x_K; x_{K+1}\}$ is a Lehmer pair of zeros of H_0.□

Finally, we establish our new result, Theorem 2.2 below. If $\Lambda \geq 0$, the lower bound of (2.18) is trivially true. Hence, assume, as in Lemmas 2.2 and 2.3, that $\Lambda < 0$. We note that λ_k, as defined in (1.13), is a monotone decreasing function of $g_k(0)$ (if $\Delta_k^2 \cdot g_k(0) < 4/5$). Hence the upper bound for $g_K(0)$ in (2.16), when used to determine λ_k in (1.13), gives the lower bound $-5.895 \cdot 10^{-9}$ of (2.18) for Λ, as claimed in the Abstract above.

THEOREM 2.2. *A lower bound for the de Bruijn-Newman constant Λ is*

$$-5.895 \cdot 10^{-9} < \Lambda. \tag{2.18}$$

As remarked in Csordas, Smith, and Varga [4], the lower bound for Λ in (2.18) is quite *insensitive* to upper estimates of $g_K(0)$. This can be seen from the following Taylor series of λ_K of (1.13), in terms of $\Delta_K^2 g_K(0)$ and its powers:

$$\lambda_K = -\frac{\Delta_K^2}{8} - \frac{\Delta_K^4 g_K(0)}{64} - \frac{\Delta_K^6 g_K^2(0)}{128} - \frac{11\Delta_K^8 g_K^3(0)}{2048} - \cdots\ , \tag{2.19}$$

where we note, from (2.17), that just the first term of (2.19) is

$$-\frac{\Delta_K^2}{8} = -\ 5.893\ 679\ldots \cdot 10^{-9}.$$

3. Appendix: Proof of Lemma 2.1. By (2.1), we can write $N(T) = s(T) + e(T)$, where

$$s(T) := \left(\frac{T}{2\pi}\right)\log\left(\frac{T}{2\pi}\right) - \frac{T}{2\pi} + \frac{7}{8} \qquad (T \geq 2). \tag{3.1}$$

Then

$$s(T+1) - s(T) = \left(\frac{T+1}{2\pi}\right)\log\left(\frac{T+1}{2\pi}\right) - \left(\frac{T+1}{2\pi}\right) - \left(\frac{T}{2\pi}\right)\log\left(\frac{T}{2\pi}\right) + \left(\frac{T}{2\pi}\right).$$

Writing $\log\left(\frac{T+1}{2\pi}\right) = \log\left(\frac{T}{2\pi}\right) + \log\left(1+\frac{1}{T}\right) = \log\left(\frac{T}{2\pi}\right) + \frac{1}{T} - \frac{1}{2T^2} + \frac{1}{3T^3} - \cdots$, we find that

$$\begin{aligned} s(T+1) - s(T) &= \tfrac{\log T - \log 2\pi}{2\pi} + \tfrac{1}{2\pi}\left\{1 + \tfrac{1}{2T} - \tfrac{1}{6T^2} + \tfrac{1}{12T^3} - \cdots\right\} - \tfrac{1}{2\pi} \\ &= \tfrac{\log T - \log 2\pi}{2\pi} + \tfrac{1}{2\pi}\left\{\tfrac{1}{2T} - \tfrac{1}{6T^2} + \tfrac{1}{12T^3} - \cdots\right\} < \tfrac{\log T - \log 2\pi}{2\pi} + \tfrac{1}{4\pi T}, \end{aligned}$$

where the upper bound arises from taking the first term of the alternating series above. Hence by (2.2),

$$\begin{aligned} N(T+1) - N(T) &< \frac{\log T}{2\pi} - \frac{\log 2\pi}{2\pi} + \frac{1}{4\pi T} + |e(T+1)| + |e(T)| \\ &< \frac{\log T}{2\pi} - \frac{\log 2\pi}{2\pi} + \frac{1}{4\pi T} + 0.137\left(2\log T + \log\left(1 + \frac{1}{T}\right)\right) \\ &+ 0.886 \log\log(T+1) + 8.70 \qquad (T \geq 2). \end{aligned}$$

Using the upper bound $\log(1+\frac{1}{T}) < \frac{1}{T}$ and evaluating the constants, this gives

$$N(T+1) - N(T) \quad < \quad 0.433\ 154\ 943 \log T + 0.886 \log\log(T+1) + 8.407\ 492\ 780 + \frac{0.216\ 577\ 472}{T}. \tag{3.2}$$

It can be easily seen that

$$0.886 \log\log(T+1) \le \alpha \log T \text{ for } \alpha := 0.134\ 874\ 935 \quad (T \ge 3 \cdot 10^8), \tag{3.3}$$

and

$$8.407\ 492\ 780 \le \beta \log T \text{ for } \beta := 0.430\ 727\ 320 \qquad (T \ge 3 \cdot 10^8). \tag{3.4}$$

Thus, inserting the bounds of (3.3) and (3.4) in (3.2) gives

$$N(T+1) - N(T) < 0.998\ 757\ 198 \log T + \frac{0.216\ 577\ 472}{T} < \log T \ (T \ge 3 \cdot 10^8), \tag{3.5}$$

which is the desired result of (2.3) of Lemma 2.1. □

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