

EFFECTIVE APPROXIMATION OF HEAT FLOW EVOLUTION OF THE RIEMANN ξ FUNCTION, AND AN UPPER BOUND FOR THE DE BRUIJN-NEWMAN CONSTANT

D.H.J. POLYMATH

ABSTRACT. For each $t \in \mathbb{R}$, define the entire function

$$H_t(z) := \int_0^\infty e^{tu^2} \Phi(u) \cos(zu) du$$

where Φ is the super-exponentially decaying function

$$\Phi(u) := \sum_{n=1}^\infty (2\pi^2 n^4 e^{9u} - 3\pi n^2 e^{5u}) \exp(-\pi n^2 e^{4u}).$$

This is essentially the heat flow evolution of the Riemann ξ function. From the work of de Bruijn and Newman, there exists a finite constant Λ (the *de Bruijn-Newman constant*) such that the zeroes of H_t are all real precisely when $t \geq \Lambda$. The Riemann hypothesis is equivalent to the assertion $\Lambda \leq 0$; recently, Rodgers and Tao established the matching lower bound $\Lambda \geq 0$. Ki, Kim and Lee established the upper bound $\Lambda < \frac{1}{2}$.

In this paper we establish several effective estimates on $H_t(x + iy)$ for $t \geq 0$, including some that are accurate for small or medium values of x . By combining these estimates with numerical computations, we are able to obtain a new upper bound $\Lambda \leq 0.22$ unconditionally, as well as improvements conditional on further numerical verification of the Riemann hypothesis. We also obtain some new estimates controlling the asymptotic behavior of zeroes of $H_t(x + iy)$ as $x \rightarrow \infty$.

1. INTRODUCTION

Let $H_0: \mathbb{C} \rightarrow \mathbb{C}$ denote the function

$$(1) \quad H_0(z) := \frac{1}{8} \xi\left(\frac{1}{2} + \frac{iz}{2}\right),$$

where ξ denotes the Riemann ξ function

$$(2) \quad \xi(s) := \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \zeta(s)$$

(after removing all singularities) and ζ is the Riemann ζ function. Then H_0 is an entire even function with functional equation $H_0(\bar{z}) = \overline{H_0(z)}$, and the Riemann hypothesis is equivalent to the assertion that all the zeroes of H_0 are real.

It is a classical fact (see [25, p. 255]) that H_0 has the Fourier representation

$$H_0(z) = \int_0^\infty \Phi(u) \cos(zu) du$$

where Φ is the super-exponentially decaying function

$$(3) \quad \Phi(u) := \sum_{n=1}^\infty (2\pi^2 n^4 e^{9u} - 3\pi n^2 e^{5u}) \exp(-\pi n^2 e^{4u}).$$

The sum defining $\Phi(u)$ converges absolutely for negative u also. From Poisson summation one can verify that Φ satisfies the functional equation $\Phi(u) = \Phi(-u)$ (i.e., Φ is even).

De Bruijn [4] introduced (with somewhat different notation) the more general family of functions $H_t: \mathbb{C} \rightarrow \mathbb{C}$ for $t \in \mathbb{R}$, defined by the formula

$$(4) \quad H_t(z) := \int_0^\infty e^{tu^2} \Phi(u) \cos(zu) du.$$

As noted in [8, p.114], one can view H_t as the evolution of H_0 under the backwards heat equation $\partial_t H_t(z) = -\partial_{zz} H_t(z)$. As with H_0 , each of the H_t are entire even functions with functional equation $H_t(\bar{z}) = \overline{H_t(z)}$; from the super-exponential decay of $e^{tu^2} \Phi(u)$ we see that the H_t are in fact entire of order 1. It follows from the work of Pólya [18] that if H_t has purely real zeroes for some t , then $H_{t'}$ has purely real zeroes for all $t' > t$; de Bruijn showed that the zeroes of H_t are purely real for $t \geq 1/2$. Newman [13] strengthened this result by showing that there is an absolute constant $-\infty < \Lambda \leq 1/2$, now known as the *De Bruijn-Newman constant*, with the property that H_t has purely real zeroes if and only if $t \geq \Lambda$. The Riemann hypothesis is then clearly equivalent to the upper bound $\Lambda \leq 0$. Recently in [20] the complementary bound $\Lambda \geq 0$ was established, answering a conjecture of Newman [13], and improving upon several previous lower bounds for Λ [5, 14, 7, 6, 15, 21]. Furthermore, Ki, Kim, and Lee [9] sharpened the upper bound $\Lambda \leq 1/2$ of de Bruijn [4] slightly to $\Lambda < 1/2$.

