Proceedings of Symposia in Applied Mathematics
Volume 48, 1994

Lehmer Pairs of Zeros and the Riemann ξ-Function

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Dedicated to the memory of Professor Derrick H. Lehmer

ABSTRACT. A rigorous formulation is given for a pair of consecutive simple zeros of the Riemann ξ-function to be a "Lehmer pair" of zeros. It is shown that Lehmer pairs exist, and that each such pair gives a lower bound for the de Bruijn-Newman constant Λ (where the Riemann Hypothesis is equivalent to $\Lambda \leq 0$). This is applied to provide the following new lower bound for Λ:

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

The theoretical contribution of this note is a proof (based on a result of Littlewood) that if infinitely many Lehmer pairs of zeros exist, then $0 \leq \Lambda$, which is an improved version of a recent result of ours.

Let

$$H_t(x) := \int_0^\infty e^{tu^2}\, \Phi(u) \cos(xu) du \qquad (t \in \mathbb{R}; x \in \mathbb{C}), \tag{1}$$

where

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

Then H_0 is essentially Riemann's ξ-function, and the *Riemann Hypothesis is equivalent to the statement that all zeros of H_0 are real* (cf. p. 255 of [**T**]).

In 1950, de Bruijn [**B**] established that $H_t(x)$ has only real zeros for $t \geq 1/2$, and that if $H_t(x)$ has only real zeros for some real t, then $H_{t'}(x)$ also has only real zeros for any $t' \geq t$. Subsequently, C.M. Newman [**N**] showed in 1976 that there is a real constant $\Lambda \leq 1/2$ such that H_t has only real zeros if and only if

1991 *Mathematics Subject Classification.* Primary 30D10; Secondary 11M26.

Support by the National Science Foundation for this research is gratefully acknowledged.

The detailed version of this paper will appear elsewhere.

$t \geq \Lambda$. This constant Λ is now called the *de Bruijn-Newman constant*, and the Riemann Hypothesis is equivalent to the statement that $\Lambda \leq 0$.

In 1956, Lehmer [**L**] found two simple zeros of the Riemann ζ-function on the critical line which were exceptionally close to one another. This has been referred to in the literature as "*Lehmer's near counterexample*" to the Riemann Hypothesis (cf. p. 177 of [**E**]). The zeros of H_0 corresponding to these zeros are

$$x_{6709}(0) = 14,010.125\,732\ldots, \quad x_{6710}(0) = 14,010.201\,129\ \ldots. \tag{3}$$

Here, and below, we find it convenient to use the above numbering system where the zeros of H_t in Re $z > 0$ are numbered according to increasing modulus, and where, from the evenness of H_t, one has $x_{-j}(t) := -x_j(t)$ $(j = 1, 2, \ldots)$.

Differentiation under the integral sign in equation (1) shows that $H_t(x)$ satisfies the backward heat equation:

$$\frac{\partial H_t(x)}{\partial t} = -\frac{\partial^2 H_t(x)}{\partial x^2} \qquad (x, t \text{ real}).$$

From this, it is clear that if H_{t_0} has a local extremum at x_0 with $H_{t_0}(x_0) = 0$, and if $\epsilon > 0$ is sufficiently small, then H_t has no real zeros near x_0 for $t_0 - \epsilon < t < t_0$. But H_t must continue to have at least two zeros near x_0, so it follows that $t_0 \leq \Lambda$ since these zeros are necessarily nonreal. Similar considerations apply when H_{t_0} has a multiple zero of odd multiplicity, proving the following proposition.

PROPOSITION 1. *Suppose that H_{t_0} has a multiple real zero. Then $t_0 \leq \Lambda$. In particular, if $t > \Lambda$, then the zeros of H_t are real and simple.*

We next give a rigorous formulation of the notion of a "close pair" of zeros.

DEFINITION 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

$$\Delta_k := x_{k+1}(0) - x_k(0). \tag{4}$$

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

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

where

$$g_k(0) := \sum_{j \neq k, k+1}{}' \left\{ \frac{1}{(x_k(0) - x_j(0))^2} + \frac{1}{(x_{k+1}(0) - x_j(0))^2} \right\}; \tag{6}$$

here (and below), the prime in the summation means that $j \neq 0$, and the summation in (6) extends over all positive and negative integers j with $j \neq k, k+1$.

From density considerations, consecutive pairs $\{x_{k_i}(0);\ x_{k_i+1}(0)\}$ of real zeros of H_0 can be found for which $\lim_{i \to \infty} \Delta_{k_i} = 0$. We remark however that inequality (5) is not solely dependent on Δ_k, so that a Lehmer pair of zeros of H_0 requires more than just close pairs of zeros.

