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THE LAGUERRE INEQUALITIES WITH APPLICATIONS TO A PROBLEM ASSOCIATED WITH THE RIEMANN HYPOTHESIS

G. CSORDAS [1,3], A. RUTTAN [2] and R.S. VARGA [2,3]

[1] *Department of Mathematics, University of Hawaii, Honolulu, HI 96822, U.S.A.*
[2] *Institute for Computational Mathematics, Kent State University, Kent, OH 44242, U.S.A.*
[3] *Research supported by the National Science Foundation.*

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We investigate here a new numerical method, based on the Laguerre inequalities, for determining lower bounds for the de Bruijn-Newman constant Λ, which is related to the Riemann Hypothesis. (Specifically, the truth of the Riemann Hypothesis would imply that $\Lambda \leqslant 0$.) Unlike previous methods which involved either finding nonreal zeros of associated Jensen polynomials or finding nonreal zeros of a certain real entire function, this new method depends only on evaluating, in real arithmetic, the Laguerre difference

$$L_1(H_\lambda(x)) := (H_\lambda'(x))^2 - H_\lambda(x) \cdot H_\lambda''(x) \quad (x, \lambda \in \mathbb{R}),$$

where $H_\lambda(z) := \int_0^\infty e^{\lambda t^2} \Phi(t) \cos(tz)\, dt$ is a real entire function. We apply this method to obtain the new lower bound for Λ,

$$-0.0991 < \Lambda,$$

which improves all previously published lower bounds for Λ.

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1. Introduction

The purpose of this paper is twofold: (i) to give a new constructive method for finding lower bounds for the de Bruijn-Newman constant Λ, which is related to the Riemann Hypothesis, and (ii) to apply this method to obtain a new lower bound for Λ.

For background, if $\zeta(z)$ denotes the Riemann ζ-function, it is known (cf. Titchmarsh [18, pp. 13, 30, and 45]) that $\zeta(z)$ has the "trivial" simple real zeros $\{-2k\}_{k=1}^{\infty}$, and all remaining zeros, which are nonreal and infinite in number, lie in the "critical" strip $0 < \operatorname{Re} z < 1$. The Riemann Hypothesis is the statement that all the zeros of $\zeta(z)$ in this critical strip lie precisely on the line $\operatorname{Re} z = 1/2$. With Riemann's definition of his ξ-function, i.e.,

$$\xi(iz) := \frac{1}{2}\left(z^2 - \frac{1}{4}\right)\pi^{-z/2-1/4}\Gamma\left(\frac{z}{2} + \frac{1}{4}\right)\zeta\left(z + \frac{1}{2}\right), \tag{1.1}$$

it can be seen from (1.1) that the *Riemann Hypothesis is equivalent to the statement that all zeros of* $\xi(z)$ *are real*. It is further known that $\xi(z)$ is an even entire function of order 1 (cf. [18, pp. 16, 29]), and that $\xi(z)$ admits the integral representation (cf. Pólya [14, p. 11] or [18, p. 255]) of the form

$$\xi\left(\frac{x}{2}\right)/8 = \int_0^\infty \Phi(t) \cos(xt) \, dt \quad (x \in \mathbb{C}), \tag{1.2}$$

where

$$\Phi(t) := \sum_{n=1}^{\infty} (2\pi^2 n^4 e^{9t} - 3\pi n^2 e^{5t}) \exp(-\pi n^2 e^{4t}) \quad (0 \leqslant t < \infty). \tag{1.3}$$

For properties of $\Phi(t)$, we have (cf. Pólya [14] or Csordas, Norfolk, and Varga [4, Theorem A]) that

$$\begin{cases} \text{(i)} & \Phi(z) \text{ is analytic in the strip } |\operatorname{Im} z| < \pi/8; \\ \text{(ii)} & \Phi(t) = \Phi(-t) \text{ and } \Phi(t) > 0 \quad (t \in \mathbb{R}); \\ \text{(iii)} & \text{for any } \epsilon > 0, \ \lim_{t \to \infty} \Phi^{(n)}(t) \exp[(\pi - \epsilon) e^{4t}] = 0 \quad (n = 0, 1, \cdots). \end{cases}$$

As in Csordas, Norfolk, and Varga [5], the entire function $H_\lambda(x)$ is defined by

$$H_\lambda(x) := \int_0^\infty e^{\lambda t^2} \Phi(t) \cos(xt) \, dt \quad (\lambda \in \mathbb{R}; \ x \in \mathbb{C}), \tag{1.5}$$

so that from (1.2),

$$H_0(x) = \xi\left(\frac{x}{2}\right)/8. \tag{1.6}$$

It was shown in [5, Appendix A] that for each real λ, $H_\lambda(x)$, as defined in (1.5), is an even real entire function of order 1 and of maximal type (i.e., its type (cf. Boas [1, p. 8]) is infinite). We note from (1.6), that *the Riemann Hypothesis is equivalent to the statement that all zeros of* $H_0(x)$ *are real*.

Next, de Bruijn [3] in 1950 established that

$$\begin{cases} \text{(i)} & H_\lambda(x) \text{ has only real zeros for } \lambda \geqslant 1/2; \\ \text{(ii)} & \text{if } H_\lambda(x) \text{ has only real zeros for some real } \lambda, \text{ then} \\ & H_{\lambda'}(x) \text{ also has only real zeros for any } \lambda' \geqslant \lambda. \end{cases} \tag{1.7}$$

In particular, we see from (1.7(ii)) that if the Riemann Hypothesis is true, then $H_\lambda(x)$ must possess only real zeros for any $\lambda \geqslant 0$. In 1976, C.M. Newman [11] showed that there exists a real number Λ, satisfying $-\infty < \Lambda \leqslant 1/2$, such that

$$\begin{cases} \text{(i)} & H_\lambda(x) \text{ has only real zeros if and only if } \lambda \geqslant \Lambda; \\ \text{(ii)} & H_\lambda(x) \text{ has some nonreal zeros if and only if } \lambda < \Lambda. \end{cases} \tag{1.8}$$

This constant Λ has been called in [5] the *de Bruijn-Newman constant*. Note that *if* the Riemann Hypothesis is true, then from (1.8(i)), Λ would satisfy $\Lambda \leqslant 0$. (In [11], Newman offers the complementary conjecture that $\Lambda \geqslant 0$.)

Because of the relationship of Λ to the Riemann Hypothesis, there has been recent interest in determining lower bounds for Λ. The first constructive lower bound,

$$-50 < \Lambda,$$

was given in 1988 in [5]. Subsequently, te Riele [16] has given in 1991 strong numerical evidence that

$$-5 < \Lambda.$$

Most recently, Varga, Norfolk, and Ruttan [19] have shown that

$$-0.385 < \Lambda,$$

using a tracking technique which yielded a nonreal zero of the function $F_\lambda(z)$, defined by

$$F_\lambda(z) := \int_0^\infty e^{\lambda t^2} \Phi(t) \cosh(t\sqrt{z})\, dt \quad (\lambda \in \mathbb{R};\ z \in \mathbb{C}),$$

where the entire function F_λ of (1.9) and H_λ of (1.5) are related (cf. [19]) through

$$F_\lambda(-z^2) = H_\lambda(z) \quad (\lambda \in \mathbb{R};\ z \in \mathbb{C}). \tag{1.10}$$

As stated earlier, our purpose here is to define a new constructive method for finding lower bounds for Λ, and to apply this method to obtain a new lower bound for Λ. This new lower bound, to be established in §3, is the result of

THEOREM 1

If Λ is the de Bruijn-Newman constant, then

$$-0.0991 < \Lambda. \tag{1.11}$$

In the next section, we define the functions in the Laguerre-Pólya class and the Laguerre differences.

2. The Laguerre-Pólya Class and the Laguerre inequalities

Since $H_\lambda(x)$ of (1.5) is a real entire function of order 1, then the relation in (1.10) shows that the function $F_\lambda(z)$ of (1.9) is a real entire function of order 1/2. Consequently (cf. [1, p. 24]), $F_\lambda(z)$ has infinitely many zeros which, with (1.10), implies that $H_\lambda(x)$ also has infinitely many zeros. Denoting the zeros of $F_\lambda(z)$ by $\{z_n(\lambda)\}_{n=1}^\infty$, then as none of these zeros can be at the origin since (cf. (1.4(ii)))

$$F_\lambda(0) = \int_0^\infty e^{\lambda t^2} \Phi(t)\, dt > 0 \quad (\lambda \in \mathbb{R}),$$

these zeros of $F_\lambda(z)$ can be arranged so that

$$0 < |z_1(\lambda)| \leqslant |z_2(\lambda)| \cdots \quad (\lambda \in \mathbb{R}).$$

Hence, the Hadamard factorization theorem, applied to $F_\lambda(z)$, gives that $F_\lambda(z)$ can be represented as

$$F_\lambda(z) = C(\lambda) \prod_{n=1}^{\infty} \left(1 - \frac{z}{z_n(\lambda)}\right), \quad \text{where } \sum_{n=1}^{\infty} |z_n(\lambda)|^{-1} < \infty. \tag{2.1}$$

Thus, from (1.10), the entire function $H_\lambda(x)$ can be similarly expressed in the form

$$H_\lambda(x) = C(\lambda) \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{x_n^2(\lambda)}\right) \quad (\lambda \in \mathbb{R},\ x_n^2(\lambda) := -z_n(\lambda)), \tag{2.2}$$

where $0 < |x_1(\lambda)| \leqslant |x_2(\lambda)| \leqslant \cdots$, with $\sum_{n=1}^{\infty} |x_n(\lambda)|^{-2} < \infty$.