In this paper we improve the upper bound:

Theorem 1.1 (New upper bound). *We have $\Lambda \leq 0.22$.*

The proof of Theorem 1.1 combines numerical verification with some new asymptotics and observations about the H_t which may be of independent interest. Firstly, by analyzing the dynamics of the zeroes of H_t , we establish in Section 3 the following criterion for obtaining upper bounds on Λ :

Theorem 1.2 (Upper bound criterion). *Suppose that $t_0, X > 0$ and $0 < y_0 \leq 1$ obey the following hypotheses:*

- (i) *(Numerical verification of RH at initial time 0) There are no zeroes $\zeta(\sigma + iT) = 0$ with $\frac{1+y_0}{2} \leq \sigma \leq 1$ and $0 \leq T \leq \frac{X}{2}$.*
- (ii) *(Asymptotic zero-free region at final time t_0) There are no zeroes $H_{t_0}(x + iy) = 0$ with $x \geq X + \sqrt{1 - y_0^2}$ and $y_0 \leq y \leq \sqrt{1 - 2t_0}$.*
- (iii) *(Barrier at intermediate times) There are no zeroes $H_t(x + iy) = 0$ with $X \leq x \leq X + \sqrt{1 - y_0^2}$, $\sqrt{y_0^2 + 2(t_0 - t)} \leq y \leq \sqrt{1 - 2t}$, and $0 \leq t \leq t_0$.*

Then $\Lambda \leq t_0 + \frac{1}{2}y_0^2$.

Informally, hypothesis (i) implies that at time $t = 0$, there are no zeroes $H_t(x + iy) = 0$ with large values of y to the left of the barrier region in (iii). The absence of zeroes in that barrier, together with a continuity argument and an analysis of the time derivative of each zero, can then be used to show that for later times $0 < t \leq t_0$, there continue to be no zeroes $H_t(x + iy) = 0$ with large values of y to the left of the barrier; see Figure 1. Hypothesis (ii) then gives the complementary assertion to the right of the barrier, and one can use an existing theorem of de Bruijn (Theorem 3.2) to conclude.

In practice, we have found it convenient numerically to replace the barrier region in Theorem 1.2 with the larger and simpler region

$$X \leq x \leq X + 1; \quad y_0 \leq y \leq 1; \quad 0 \leq t \leq t_0.$$

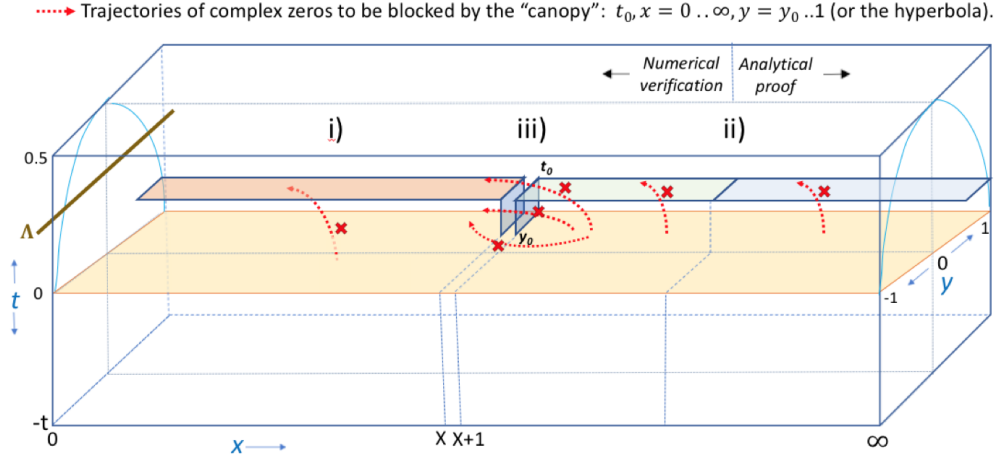


FIGURE 1. A visualization of Theorem 1.2. If at time t_0 one can show that there are no zeroes $H_t(x + iy) = 0$ in the “canopy” $0 \leq x < \infty$, $y_0 \leq y \leq 1$, then a theorem of de Bruijn allows one to conclude the desired bound $\Lambda \leq t_0 + \frac{1}{2}y_0^2$. The hypothesis (i) prevents zeroes hitting this canopy from an initial position to the left of the barrier; the hypothesis (iii) prevents zeroes from lying in the canopy to the right of the barrier; and the hypothesis (ii) prevents zeroes from starting to the right of the barrier and reaching the canopy to the left of the barrier.