With the above notations, our main result can be stated as

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

$$\lambda_k := \frac{(1 - \frac{5}{4}\Delta_k^2 \cdot g_k(0))^{4/5} - 1}{8 g_k(0)}, \tag{7}$$

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

$$\lambda_k \leq \Lambda. \tag{8}$$

The details of the proof can be found in [**CSV**]; here we just indicate the method. The first step is to show that if $t_0 \geq t > \Lambda$ and if $x_k(t)$ and $x_{k+1}(t)$ are two consecutive simple positive zeros of H_t, then

$$x'_{k+1}(t) - x'_k(t) = \frac{4}{[x_{k+1}(t) - x_k(t)]} - f_k(t) \cdot [x_{k+1}(t) - x_k(t)], \tag{9}$$

where

$$f_k(t) := \sum_{j \neq k, k+1}{}' \frac{2}{[x_k(t) - x_j(t)][x_{k+1}(t) - x_j(t)]}. \tag{10}$$

If the second term on the right side of (9) were zero, then its solution would be

$$(x_{k+1}(t) - x_k(t))^2 - (x_{k+1}(t_0) - x_k(t_0))^2 = 8(t - t_0). \tag{11}$$

It would follow that H_t has a multiple real zero for $\hat{t} := t_0 - (x_{k+1}(t_0) - x_k(t_0))^2/8$, and thus $\hat{t} \leq \Lambda$ by Proposition 1. This method of establishing a lower bound for Λ remains valid if f_k is not "too large". The assumption that $\{x_k(0); x_{k+1}(0)\}$ is a Lehmer pair is what is required to provide a suitable estimate for f_k.

COROLLARY 1. *If* H_0 *has infinitely many Lehmer pairs of zeros, then* $0 \leq \Lambda$.

PROOF. If H_0 has any nonreal zeros, then $\Lambda > 0$ by definition. Hence, we may assume that H_0 has only real zeros. This implies that $g_k(0) > 0$. Now it follows from a result of Littlewood (see p. 224 of [**T**]) that the separation between the real parts of consecutive zeros of H_0 tends to zero, and so $\lim_{k \to \infty} \Delta_k = 0$, since we are assuming H_0 has only real zeros. Suppose that $\{x_{k_i}(0); x_{k_i+1}(0)\}$ are Lehmer pairs of zeros of H_0. A straightforward calculation using (7) yields that

$$-\frac{5}{32}\,\Delta_{k_i}^2 < \lambda_{k_i} < -\frac{1}{8}\,\Delta_{k_i}^2, \tag{12}$$

and consequently $\lim_{i \to \infty} \lambda_{k_i} = 0$. Hence $0 \leq \Lambda$, by Theorem 1. □

Corollary 1 above is a strengthened version of Corollary 1 of [**CSV**]. It gives credence to the conjecture of Newman [**N**] that $0 \leq \Lambda$. Note that the existence of infinitely many Lehmer pairs, as in Corollary 1, would *not* disprove the Riemann Hypothesis, but would (paraphrasing Newman [**N**]) yield a "quantitative version of the dictum that the Riemann Hypothesis, if true, is only barely so".

Theorem 1 might seem to be a purely *theoretical* result, since its application requires first showing that a given pair $\{x_k(0); x_{k+1}(0)\}$ of zeros of H_0 is a *Lehmer pair* by showing that inequality (5) is satisfied. But this inequality involves *all* (real or complex) zeros of H_0 (cf. (5) and (6)), and these zeros are certainly not all known. Fortunately, given accurate values for a sufficient number of zeros of H_0 on either side of the given pair $\{x_k(0); x_{k+1}(0)\}$, we can provide an upper bound for $g_k(0)$ which may be sufficient for satisfying (5).

Indeed, this is the case for Lehmer's pair of zeros of H_0 given in (3). Our calculations, using the tabulations of te Riele [**R**], show (see §4 of [**CSV**]) that

$$\Delta_{6709}^2 \cdot g_{6709}(0) < 6.936 \cdot 10^{-3} < 4/5, \tag{13}$$

so that this pair of zeros is a Lehmer pair of zeros. Applying Theorem 1 then yields the following lower bound for Λ:

$$-7.113 \cdot 10^{-4} < \Lambda, \tag{14}$$

which improves all previously known lower bounds for Λ (cf. [**CSV**]).

From A.M. Odlyzko's tabulation of the zeros of $\zeta(z)$ on the critical line [**O**], the minimum value of Δ_k for $1 \le k \le 2 \cdot 10^6$ occurs when $k = 1,115,578$. In the same manner, it is shown in §5 of [**CSV**] that

$$\Delta_{1,115,578}^2 \cdot g_{1,115,578}(0) < 3.001 \cdot 10^{-4} < 4/5, \tag{15}$$

and so $\{x_{1,115,578}(0); x_{1,115,579}(0)\}$ is a Lehmer pair. Applying Theorem 1 to this pair yields the lower bound $-4.379 \cdot 10^{-6} < \Lambda$, as claimed in the Abstract.

Acknowledgment. We heartily thank Dr. A.M. Odlyzko for his kindness in providing us the zeros of $\zeta(z)$ used in the computation above.

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