Next, the *Laguerre-Pólya class* is defined as the collection of all entire functions $f(x)$ which can be expressed in the following form:

$$f(x) = C\, e^{-\alpha x^2 + \beta x} x^n \prod_{j=1}^{w} \left(1 - \frac{x}{x_j}\right) e^{x/x_j} \quad (0 \leqslant w \leqslant \infty), \tag{2.3}$$

where $\alpha \geqslant 0$, β and C are real numbers, n is a nonnegative integer, and the x_j's are real and nonzero which satisfy $0 < |x_1| \leqslant |x_2| \leqslant \cdots$ and $\sum_{j=1}^{w} x_j^{-2} < \infty$. (For any such entire function $f(x)$, we write $f \in \mathscr{L}-\mathscr{P}$.) With this notation, it follows from (2.2) that (1.8) can be equivalently expressed succinctly as

$$H_\lambda \in \mathscr{L}-\mathscr{P} \quad \text{if and only if } \lambda \geqslant \Lambda. \tag{2.4}$$

By way of notation, for any real entire function $g(x)$, we set

$$L_n(g(x)) := \frac{1}{(2n)!} \sum_{k=0}^{2n} (-1)^{k+n} \binom{2n}{k} g^{(k)}(x) g^{(2n-k)}(x)$$
$$(x \in \mathbb{R};\ n = 0, 1, \cdots), \tag{2.5}$$

and we term $L_n(g(x))$ the n^{th} *Laguerre difference* for $g(x)$. The following result of Csordas and Varga [6], giving necessary and sufficient conditions in terms of Laguerre differences for certain real entire functions to be in the Laguerre-Pólya class, extends results of Obreschkoff [12], Patrick [13], and Skovgaard [17].

THEOREM A ([6])

Let

$$f(z) = e^{-\alpha z^2} g(z), \tag{2.6}$$

where $\alpha > 0$ *and where* $g(z)(\not\equiv 0)$ *is a real entire function of genus* 0 *or* 1. *Then,* $f \in \mathscr{L}-\mathscr{P}$ *if and only if* (*cf.* (2.5))

$$L_n(f^{(p)}(x)) \geqslant 0 \quad (x \in \mathbb{R};\ n = 0, 1 \cdots;\ p = 0, 1, \cdots). \tag{2.7}$$

If $n=1$ and $p=0$, then (2.7) of Theorem A reduces from (2.5) to

$$L_1(f(x)) = (f'(x))^2 - f(x)f''(x) \geqslant 0 \quad (x \in \mathbb{R}), \tag{2.8}$$

and the inequality (2.8) is called, in the literature, the *Laguerre inequality* for $f(x)$. Thus, Theorem A asserts, in particular, that if $f \in \mathscr{L}-\mathscr{P}$, then the Laguerre inequality of (2.8) necessarily holds. Clearly, (2.8) is only a *necessary condition* for a real entire function $f(x)$ to belong to the Laguerre-Pólya class. Indeed, if

$$h(x) := e^x - e^{2x}, \text{ so that } h^{(p)}(x) = e^x - 2^p e^{2x} \quad (p = 0, 1, \cdots), \tag{2.9}$$

then

$$L_1(h^{(p)}(x)) = 2^p e^{3x} > 0 \quad (x \in \mathbb{R};\ p = 0, 1, \cdots), \tag{2.10}$$

so that $h(x)$, as well as *all* its derivatives, satisfy the Laguerre inequality of (2.8). But, it is evident that $h^{(p)}(x)$ is not an element in $\mathscr{L}-\mathscr{P}$ for any $p = 0, 1, \cdots$, since $h^{(p)}(x)$, from (2.9), has the *nonreal* zeros $-p \log 2 + 2\pi i k$ ($k = \pm 1, \pm 2, \cdots$).

On combining (2.4) and the special case $n=1$ and $p=0$ of (2.8) from Theorem A, we immediately have the result of

PROPOSITION 2

Suppose that, for some real λ and for some real x, the real entire function H_λ of (1.5) *satisfies*

$$L_1(H_\lambda(x)) < 0. \tag{2.11}$$

Then (cf. (2.4)),

$$\lambda < \Lambda. \tag{2.12}$$

The proof of Theorem 1 in §3 is explicitly based on Proposition 2, where, for the particular choice $\hat{\lambda} := -0.0991$ and for a particular real X (cf. (3.12)), it will be shown that $L_1(H_{\hat{\lambda}}(X)) < 0$; whence (cf. (2.12)), $\hat{\lambda} < \Lambda$, which is the desired result of (1.11) of Theorem 1.

It may be asked here why the *particular* Laguerre difference $L_1(g)$ in (2.11) was singled out in Proposition 2, since, from Theorem A, *any* Laguerre difference $L_n(g)$ with $L_n(H_\lambda(x)) < 0$ could have been used. A reason for this choice is given in Lemma 3 below.

LEMMA 3

Let $g(x)$ be a real entire function, and define

$$f(x) := \left[(x-\alpha)^2 + \beta^2\right]^m g(x) \quad (\alpha \in \mathbb{R},\ \beta > 0,\ m \text{ a positive integer}), \tag{2.13}$$

so that $\alpha \pm i\beta$ *are two nonreal zeros of order* m *of* $f(x)$. *If* $g(\alpha) \neq 0$, *then*

$$L_1(f(\alpha)) = -2m\beta^{4m-2}(g(\alpha))^2 + \beta^{4m}L_1(g(\alpha)). \tag{2.14}$$

Thus, if

$$M := \begin{cases} \dfrac{2m(g(\alpha))^2}{L_1(g(\alpha))}, & \text{if} \quad L_1(g(\alpha)) > 0, \\ +\infty, & \text{if} \quad L_1(g(\alpha)) \leqslant 0. \end{cases} \tag{2.15}$$

then

$$L_1(f(\alpha)) < 0 \text{ for all } 0 < \beta < M. \tag{2.16}$$

Proof

A straightforward calculation using logarithmic differentiation and the fact that $f(\alpha) = \beta^{2m}g(\alpha)$, directly gives (2.14), which, with (2.15), then yields (2.16). □

The result (2.16) of Lemma 3 can be paraphrased as follows: a pair of conjugate complex zeros $\alpha \pm i\beta$ of $f(x)$ of (2.13), when $\beta > 0$ is sufficiently small, forces $L_1(f(\alpha))$ to be negative. This will play an essential role in our new numerical method for finding lower bounds for the de Bruijn-Newman constant Λ, which will be described in detail in §4.

3. Proof of Theorem 1

It is known, from the impressive computations of van de Lune, te Riele, and Winter [9], that the first $T := 1{,}500{,}000{,}001$ nontrivial zeros of the Riemann ζ-function in the upper critical strip $0 < \text{Re } z < 1$ with $\text{Im } z > 0$, are all of the form

$$\rho_n := \tfrac{1}{2} + i\gamma_n \text{ where } 0 < \gamma_1 < \gamma_2 < \cdots < \gamma_T, \tag{3.1}$$

and that all these zeros are *simple*, i.e., $\zeta'(\rho_n) \neq 0$. This, coupled with (1.1) and (1.6), gives (since $H_\lambda(x)$ is an even function for any λ real) that

$$\begin{cases} \text{(i)} \quad H_0(-2\gamma_n) = 0 \quad (n = 1, 2, \ldots, T), \text{ and} \\ \text{(ii)} \quad H_0'(-2\gamma_n) \neq 0 \quad (n = 1, 2, \cdots, T). \end{cases} \tag{3.2}$$

Since the zeros $\{\rho_n\}_{n=1}^T$ of $\zeta(z)$ in (3.1) are all simple, then

$$\tau_n := |\rho_n \zeta'(\rho_n)|^{-1} \tag{3.3}$$

is a well-defined positive real number for each $n = 1, 2, \cdots, T$. Thus, from (1.1), (1.6) and (3.3), a calculation shows that

$$|H_0'(-2\gamma_n)| = \frac{|\rho_n| \cdot |\Gamma(\rho_n/2)|}{32\pi^{1/4}\tau_n} \quad (n = 1, 2, \cdots, T), \tag{3.4}$$

where the relationship in (3.4) will be used below.