We will obtain Theorem 1.1 by applying Theorem 1.2 with the specific numerical choices $t_0 = 0.2$, $X = 6 \times 10^{10} + 83952 - 0.5$, and $y_0 = 0.2$. The reason we choose X close to 6×10^{10} is that this is near the limit of known numerical verifications of the Riemann hypothesis such as [17], which we need for the hypothesis (i) of the above theorem; the shift $83952 - 0.5$ is in place to make the partial Euler product $\prod_{p \leq 11} \left(1 - \frac{1}{p^{\frac{1-iX}{2}}}\right)^{-1}$ large, which helps in keeping the functions $H_t(x + iy)$, $H_{t_0}(x + iy)$ large in magnitude, which in turn is helpful for numerical verifications of (ii) and (iii); see also Figure 11. The choices $t_0 = 0.2$, $y_0 = 0.2$ are then close to the limit of our ability to numerically verify hypothesis (ii) for this choice of X . (The hypothesis (iii) is also verified numerically, but can be done relatively quickly compared to (ii), and so does not present the main bottleneck to further improvements to Theorem 1.1.) Further upper bounds to Λ can be obtained if one assumes the Riemann hypothesis to hold up to larger heights than that in [17]: see Section 11.

To verify (ii) and (iii), we need efficient approximations (of Riemann-Siegel type) for $H_t(x + iy)$ in the regime where t, y are bounded and x is large. For sake of numerically explicit constants, we will focus attention on the region

$$(5) \quad 0 < t \leq \frac{1}{2}; \quad 0 \leq y \leq 1; \quad x \geq 200,$$

though the results here would also hold (with different explicit constants) if the numerical quantities $\frac{1}{2}$, 1, 200 were replaced by other quantities.

A key difficulty here is that $H_t(x + iy)$ decays exponentially fast in x (basically because of the Gamma factor in (2)); see Figure 3. This means that any direct attempt to numerically establish a zero-free region for $H_t(x + iy)$ for large x would require enormous amounts of numerical precision. To get around this, we will first renormalise the function $H_t(x + iy)$ by dividing it by a nowhere vanishing explicit function $B_t(x + iy)$ (basically a variant of the aforementioned Gamma factor) that removes this decay. To describe this function, we first introduce the function $M_0 : \mathbb{C} \setminus (-\infty, 1] \rightarrow \mathbb{C} \setminus \{0\}$ defined by the formula

$$(6) \quad M_0(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \sqrt{2\pi} \exp\left(\left(\frac{s}{2} - \frac{1}{2}\right) \text{Log} \frac{s}{2} - \frac{s}{2}\right),$$

where Log denotes the standard branch of the complex logarithm, with branch cut at the negative axis and imaginary part in $(-\pi, \pi]$. One may interpret $M_0(s)$ as the Stirling approximation to the factor $\frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right)$ appearing in (1), (2); it decays exponentially as one moves to infinity $s \rightarrow \pm i\infty$ along the critical strip. We may form a holomorphic branch $\log M_0 : \mathbb{C} \setminus (-\infty, 1] \rightarrow \mathbb{C}$ of the logarithm of M_0 by the formula

$$(7) \quad \log M_0(s) := \text{Log} s + \text{Log}(s-1) - \frac{s}{2} \log \pi + \log \frac{\sqrt{2\pi}}{16} + \left(\frac{s}{2} - \frac{1}{2}\right) \text{Log} \frac{s}{2} - \frac{s}{2};$$

differentiating this, we see that the logarithmic derivative $\alpha : \mathbb{C} \setminus (-\infty, 1] \rightarrow \mathbb{C}$ of this function, defined by

$$(8) \quad \alpha := (\log M_0)' = \frac{M_0'}{M_0}$$

is given explicitly by the formula

$$(9) \quad \begin{aligned} \alpha(s) &= \frac{1}{s} + \frac{1}{s-1} - \frac{1}{2} \log \pi + \frac{1}{2} \log \frac{s}{2} - \frac{1}{2s} \\ &= \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2} \log \frac{s}{2\pi}. \end{aligned}$$