In Table 1 of te Riele [15], one finds the numbers $\{\gamma_n\}_{n=1}^{15,000}$, accurate to approximately 28 significant digits, and in Table 2 of [15], one finds the numbers $\{\tau_n\}_{n=1}^{15,000}$, accurate to approximately 10 significant digits. Concentrating on the particularly close pair of zeros of $\zeta(z)$, namely

$$\rho_{212} = \tfrac{1}{2} + \mathrm{i}\gamma_{212} \quad \text{and } \rho_{213} = \tfrac{1}{2} + \mathrm{i}\gamma_{213}, \tag{3.5}$$

we have, from [15, Table 1], that

$$\begin{cases} \gamma_{212} = 415.\,01880\ 97551\ 55115\ 64631\ 92115, \\ \gamma_{213} = 415.\,45521\ 49962\ 94598\ 85712\ 87825, \end{cases} \tag{3.6}$$

while from [15, Table 2], we have (cf. (3.3))

$$\begin{cases} \tau_{212} = 0.14878\ 74760 \times 10^{-2} \\ \tau_{213} = 0.12561\ 94402 \times 10^{-2}. \end{cases} \tag{3.7}$$

Hence, with the complex form of Stirling's formula (cf. Henrici [7, p. 377]), i.e.,

$$\Gamma(z) = \sqrt{2\pi}\ \exp\left[\left(z - \tfrac{1}{2}\right) \ln z - z\right] \mathrm{e}^{J(z)}, \tag{3.8}$$

where the Binet function $J(z)$ in (3.8) has the asymptotic representation (cf. [7, p. 359])

$$J(z) \approx \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5} - \frac{1}{1680z^7} + \cdots$$
$$(z \to \infty \text{ with } |\arg z| \leqslant \pi/2), \tag{3.9}$$

it is possible from (3.4) to estimate $|H_0'(-2\gamma_{212})|$ and $|H_0'(-2\gamma_{213})|$. Indeed, we find that

$$\begin{cases} |H_0'(-2\gamma_{212})| = 1.18968\ldots \times 10^{-138}, \\ |H_0'(-2\gamma_{213})| = 1.00098\ldots \times 10^{-138}. \end{cases} \tag{3.10}$$

It is the *smallness* of the two numbers in (3.10) which prompted our use of *high-precision* in our numerical calculations, to be discussed in §4 and §5.

This brings us to the

Proof of Theorem 1

With (1.5), we see that

$$\begin{cases} H_\lambda(x) = \int_0^\infty e^{\lambda t^2}\Phi(t)\cos(xt)\,dt, \\ H_\lambda'(x) = -\int_0^\infty t\,e^{\lambda t^2}\Phi(t)\sin(xt)\,dt, \\ H_\lambda''(x) = -\int_0^\infty t^2\,e^{\lambda t^2}\Phi(t)\cos(xt)\,dt. \end{cases} \tag{3.11}$$

For the particular values

$$X := -830.51222\ 23698\ 70977\ 76903\ 53 \text{ and } \hat{\lambda} := -0.0991, \tag{3.12}$$

the integrals $\{H_{\hat\lambda}^{(j)}(X)\}_{j=0}^{2}$ from (3.11) were numerically determined, each to an absolute accuracy (cf. §6) of 10^{-200} using 210 digit floating point arithmetic. The calculated approximations are

$$\left.\begin{aligned} H_{\hat\lambda}(X) \doteqdot -6.69844\ &92854\ 36698\ 50022\ 46215\ 55350\ 75726\ 97379\ 36465 \\ &24345\ 31495\ 72840\ 88049\ 22773\ 35031\ 74716\ 55792 \\ &12935\ 13450\ 08355\ 25610\ 96074\ 40992\ 74294\ 85514 \\ &96610\ 14950\ 89343\ 68820\ 06031\ 51781\ 54358\ 86512 \\ &57173\ 87696\ 46318\ 14500\ 26289\ 08756\ 4258\quad E\text{-}143, \\ H_{\hat\lambda}'(X) \doteqdot -8.30046\ &96964\ 81693\ 93998\ 18551\ 31834\ 89533\ 94361\ 64158 \\ &17471\ 35631\ 81922\ 57659\ 58807\ 08167\ 39482\ 48240 \\ &64016\ 57319\ 47243\ 57671\ 23339\ 45055\ 51722\ 18218 \\ &74313\ 34850\ 98125\ 67169\ 99313\ 90861\ 09051\ 59390 \\ &33845\ 43089\ 00053\ 68532\ 20245\ 75207\ 1103\quad E\text{-}156, \\ H_{\hat\lambda}''(X) \doteqdot -2.29889\ &40844\ 83868\ 42954\ 59661\ 54783\ 43796\ 56798\ 41808 \\ &60451\ 74239\ 61487\ 51577\ 21096\ 52957\ 35073\ 02363 \\ &25673\ 65141\ 03585\ 83713\ 33482\ 17015\ 95085\ 22944 \\ &85914\ 18790\ 21836\ 12152\ 38568\ 11604\ 93831\ 13554 \\ &75425\ 73952\ 49006\ 47667\ 45243\ 55758\ 0477\quad E\text{-}138. \end{aligned}\right\} \tag{3.13}$$

The magnitude of these numbers, together with the magnitude of the absolute error of the calculation, yields that the approximations given in (3.13) must agree with the actual values of $H_{\hat\lambda}(x)$, $H_{\hat\lambda}'(x)$ and $H_{\hat\lambda}''(x)$ to at least 43 significant digits ($43 = 200 - 156 - 1$). With these numbers $\{H_{\hat\lambda}^{(j)}(X)\}_{j=0}^{2}$, the Laguerre difference, $L_1(H_{\hat\lambda}(X))$, was determined (cf. (2.8)):

$$L_1(H_{\hat\lambda}(X)) := \left(H_{\hat\lambda}'(X)\right)^2 - H_{\hat\lambda}(X)\cdot H_{\hat\lambda}''(X) = -1.53990\ldots\times 10^{-280} < 0. \tag{3.14}$$

As $L_1(H_\lambda(X)) < 0$, it follows from (2.12) of Proposition 2 that

$$-0.0991 < \Lambda, \tag{3.15}$$

the desired result of Theorem 1. □

4. The Laguerre difference method

Before giving in §6 the details on how the integrals of (3.13) were computed and how the accuracies of these numbers can be guaranteed, we describe in this section our new Laguerre difference method, from which the numbers, appearing so mysteriously in (3.12), arose. In addition to this method's dependence on the Laguerre difference $L_1(f(x))$ of (2.8), it also depends on Lemma 4 and its Corollary, which are given below. We remark that Lemma 4 is an extension, for our purposes, of the classical Laguerre theorem on the separation of zeros of certain entire functions (cf. [1, p. 23]).

LEMMA 4

Let $f(x)$ be a real entire function of the form

$$f(x) = C\,\mathrm{e}^{-\alpha x^2+\beta x} \prod_{k=1}^{\infty}\left(1-\frac{x}{x_k}\right)\mathrm{e}^{x/x_k} \prod_{j=1}^{w}\left(1-\frac{x}{z_j}\right)\mathrm{e}^{x/z_j} \prod_{j=1}^{w}\left(1-\frac{x}{\bar{z}_j}\right)\mathrm{e}^{x/\bar{z}_j}, \tag{4.1}$$

where $\alpha \geqslant 0$, $C \neq 0$ and β are real numbers, the x_k's are nonzero real numbers $(1 \leqslant k \leqslant \infty)$ and the z_j's are nonzero complex numbers $(1 \leqslant j \leqslant w$, where $0 \leqslant w \leqslant \infty)$ which satisfy $\sum_{k=1}^{\infty} 1/x_k^2 < \infty$ and $\sum_{j=1}^{w} 1/|z_j|^2 < \infty$. Assume that there is a finite real interval $[A, B]$ with $B - A > 2$, such that

all zeros of $f(x)$ in the vertical strip $A \leqslant \mathrm{Re}\ x \leqslant B$ are real and simple, (4.2)

and that all the complex zeros z_j of $f(z)$ satisfy

$$|\mathrm{Im}\ z_j| < 1 \quad (1 \leqslant j \leqslant w). \tag{4.3}$$

Then,

$$L_1(f(x)) := (f'(x))^2 - f(x)\cdot f''(x) > 0 \text{ for all } x \in [A+1, B-1]. \tag{4.4}$$

Moreover, if x_n and x_{n+1} (with $x_{n+1} > x_n$) are any two consecutive real zeros of $f(x)$ in the interval $[A+1, B-1]$, then $f'(x)$ has exactly one zero in the interval (x_n, x_{n+1}).

Proof

Setting $z_j := \alpha_j + \mathrm{i}\beta_j$ $(\alpha_j, \beta_j \in \mathbb{R};\ 1 \leqslant j \leqslant w)$, then logarithmic differentiation of f(x) in (4.1) gives, from the definition of $L_1(f(x))$, that

$$L_1(f(x)) = (f(x))^2 \left\{ 2\alpha + \sum_{k=1}^{\infty} \frac{1}{(x-x_k)^2} + 2\sum_{j=1}^{w} \frac{(x-\alpha_j)^2 - \beta_j^2}{\left[(x-\alpha_j)^2 + \beta_j^2\right]^2} \right\}.$$

If $w = 0$ (i.e., the last two products of (4.1) are vacuous), we see from (4.5) that $L_1(f(x)) > 0$ for all real x, which is stronger than the desired result of (4.4). If $w > 0$, then the hypotheses of (4.2) and (4.3) imply that

$$(x-\alpha_j)^2 - \beta_j^2 > 0 \text{ for any } x \in [A+1,\ B-1] \text{ and any } j \text{ with } 1 \leqslant j \leqslant w,$$

which, from (4.5), gives the desired result of (4.4).

For the final assertion of Lemma 4, let x_n and x_{n+1} (with $x_n < x_{n+1}$) be any two consecutive zeros of f in $[A+1,\ B-1]$. Then, f is of one sign in $(x_n,\ x_{n+1})$ and by Rolle's Theorem, f' has an odd number ($\geqslant 1$) of zeros in $(x_n,\ x_{n+1})$. Suppose, on the contrary, that f' has more than one zero on $(x_n,\ x_{n+1})$, say 3 consecutive zeros, a, b and c, with $x_n < a < b < c < x_{n+1}$, where f' is of one sign in $(a,\ b)$. From (4.4), a, b, and c are each necessarily simple zeros of f' in $[A+1,\ B-1]$. From Rolle's theorem again, f'' has an odd number of zeros in $(a,\ b)$, and so, in particular, since f' is of one sign on $(a,\ b)$, then

$$f''(a) \cdot f''(b) < 0 \quad \text{with } f'(a) = 0 = f'(b). \tag{4.6}$$

Thus, it follows from (4.6) that

$$\begin{aligned} L_1(f(a)) \cdot L_1(f(b)) &= [-f(a)f''(a)] \cdot [-f(b) \cdot f''(b)] \\ &= [f(a)f(b)](f''(a)f''(b)) < 0, \end{aligned} \tag{4.7}$$

since f is of one sign on $(x_n,\ x_{n+1})$, i.e., $f(a)f(b) > 0$. But as a and b are points of $[A+1,\ B-1]$, this contradicts (4.4). □

To apply Lemma 4, consider the Riemann ξ-function of (1.1). It can be verified from (1.1) that, since all the nonreal zeros of $\zeta(z)$ lie in the critical strip $0 < \text{Re } z < 1$, all (real or complex) zeros of $\xi(x)$ necessarily lie in the horizontal strip $|\text{Im z}| < 1/2$. With (1.6), this implies that all (real or complex) zeros of $H_0(x)$ lie in the horizontal strip

$$|\text{Im } z| < 1, \tag{4.8}$$

which similarly appears in hypothesis (4.3) of Lemma 4. As was mentioned in §1, $H_0(x)$ is an even real entire function, of order one, so H_0 satisfies the hypothesis of Lemma 4, up to the determination of an appropriate interval $[A,\ B]$. But from the numerical results of van de Lune, te Riele, and Winter [9], it is known that for

$$\mu := 545,\ 439,\ 823.215, \tag{4.9}$$

there are precisely $T := 1,\ 500,\ 000,\ 001$ simple zeros of ζ, in $0 < \text{Re } z < 1$ and $0 < \text{Im } z < \mu$, which lie exactly on $\text{Re } z = 1/2$. Hence, with the identities of

(1.1), and (1.6), it follows that H_0 has only real simple zeros (numbering $2T =$ 3, 000, 000, 002) in the vertical strip $-2\mu \leqslant \text{Re } z \leqslant 2\mu$, and applying Lemma 4 with $A = -2\mu$ and $B = 2\mu$ gives the

COROLLARY

For the entire function $H_0(x) := \xi(x/2)$,

$$L_1(H_0(x)) > 0 \text{ on } [-2\mu + 1, 2\mu - 1], \quad (2\mu = 1.0908 \ldots 10^9), \tag{4.10}$$

where μ *is defined in* (4.9). *Moreover, between any two consecutive real zeros of* H_0 *in* $[-2\mu + 1, 2\mu - 1]$, H_0' *has exactly one zero.*

We now describe our *Laguerre difference method*. For the initial value $\lambda = 0$, take any two consecutive real zeros of H_0, say $-2\gamma_{n+1}$ and $-2\gamma_n$, where it is assumed that

$$\gamma_{n+1} < \mu - 1/2, \tag{4.11}$$

so that Lemma 4 applies to H_0. (The numerical example in §3 corresponds to the choice $n = 212$, and as $\gamma_{213} = 415.455\ldots$ from (3.6), (4.11) is trivially satisfied in this case!) From the Corollary of Lemma 4, there is a *unique* real $x(0)$, satisfying $-2\gamma_{n+1} < x(0) < -2\gamma_n$, for which

$$H_0'(x(0)) = 0, \tag{4.12}$$

and $x(0)$ was iteratively determined using Newton's method, i.e.,

$$y_{j+1} := y_j - \frac{H_0'(y_j)}{H_0''(y_j)} \quad (j = 1, 2, \cdots), \tag{4.13}$$

where $\lim_{j\to\infty} y_j = x(0)$. (Note that this use of Newton's method requires the simultaneous evaluation of the integrals $H_0'(y_j)$ and $H_0''(y_j)$, so that in the process of determining $x(0)$, the numbers $H_0'(x(0))$ and $H_0''(x(0))$ are also determined.) Then, on evaluating $H_0(x(0))$, the Laguerre difference, with (4.12), satisfies

$$\begin{aligned} L_1(H_0(x(0))) &:= (H_0'(x(0)))^2 - H_0(x(0)) \cdot H_0''(x(0)) \\ &= -H_0(x(0)) \cdot H_0''(x(0)). \end{aligned} \tag{4.14}$$

For this initial choice of $\lambda = 0$, the above quantity is evidently positive from Lemma 4. Consequently, neither $H_0(x(0))$ nor $H_0''(x(0))$ is zero; whence, $x(0)$ is a simple zero of H_0'. Then, $\lambda = 0$ was decreased by a sufficiently small amount to $\lambda_1 < 0$, so that in analogy with (4.12), a number $x(\lambda_1)$ (close to $x(0)$) exists for which

$$H_{\lambda_1}'(x(\lambda_1)) = 0. \tag{4.15}$$

Then, $x(\lambda_1)$ was determined using Newton's method, which again required for

Newton's method the simultaneous evaluation of the integrals $H'_{\lambda_1}(x)$ an $H''_{\lambda_1}(x(\lambda_1))$ and (4.15),

$$L_1\big(H_{\lambda_1}(x(\lambda_1))\big) = -H_{\lambda_1}(x(\lambda_1))H''_{\lambda_1}(x(\lambda_1)) \tag{4.16}$$

was determined. If the Laguerre difference (4.16) was nonnegative, λ_1 wa further decreased, and this process was terminated when a real value of $\lambda <$ was found for which $L_1(H_\lambda(x(\lambda))$ was negative. As indicated by the reasoning i §2, the initial pair of real zeros (when $\lambda = 0$), namely $-2\gamma_{213}$ and $-2\gamma_{212}$ c $H_0(x)$, had, in the process of decreasing λ from zero, become two *nonrea* complex conjugate zeros of $H_\lambda(x)$, which produced the lower bound of Λ c Theorem 1.

We emphasize that this Laguerre difference, when applied to *arbitrar* consecutive pairs of zeros of $H_0(x)$, will generally *fail* to produce a value c $\lambda < 0$ and an $x(\lambda)$ for which $L_1(H_\lambda(x(\lambda)) < 0$. Certain consecutive pairs of zero of $H_0(x)$, from which the method begins, *do*, on the other hand, produce lowe bounds for the de Bruijn-Newman constant Λ. This is discussed in the nex section.

5. General comments for future numerical work

It is our opinion that the method proposed here, based on the *real* arithmeti calculation of $\{H_\lambda^{(j)}(x)\}_{j=0}^{2}$ and the Laguerre difference $L_1(H_\lambda(x))$, has computa tional advantages over the two techniques, using *complex* arithmetic, which wer previously used to find lower bounds for the de Bruijn-Newman Λ. The firs technique, used by Csordas, Norfolk, and Varga [5] to produce the lower boun

$$-50 < \Lambda, \tag{5.1}$$

and its improvement by the Riele [16] to

$$-5 < \Lambda, \tag{5.2}$$

in essence sought nonreal zeros of associated Jensen polynomials, as defined i [5], by tracking a particular pair of zeros, $x_4(\lambda)$ and $x_5(\lambda)$ of $H_\lambda(x)$, starting wit

$$x_4(0) := -2\gamma_4 = -60.84975\ldots \text{and } x_5(0) := -2\gamma_5 = -65.87012\ldots, \tag{5.3}$$

as λ decreased from zero. Similarly, in Varga, Norfolk, and Ruttan [19], tracking procedure (not involving Jensen polynomials) of nonreal zeros wa applied to the function $F_\lambda(x)$ of (1.9), starting in essence with the particular pai of zeros of $x_{34}(0)$ and $x_{35}(0)$ of $H_\lambda(x)$ as λ decreased from zero, where initiall

$$x_{34}(0) = -2\gamma_{34} = -222.05907\ldots \text{and } x_{35}(0) = -2\gamma_{35} = -223.74931\ldots. \tag{5.4}$$

This produced the lower bound of [19] of

$$-0.385 < \Lambda. \tag{5.5}$$

Using the new Laguerre difference method of this paper, we repeated the above calculations by also starting with the initial pair of zeros of (5.3), and this produced the *improvement* of (5.1) and (5.2) to

$$-3.9 < \Lambda; \tag{5.6}$$

similarly, the Laguerre difference method, starting with the initial pair of zeros of (5.4), produced the improvement of (5.5) to

$$-0.38 < \Lambda. \tag{5.7}$$

We wish to also comment here on the possibility of using this Laguerre difference method to produce even *better* lower bounds than reported in (1.11) of Theorem 1. In each case mentioned above, we had applied this Laguerre difference method, starting (at $\lambda = 0$) with a pair of successive zeros of $H_0(x)$, say $-2\gamma_n$ and $-2\gamma_{n+1}$, for which γ_n and γ_{n+1} were *close*. Because these starting values were crucial, we give in Table A below *all* the successive values of γ_n $(2 \leqslant n \leqslant 15{,}000)$, where, if

$$\Delta_j := \gamma_{j+1} - \gamma_j \quad (j = 1, 2, \cdots, T-1;\ T := 1{,}500{,}000{,}001),$$

then the difference Δ_n was *smaller* than *all* previous differences Δ_j, i.e.,

$$\Delta_n < \min_{1 \leqslant j \leqslant n-1} \Delta_j, \tag{5.8}$$

and we call the differences Δ_n satisfying (5.8) *super differences*. In our Table A (all of whose entries are truncated to five decimal places), we also estimate $|H_0'(-2\gamma_n)|$. These estimates of $|H_0'(-2\gamma_n)|$ are derived from (3.4), using (3.8) and (3.9). It is at this point that the numbers τ_n of (3.3) are used. We remark that all entries in in Table A can be deduced from Tables 1 and 2 of te Riele [15], on using (3.4).

The lower bound of (1.11) for Λ of this paper specifically came from applying this Laguerre difference method (with the starting values $\lambda = 0$ and the two zeros $-2\gamma_{212}$ and $-2\gamma_{213}$ of $H_0(x)$), determined from the row corresponding to $n = 212$ of Table A. There is every reason to believe that the application of this new method to subsequent rows of Table A, will produce further *improved* lower bounds for Λ. However, the last column of Table A, which gives values of $|H_0'(-2\gamma_n)|$, indicates that the associated calculations must be done with successively *greater precision*, and such calculations will undoubtedly require significantly more computer time! (For example, to apply this method to the starting values associated with the row for $n = 1496$ of Table A, one would have to carry out all computations with approximately 750 floating point significant digits.)

We remark that the last column, of $|H_0'(-2\gamma_n)|$, of Table A depends specifically on the numbers $\{\tau_n\}_{n=1}^{15{,}000}$ which were compiled in Table 2 of Riele [15], and, to our knowledge, this compilation has not been extended beyond $n = 15{,}000$. However, it may be of interest to the readers to have a listing

Table A
Super differences ($2 \leqslant n \leqslant 15{,}0000$)

n	γ_n	$\Delta := \gamma_{n+1} - \gamma_n$	$\lvert H_0'(-2\gamma_n)\rvert$
2	21.02203	3.98881	1.10936E-6
4	30.42487	2.51018	1.50731E-9
7	40.91871	2.40835	7.62215E-13
9	48.00515	1.76868	4.05787E-15
13	59.34704	1.48473	7.06392E-19
19	75.70469	1.44014	3.64154E-24
24	87.42527	1.38383	4.76349E-28
27	94.65134	1.21929	1.54247E-30
34	111.02953	0.84512	5.68260E-36
63	169.09451	0.81746	1.79231E-55
71	184.87446	0.72431	8.44906E-61
91	220.71491	0.71578	6.77870E-73
135	294.96536	0.60788	4.48141E-98
159	333.64537	0.56597	6.04617E-111
186	375.82591	0.49817	2.05820E-125
212	415.01880	0.43640	1.18968E-138
298	540.21316	0.41822	2.76261E-181
315	564.16087	0.34517	2.38099E-189
363	630.47388	0.33189	5.92345E-212
453	750.65595	0.31043	1.27457E-252
693	1054.78103	0.22110	2.09575E-356
922	1329.04351	0.16150	6.01580E-450
1496	1977.17394	0.09750	1.48834E-670
3777	4292.72644	0.09081	3.82866E-1460
4765	5229.19855	0.04325	2.24581E-1779
6709	7005.06286	0.03769	6.40373E-2385

beyond $n = 15{,}000$ of those *super differences* Δ_n which satisfy (5.8). This is given in Table B below for *all* $15{,}000 < n \leqslant 2{,}000{,}000$, where the numbers in Table B were kindly supplied to us by Dr. A.M. Odlyzko (A.T.&T. Bell Laboratories).

Table B
Super differences ($15{,}000 < n \leqslant 2 \cdot 10^6$)

n	γ_n	$\Delta_n := \gamma_{n+1} - \gamma_n$
18,859	17,143.78653	0.03530
44,555	36,510.16638	0.02953
73,997	57,273.66193	0.02583
82,552	63,137.21153	0.02085
87,761	66,678.07585	0.01948
95,248	71,732.90120	0.01470
354,769	234,016.89498	0.01305
415,587	270,071.29406	0.00863
420,891	273,193.66313	0.00570
1,115,578	663,318.50831	0.00295

Tables A and B indicate that the number of such super differences Δ_n which satisfy (5.8), is quite small!

6. Computation of $H_\lambda(x)$

Recalling from (1.5) and (1.3) that $H_\lambda(x) := \int_0^\infty e^{\lambda t^2}\Phi(t)\cos(xt)\,dt$, and $\Phi(t) := \sum_{n=1}^\infty (2\pi^2 n^4 e^{9t} - 3\pi n^2 e^{5t})\exp(-\pi n^2 e^{4t})$, we will, in this section, describe how one can obtain rigorous approximations to $H_\lambda(x)$, $H'_\lambda(x)$, and $H''_\lambda(x)$ to more than 43 significant decimal digits when $\lambda = -0.0991$ and $x = X$, as given in (3.12). Since the analysis is essentially the same for all of these functions, we will discuss only the approximation of $H''_\lambda(x)$.

We approximate $H''_\lambda(x)$ by computing

$$H''_\lambda(x)^\# := \left(T\left(-t^2 e^{\lambda t^2}\hat{\Phi}(t)\cos(xt), h, n\right)\right)^\#, \tag{6.1}$$

where

$$\hat{\Phi}(t) := \sum_{n=1}^{16} (2\pi^2 n^4 e^{9t} - 3\pi n^2 e^{5t})\exp(-\pi n^2 e^{4t}) \tag{6.1'}$$

is the truncation of the series for $\Phi(t)$, and where $T(f(t), n, h)$ is a modification of the trapezoidal rule approximation to $f(t)$ using the $n+1$ points $0, h, 2h, \ldots, nh$. That is,

$$T\left(-t^2 e^{\lambda t^2}\hat{\Phi}(t)\cos(xt), h, n\right)$$
$$:= h\left\{\tfrac{1}{2}\left[-t^2 e^{\lambda t^2}\hat{\Phi}(t)\cos(xt)\right]_{t=0} + \sum_{k=1}^{n}\left[-(kh)^2 e^{\lambda k^2 h^2}\hat{\Phi}(kh)\cos(khx)\right]\right\}. \tag{6.2}$$

Here, $H''_\lambda(x)^\#$ denotes the *computed* value of the quantity in (6.2). In the actual computations, we used

$$h = \frac{1}{8192} \text{ and } n = 16384, \text{ so that } nh = 2. \tag{6.2'}$$

From the triangle inequality, we obtain

$$\left|H''_\lambda(x) - H''_\lambda(x)^\#\right|$$
$$\leqslant \left|H''_\lambda(x)^\# - T\left(-t^2 e^{\lambda t^2}\hat{\Phi}(t)\cos(xt), h, n\right)\right| \tag{6.3a}$$
$$+\left|T\left(-t^2 e^{\lambda t^2}\hat{\Phi}(t)\cos(xt), h, n\right) - T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, n\right)\right| \tag{6.3b}$$

$$+\left|T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, n\right) - T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, \infty\right)\right| \tag{6.3c}$$

$$+\left|T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, \infty\right) - H_\lambda''(x)\right|. \tag{6.3d}$$

The remainder of this section will be devoted to showing that the sum of the terms in (6.3a), (6.3b), (6.3c), and (6.3d) does not exceed 1.45×10^{-201} when $H_\lambda''(x)^{\#}$ is computed using 210 digit floating point arithmetic.

Before considering a bound for (6.3a), whose size must depend directly on the nature of the underlying arithmetic, we will consider (6.3b), (6.3c) and (6.3d), which can be bounded analytically without regard to arithmetic details.

WE FIRST DETERMINE AN UPPER BOUND FOR THE TERM IN (6.3d).

Fortunately, because the integrand of $H_\lambda''(x)$ of (3.11) is an even function which is (cf. (1.4i)) analytic in the strip $|\mathrm{Im}\, z| < \pi/8$, it follows from the work of Martensen [10] and Kress [8] that the familiar trapezoidal rule approximation (on a uniform mesh of size h) of $H_\lambda''(x)$, defined by

$$\begin{aligned} &T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, \infty\right) \\ &:= h\left\{\tfrac{1}{2}\left[-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt)\right]_{t=0} \right. \\ &\qquad \left. + \sum_{k=1}^{\infty}\left[-(kh)^2\, e^{\lambda k^2 h^2}\Phi(kh)\cos(khx)\right]\right\}, \end{aligned} \tag{6.4}$$

converges *exponentially rapidly* to $H_\lambda''(x)$ as h decreases to 0, i.e., (cf. [8, Theorem 2.2 with $p=0$])

$$\begin{aligned} &\left|T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, \infty\right) - H_\lambda''(x)\right| \\ &\leqslant \frac{\exp(-\alpha\pi/h)\cosh(\alpha x)\, e^{-\alpha^2\lambda}}{\sinh(\alpha\pi/h)} \int_0^\infty \left|(s+\mathrm{i}\alpha)^2 \Phi(s+\mathrm{i}\alpha)\right| \mathrm{d}s, \end{aligned} \tag{6.5}$$

for any $\lambda \leqslant 0$ and for any α with $0 < \alpha < \pi/8 = 0.39269\ldots$, where the path of integration in (6.5) is the nonnegative real axis. It directly follows from the definition of $\Phi(t)$ that the integrand in (6.5) is bounded above by

$$(s^2+\alpha^2)\sum_{n=1}^{\infty}(2\pi^2 n^4\, e^{9s} + 3\pi n^2\, e^{5s})\exp(-\pi n^2\, e^{4s}\cos 4\alpha) \quad (s \geqslant 0), \tag{6.6}$$

and on observing that $3n^2\pi\, e^{5s} < n^4\pi^2\, e^{9s}$ for all $s \geqslant 0$ and all $n \geqslant 1$, we see that the integrand in (6.5) is bounded above by

$$3\pi^2(s^2+\alpha^2)\, e^{9s}\sum_{n=1}^{\infty} n^4 \exp(-\pi n^2\, e^{4s}\cos 4\alpha). \tag{6.7}$$

Setting

$$\hat{\alpha} := \tfrac{1}{4} \arccos\left(\frac{5}{3\pi} \ln(2)\right) = 0.29855\ldots \left(< \frac{\pi}{8}\right), \tag{6.8}$$

it can be verified that the ratio of successive terms in the summand given in (6.7), with $\alpha = \hat{\alpha}$, is at most $1/2$ for all $n \geqslant 1$ and all $s \geqslant 0$. Consequently,

$$\begin{aligned} \left|(s+\mathrm{i}\hat{\alpha})^2 \Phi(s+\mathrm{i}\hat{\alpha})\right| &\leqslant 3\pi^2(s^2+\hat{\alpha}^2)e^{9s} \exp(-\pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha}) \sum_{k=1}^{\infty} \left(\tfrac{1}{2}\right)^{(k-1)} \\ &\leqslant 6\pi^2(s^2+\hat{\alpha}^2)\, \mathrm{e}^{9s} \exp(-\pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha}). \end{aligned} \tag{6.9}$$

Therefore, from (6.5),

$$\begin{aligned} &\left|T(-t^2\, \mathrm{e}^{\lambda t^2}\Phi(t) \cos(xt),\, h,\, \infty) - H_\lambda''(x)\right| \\ &\quad \leqslant 6\pi^2 \left(\frac{\exp(-\hat{\alpha}\pi/h) \cosh(\hat{\alpha}x)\, \mathrm{e}^{-\hat{\alpha}^2\lambda}}{\sinh(\hat{\alpha}\pi/h)}\right) \\ &\qquad \times \int_0^\infty (s^2+\hat{\alpha}^2)\, \mathrm{e}^{9s} \exp(-\pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha})\, \mathrm{d}s \quad (\lambda \leqslant 0). \end{aligned} \tag{6.10}$$

For any positive integer k, set $I_k := \int_0^\infty \mathrm{e}^{4ks} \exp(-\pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha})\, \mathrm{d}s$, where $\hat{\alpha}$ is defined in (6.8). With the change of variables $u := \pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha}$, this integral becomes

$$I_k = \frac{1}{4(\pi \cos 4\hat{\alpha})^k} \int_{\pi \cos 4\hat{\alpha}}^\infty u^{k-1}\, \mathrm{e}^{-u}\, \mathrm{d}u.$$

Since from (6.8), the lower limit of integration satisfies $\pi \cos 4\hat{\alpha} = 1.15524\ldots > 0$, then evidently

$$I_k \leqslant \frac{1}{4(\pi \cos 4\hat{\alpha})^k} \int_0^\infty u^{k-1}\, \mathrm{e}^{-u}\, \mathrm{d}u = \frac{(k-1)!}{4(\pi \cos 4\hat{\alpha})^k}, \tag{6.11}$$

for all $k = 1, 2, \ldots$. Consequently, for $k = 3$ (so that $4k - 9 > 0$),

$$\begin{aligned} &\int_0^\infty (s^2+\alpha^2)\, \mathrm{e}^{9s} \exp(-\pi\, \mathrm{e}^{4s} \cos 4\hat{\alpha})\, \mathrm{d}s \\ &\quad \leqslant \max_{s \geqslant 0} \{(s^2+\hat{\alpha}^2)\, \mathrm{e}^{-3s} I_3\} \leqslant \frac{2}{4(\pi \cos 4\hat{\alpha})^3} \max_{s \geqslant 0} \{(s^2+\hat{\alpha}^2)\, \mathrm{e}^{-3s}\}. \end{aligned} \tag{6.12}$$

It is easily verified by the calculus that

$$\max_{s \geqslant 0} \{(s^2+\hat{\alpha}^2)\, \mathrm{e}^{-3s}\} = \hat{\alpha}^2. \tag{6.13}$$

Thus, combining (6.10), (6.11), and (6.13) gives that

$$\left|T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, \infty\right) - H_\lambda''(x)\right| \leqslant 3\frac{\hat{\alpha}^2 \exp(-\hat{\alpha}\pi/h - \lambda\hat{\alpha}^2)\cosh(\hat{\alpha}x)}{\pi \sinh(\hat{\alpha}\pi/h)(\cos 4\hat{\alpha})^3} < 2.87\times 10^{-6565}, \tag{6.14}$$

for $h = 1/8192$ and for all $|x| \leqslant 1000$ and all $-1 \leqslant \lambda \leqslant 0$, which bounds the term in (6.3d). (Note that X and $\hat{\lambda}$ of (3.12) are thus covered by (6.14).)

NEXT, WE DEDUCE AN UPPER BOUND FOR THE TERM IN (6.3c).

Since $\Phi(t) > 0$, this term in (6.3c) satisfies

$$\left|T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, n\right) - T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, \infty\right)\right|$$
$$= h\left|\sum_{k=n+1}^{\infty}\left[-(kh)^2 e^{\lambda k^2h^2}\Phi(kh)\cos(khx)\right]\right| \leqslant h\sum_{k=n+1}^{\infty}(kh)^2 e^{\lambda k^2h^2}\Phi(kh). \tag{6.15}$$

Next, with the notation of [4] that $\Phi(t) := (2\pi^2 e^{9t} - 3\pi e^{5t})\exp(-\pi e^{4t}) + \Phi_1(t)$, it is known (cf. [4, eq. (3.9)]) that $\Phi_1(t) < 64\pi^2 \exp(9t - 4\pi e^{4t})$ for all $t \geqslant 0$. Thus, this inequality for $\Phi_1(t)$ gives

$$\begin{aligned} 0 < \Phi(t) &< (2\pi^2 e^{9t} - 3\pi e^{5t})\exp(-\pi e^{4t}) + 64\pi^2\exp(9t - 4\pi e^{4t}) \\ &< 2\pi^2\exp(9t - \pi e^{4t}) + 64\pi^2\exp(9t - 4\pi e^{4t}) \\ &= \pi^2(2 + 64 e^{-3\pi e^{4t}})\exp(9t - \pi e^{4t}) \quad (t \geqslant 0). \end{aligned} \tag{6.16}$$

But as $2 + 64\exp(-3\pi e^{4t}) \leqslant 2 + 64\exp(-3\pi) < 3$ for all $t \geqslant 0$, then

$$\Phi(t) < 3\pi^2 \exp(9t - \pi e^{4t}) \quad (t \geqslant 0), \tag{6.17}$$

and inserting this inequality in (6.15) gives, for all $\lambda \leqslant 0$, and all real x,

$$\left|T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, n\right) - T\left(-t^2 e^{\lambda t^2}\Phi(t)\cos(xt), h, \infty\right)\right| < 3\pi^2 h\sum_{k=n+1}^{\infty}(kh)^2\exp(9kh - \pi e^{4kh}). \tag{6.18}$$

We now proceed to establish an upper bound for

$$S := \sum_{k=n+1}^{\infty}(kh)^2\exp(9kh - \pi e^{4kh}). \tag{6.18'}$$

We begin by writing this sum as

$$\sum_{k=n+1}^{\infty}(kh)^2\exp(9kh - \pi e^{4kh}) = \sum_{k=n+1}^{\infty}\frac{1}{\exp\{-9kh + \pi e^{4kh} - 2\ln kh\}}$$
$$\leqslant \sum_{k=n+1}^{\infty}\frac{1}{K^k} = \sum_{k=n+1}^{\infty}\frac{1}{\exp(k\ln K)}. \tag{6.19}$$

If the middle inequality in (6.19) is to be true, then

$$-9kh+\pi\, e^{4kh}-2\ln kh \geqslant k\ln K=(kh)\frac{\ln K}{h} \quad (k\geqslant n+1), \tag{6.20}$$

or equivalently, on dividing by kh,

$$-9+\frac{\pi\, e^{4kh}}{kh}-\frac{2\ln kh}{kh}\geqslant\frac{\ln K}{h} \quad (k\geqslant n+1). \tag{6.21}$$

For a continuous variable s with $(n+1)h\leqslant s<\infty$, set

$$g(s):=-9+\frac{\pi\, e^{4s}-2\ln s}{s} \quad (s\geqslant (n+1)/h), \tag{6.22}$$

so that

$$g'(s)=\frac{\pi[4s-1]\, e^{4s}+2(\ln s-1)}{s^2} \quad (s\geqslant (n+1)h). \tag{6.23}$$

Now, the numerator of $g'(s)$ in (6.23), on differentiating, is seen to be strictly increasing for $s>0$. As this numerator is also positive for $s=2$, it follows that

$$g'(s)>0 \quad \text{for all } s\geqslant 2. \tag{6.24}$$

Thus, $g(s)$ is strictly increasing for $s\geqslant 2$. Consequently,

$$g(s)\geqslant g(2)=-9+\frac{\pi\, e^8-2\ln 2}{2}=4672.78470\ldots \quad (s\geqslant 2), \tag{6.25}$$

and we then *define* K by (cf. (6.21))

$$\frac{\ln K}{h}:=g(2)=-9+\frac{\pi\, e^8-2\ln 2}{2}, \tag{6.26}$$

so that

$$K=\exp\left(h\left\{-9+\frac{\pi\, e^8-2\ln 2}{2}\right\}\right). \tag{6.27}$$

Now, the final sum in (6.19) is just

$$\frac{1}{K^{n+1}\left(1-\frac{1}{K}\right)}=\frac{1}{\exp\left((n+1)h\left\{-9+\frac{\pi\, e^8-2\ln 2}{2}\right\}\right)}\cdot\frac{1}{\left(1-\frac{1}{K}\right)}. \tag{6.28}$$

But as $nh=2$ from (6.2′), the above expression is bounded above by

$$\frac{1}{\exp(-18+\pi\, e^8-2\ln 2)}\cdot\frac{1}{\left(1-\frac{1}{K}\right)}. \tag{6.29}$$

Now $\{\exp(-18+\pi\, e^8 - 2\ln 2)\}^{-1} < 1.866 \times 10^{-4059}$. Next, from (6.27) with $h = \frac{1}{8192}$, we see that $K \geqslant 1.768$, so that $(1-1/K)^{-1} < 2.301$. Thus, from (6.18) and the definition of S in (6.18′), we have

$$\left|T\left(-t^2\Phi(t)\, e^{\lambda t^2}\cos(xt),\, h,\, n\right) - T\left(-t^2\Phi(t)\, e^{\lambda t^2}\cos(xt),\, h,\, \infty\right)\right|$$
$$\leqslant 3\pi^2 h \sum_{k=n+1}^{\infty} (kh)^2 \exp(9kh - \pi\, e^{4kh}) \leqslant \frac{3\pi^2 h}{K^{n+1}\left(1-\dfrac{1}{K}\right)}$$
$$< 1.552 \times 10^{-4061}, \tag{6.30}$$

which bounds the term in (6.3c) for all $\lambda \leqslant 0$ and all real x.

WE NEXT BOUND THE TERM IN (6.3b).

First note that the general error in truncating the series for the function $\Phi(t)$ of (1.3) satisfies (cf. [4, eq. (4.6)])

$$0 < \Phi(t) - \sum_{n=1}^{N} (2\pi^2 n^4\, e^{9t} - 3\pi n^2\, e^{5t}) \exp(-\pi n^2\, e^{4t})$$
$$< \pi N^3 \exp(5t - \pi N^2\, e^{4t}),$$

for any $t \geqslant 0$ and for any positive integer N. Consequently, for the particular truncation $N = 16$ of (6.1′), we have

$$0 < \Phi(t) - \hat{\Phi}(t) < 4096\pi \exp(5t - 256\pi\, e^{4t}) \quad (t \geqslant 0). \tag{6.31}$$

For all $\lambda \leqslant 0$ and all real x, this yields

$$\left|T\left(-t^2\, e^{\lambda t^2}\hat{\Phi}(t)\cos(xt),\, h,\, n\right) - T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, n\right)\right|$$
$$\leqslant h\left\{\tfrac{1}{2}\left|t^2(\hat{\Phi}(t) - \Phi(t))\right|_{t=0} + \sum_{k=1}^{n} (kh)^2\left|\hat{\Phi}(kh) - \Phi(kh)\right|\right\}$$
$$\leqslant h \sum_{k=1}^{n} 4096\pi (kh)^2 \exp\left[5kh - 256\pi\, e^{4kh}\right]. \tag{6.32}$$

With the specific values of n and h of (6.2′), it can be verified that each term of the final sum of (6.32) is bounded above by

$$\max_{1\leqslant k\leqslant n}\left\{4096\pi (kh)^2 \exp(5kh - 256\pi\, e^{4kh})\right\}$$
$$= \left[4096\pi (kh)^2 \exp(5kh - 256\pi\, e^{4kh})\right]_{k=5} < 3.54 \times 10^{-353}. \tag{6.33}$$

Therefore, as $nh = 2$ from (6.2′),

$$\left|T\left(-t^2\, e^{\lambda t^2}\hat{\Phi}(t)\cos(xt),\, h,\, n\right) - T\left(-t^2\, e^{\lambda t^2}\Phi(t)\cos(xt),\, h,\, n\right)\right|$$
$$< 3.54 \times 10^{-353}(nh) = 7.08 \times 10^{-353}, \tag{6.34}$$

which bounds the term in (6.3b) for all $\lambda \leqslant 0$ and all real x.

Finally, we consider the numerical evaluation of

$$H_{\lambda}''(x)^{\#} := \left[h\left\{\sum_{k=1}^{n} -(kh)^2\, e^{\lambda k^2h^2}\hat{\Phi}(kh)\cos(xkh)\right\}\right]^{\#}. \tag{6.35}$$

Central to this issue is the accuracy of the cvaluation of sums and products of floating point numbers. To establish rigorous bounds on the accuracy of our floating point calculations, we will use the following well-known facts (cf. Wilkinson [20], Chapter 1). In the following theorem t represents the floating-point precision of each of the arithmetic operations.

THEOREM B

If x and y are floating point numbers and if floating point arithmetic is used, then

$$\left(x \begin{smallmatrix}+\\-\\\times\\\div\end{smallmatrix} y\right)^{\#},$$

which are defined as the computed values of

$$\left(x \begin{smallmatrix}+\\-\\\times\\\div\end{smallmatrix} y\right),$$

satisfy

$$\left(x \begin{smallmatrix}+\\-\\\times\\\div\end{smallmatrix} y\right)^{\#} = \left(x \begin{smallmatrix}+\\-\\\times\\\div\end{smallmatrix} y\right)(1+\epsilon)$$

where $|\epsilon| < 10^{-t}$. *If* $m < 10^{t}$ *and if* $x_1, x_2, \ldots, x_m$, *are floating-point numbers, then*

$$\begin{cases} (x_1 \times x_2 \times \ldots \times x_m)^{\#} = (x_1 \times x_2 \times \ldots \times x_m)(1+E) \\ \textit{where } (1-10^{-t})^{m-1} \leqslant 1+E \leqslant (1+10^{-t})^{m-1}, \end{cases} \tag{6.36}$$

and

$$\begin{cases} (x_1 + x_2 + \ldots + x_m)^{\#} = x_1(1+\nu_1) + x_2(1+\nu_2) + \ldots + x_m(1+\nu_m) \\ \textit{where } (1-10^{-t})^{m+1-r} < 1+\nu_r < (1+10^{-t})^{m+1-r},\ r = 1, 2, \ldots, m. \end{cases} \tag{6.37}$$

All calculations for this report were performed on Sun 3/80 work station using Richard Brent's MP package [2] with the floating point precision set so that the arithmetic satisfies the assumptions of the above Theorem 2 with

$t = 210$. In addition, with the floating point precision set to 210 decimal places Brent's MP package can evaluate all the elementary functions to that accuracy Moreover, if x is a floating point number, then the value of e^x produced by the MP package satisfies $(e^x)^{\#} = e^x(1+\epsilon_1)$ and $\pi^{\#} = \pi(1+\epsilon_2)$ where $|\epsilon_i| < 10^{-210}$ $i = 1, 2$, but the MP can only evaluate such functions as $\cos(x)$ and $\sin(x)$ to an *absolute error* of 10^{-210}.

Recall that to estimate (6.3a), we must determine the error involved in calculating $\hat{\Phi}(kh) = \sum_{n=1}^{16}(2\pi^2 n^4 e^{9kh} - 3\pi n^2 e^{5kh}) \exp(-\pi n^2 e^{4kh})$. To evaluate this sum, for $k = 0, 1, \ldots, n$, we compute for each j, $j = 1, \ldots, 16$, respectively

1. $(e^{2kh})^{\#} = \left((e^{kh})^{\#}(e^{kh})^{\#}\right)^{\#}$,

2. $(e^{4kh})^{\#} = \left((e^{2kh})^{\#}(e^{2kh})^{\#}\right)^{\#}$,

3. $(e^{5kh})^{\#} = \left((e^{4kh})^{\#}(e^{kh})^{\#}\right)^{\#}$,

4. $(\pi j^2)^{\#} = (\pi^{\#} j^2)^{\#}$,

5. $(\pi j^2 e^{4kh})^{\#} = \left((\pi j^2)^{\#}(e^{4kh})^{\#}\right)^{\#}$,

6. $(\exp(-\pi j^2 e^{4kh}))^{\#} = \left(\exp\left(-(\pi j^2 e^{4kh})^{\#}\right)\right)^{\#}$,

7. $(2\pi j^2 e^{4kh})^{\#} = \left(2(\pi j^2 e^{4kh})^{\#}\right)^{\#}$,

8. $(2\pi j^2 e^{4kh} - 3)^{\#} = \left((2\pi j^2 e^{4kh})^{\#} - 3\right)^{\#}$,

9. $(2\pi j^2 e^{9kh} - 3 e^{5kh})^{\#} = (2\pi j^2 e^{4kh} - 3)^{\#}(e^{5kh})^{\#}$,

10. $(2\pi^2 j^4 e^{9kh} - 3\pi j^2 e^{5kh})^{\#} = \left((\pi j^2)^{\#}(2\pi j^2 e^{9kh} - 3 e^{5kh})^{\#}\right)^{\#}$,

11. $\left((2\pi^2 j^4 e^{9kh} - 3\pi j^2 e^{5kh}) \exp(-\pi j^2 e^{4kh})\right)^{\#}$
$= \left((2\pi^2 j^4 e^{9kh} - 3\pi j^2 e^{5kh})^{\#} \exp(-\pi j^2 e^{4kh})^{\#}\right)^{\#}$.

Using only the fact that when the floating point precision is set to 210 significant digits, the MP package calculates products, differences, exponentials and π with a relative error of at most 10^{-210}, one can show that the computed value of $(2\pi^2 j^4 e^{9kh} - 3\pi j^2 e^{5kh}) \exp(-\pi j^2 e^{4kh})$ is no more than

$$(1+|\nu|)^{16}\left[2\pi^2 j^4 e^{4kh}(1+|\nu|)^{11} - 3\pi j^2\right] \exp\left(5kh - \pi j^2 e^{4kh}(1-|\nu|)^{10}\right), \tag{6.38}$$

where $|\nu| < 10^{-210}$. The maximum *relative error* produced from (6.38) is given by

$$M_2 := \max_{\substack{0 \leqslant k \leqslant n \\ 1 \leqslant j \leqslant 16}} \left\{ \frac{(1+|\nu|)^{16}\left[\frac{2}{3}\pi j^2 \,\mathrm{e}^{4kh}(1+|\nu|)^{11}-1\right] \exp\left[\pi j^2 \,\mathrm{e}^{4kh}(1-(1-|\nu|)^{10}\right]}{(\frac{2}{3}\pi j^2 \,\mathrm{e}^{4kh}-1)} - 1 \right\}.$$

As the term in braces above is strictly increasing in $\pi j^2 \,\mathrm{e}^{4kh}$ and in $|\nu|$, the maximum is thus obtained when $k = n = 16384$, $j = 16$, and $|\nu| = 10^{-210}$. Hence, as $nh = 2$ from (6.2′), we have

$$M_2 < \frac{(1+10^{-210})^{16}\left[\frac{2}{3}\pi(16)^2 \,\mathrm{e}^8(1+10^{-210})^{11}-1\right] \exp\left[\pi(16)^2 \,\mathrm{e}^8(1-(1-10^{-210})^{10}\right]}{(\frac{2}{3}\pi(16)^2 \,\mathrm{e}^8-1)} - 1,$$

which, on evaluating the right side above, gives

$$M_2 < 2.40 \times 10^{-203}.$$

A lower bound for the minimum relative error is similarly obtained, with the same modulus, so that

$$\left.\begin{aligned} &((2\pi^2 j^4 \,\mathrm{e}^{4kh} - 3\pi j^2) \exp(5kh - \pi j^2 \,\mathrm{e}^{4kh}))^{\#} \\ &\quad = (2\pi^2 j^4 \,\mathrm{e}^{4kh} - 3\pi j^2) \exp(5kh - \pi j^2 \,\mathrm{e}^{4kh})(1 + w_j), \\ &\text{where } |w_j| < 2.40 \times 10^{-203} \quad (k = 0, 1, \cdots, n;\ j = 1, 2, \cdots, 16). \end{aligned}\right\} \tag{6.39}$$

Next, on applying (6.37) of Theorem B, we have

$$\hat{\Phi}(kh)^{\#} = \sum_{j=1}^{16} (2\pi^2 j^4 \,\mathrm{e}^{4kh} - 3\pi j^2) \exp(5kh - \pi j^2 \,\mathrm{e}^{4kh})(1 + w_j)(1 + \nu_j), \tag{6.40}$$

where w_j satisfies (6.39) and where (cf. (6.37))

$$1 - 10^{-208} < (1 - 10^{-210})^{17-j} < 1 + \nu_j < (1 + 10^{-210})^{17-j} < 1 + 10^{-208}$$
$$(j = 1, 2, \cdots, 16). \tag{6.41}$$

Writing $(1 + w_j)(1 + \nu_j) =: 1 + \eta_j$, then (6.40) becomes

$$\hat{\Phi}(kh)^{\#} = \sum_{j=1}^{16} (2\pi^2 j^4 \,\mathrm{e}^{4kh} - 3\pi j^2) \exp(5kh - \pi j^2 \,\mathrm{e}^{4kh})(1 + \eta_j) \tag{6.42}$$

where, from (6.39) and (6.41),

$$|\eta_j| < 2.41 \times 10^{-203} < 10^{-202} \quad (j = 1, 2, \cdots, 16). \tag{6.43}$$

Because all the terms in the sum in (6.42) are positive, it then follows from (6.42) and (6.43) that

$$\hat{\Phi}(kh)^{\#} = \hat{\Phi}(kh)(1 + \mu_k), \quad \text{where } |\mu_k| < 10^{-202} \quad (k = 0, 1, \cdots, n). \tag{6.44}$$

Finally, we come to the calculation of

$$T\left(-t^2\hat{\Phi}(t)\,\mathrm{e}^{\hat{\lambda}t^2}\cos(Xt),\,n,\,h\right),$$

where X and $\hat{\lambda}$ are explicitly given in (3.12). To this end, we apply Theorem with $n = 16384$, noting that khX can be represented *exactly*, using 210 di floating point arithmetic. We thus obtain

$$\begin{aligned} H_{\hat{\lambda}}''(X)^{\#} &:= T\left(-t^2\hat{\Phi}(t)\,\mathrm{e}^{\hat{\lambda}t^2}\cos(Xt),\,h,\,n\right)^{\#} \\ &= -(1+\nu_1)h\sum_{k=1}^{n}\Bigg(\bigg(\Big(\big((kh)^2(1+\nu_{2,k})\big)\big(\hat{\Phi}(kh)(1+\mu_k)\big)(1+\nu_{3,k}) \\ &\quad\times\Big(\exp\Big(\hat{\lambda}(1+\nu_{4,k})\big((kh)^2(1+\nu_{2,k})\big)\Big)(1+\nu_{5,k})\Big)(1+\nu_{6,k})\bigg) \\ &\quad\times(1+\nu_{7,k})(\cos(khX)+\nu_{8,k})\Bigg)(1+\nu_{9,k}), \end{aligned} \tag{6.4}$$

where, for $0 \leqslant k \leqslant 16384$,

$$|\nu_1|,\ |\nu_{i,k}| < 10^{-210} \quad (2 \leqslant i \leqslant 8);\ |\nu_{9,k}| < 10^{-205} \quad \text{(cf. (6.37)); and}$$
$$|\mu_k| < 10^{-202}.$$

Next, with the known inequality (cf. [4, eq. (3.41)]) that

$$\max_{t\geqslant 0}\Phi(t) = \Phi(0) < \tfrac{203}{202}(2\pi^2-3)\exp(-\pi) = 0.44793\ldots, \tag{6.4}$$

on expanding $H_{\hat{\lambda}}''(X)^{\#} - T(-t^2\,\mathrm{e}^{\hat{\lambda}t^2}\Phi(t)\cos(Xt),\,h,\,n)$ and using explicitly t expression in (6.45), it can be verified in a straightforward, but tedious way, th

$$\left|H_{\hat{\lambda}}''(X)^{\#} - T\left(-t^2\,\mathrm{e}^{\hat{\lambda}t^2}\Phi(t)\cos(Xt),\,h,\,n\right)\right| < 1.44\times 10^{-201}, \tag{6.4}$$

which is a generous upper bound for the remaining term (6.3a). Combini (6.47) with our previous bounds for (6.3b)–(6.3d) then gives that

$$\begin{aligned} \left|H_{\hat{\lambda}}''(X)^{\#} - H_{\hat{\lambda}}''(X)\right| &< 2.87\times 10^{-6565} + 1.552\times 10^{-4061} + 7.08\times 10^{-353} \\ &\quad + 1.44\times 10^{-201} < 1.45\times 10^{-201}, \end{aligned} \tag{6.4}$$

i.e., $H_{\hat{\lambda}}''(X)$ can be computed to an absolute accuracy of 10^{-200}, as claimed §3.

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