For any time $t \in \mathbb{R}$, we then define the deformation $M_t : \mathbb{C} \setminus (-\infty, 1]$ of M_0 by the formula

$$(10) \quad M_t(s) := \exp\left(\frac{t}{4} \alpha(s)^2\right) M_0(s)$$

for any $t \geq 0$. In the region (5), we introduce the quantity

$$(11) \quad B_t(x + iy) := M_t\left(\frac{1+y-ix}{2}\right).$$

For fixed $t \geq 0$ and $y > 0$, $B_t(x + iy)$ is non-vanishing, and it is easy to verify the asymptotic $|B_t(x + iy)| = e^{-(\frac{\pi}{8} + o(1))x}$. As it turns out, $B_t(x + iy)$ is an asymptotic approximation to $H_t(x + iy)$ in the region (5), in the sense that

$$(12) \quad \lim_{x \rightarrow \infty} \frac{H_t(x + iy)}{B_t(x + iy)} = 1$$

for any fixed $t > 0$ and $y > 0$; see Figure 2. (However, the convergence of (12) is *not* uniform as t approaches zero.)

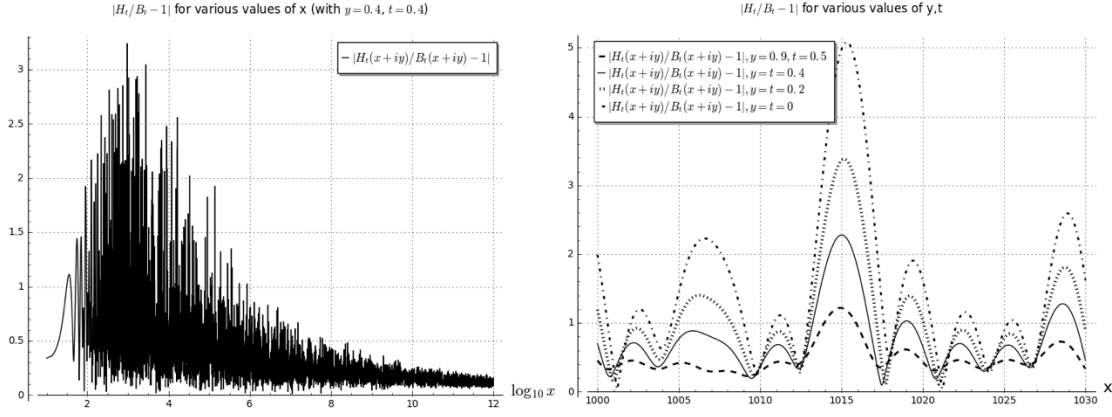


FIGURE 2. The quantity $|H_t(x+iy)/B_t(x+iy) - 1|$ when $y = t = 0.4$ and $\log_{10} x \leq 12$ (left) and when for $1000 \leq x \leq 1030$ and various choices of (y, t) (right).



FIGURE 3. The quantities $\log|H_t(x+iy)|$ and $\log|B_t(x+iy)|$ when $y = t = 0.4$ and $\log_{10} x \leq 7$. Both quantities decay like $-\frac{\pi}{8}x \approx -0.393x$.

In fact we have the following significantly more accurate approximation (of Riemann-Siegel type) with effective error estimates. For any real number X , let $O_{\leq}(X)$ denote a quantity that is bounded in magnitude by X . We also use $x_+ = \max(x, 0)$ to denote the positive part of a real number x .

Theorem 1.3 (Effective Riemann-Siegel approximation to $H_t(x+iy)$). *Let t, x, y lie in the region (5). Then we have*

$$(13) \quad \frac{H_t(x+iy)}{B_t(x+iy)} = f_t(x+iy) + O_{\leq}(e_A + e_B + e_{C,0})$$

where

$$(14) \quad f_t(x+iy) := \sum_{n=1}^N \frac{b'_n}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b'_n}{n^{s_*+\kappa}}$$

$$(15) \quad b'_n := \exp\left(\frac{t}{4} \log^2 n\right)$$

$$(16) \quad \gamma = \gamma(x+iy) := \frac{M_t\left(\frac{1-y+ix}{2}\right)}{M_t\left(\frac{1+y-ix}{2}\right)}$$

$$(17) \quad s_* = s_*(x+iy) := \frac{1+y-ix}{2} + \frac{t}{2} \alpha\left(\frac{1+y-ix}{2}\right)$$

$$(18) \quad \kappa = \kappa(x+iy) := \frac{t}{2} \left(\alpha\left(\frac{1-y+ix}{2}\right) - \alpha\left(\frac{1+y+ix}{2}\right) \right)$$

$$(19) \quad N := \left\lfloor \sqrt{\frac{x}{4\pi} + \frac{t}{16}} \right\rfloor$$

and $e_A, e_B, e_{C,0}$ are certain explicitly computable positive quantities¹ depending on t and $x+iy$. Furthermore, we have the following bounds:

$$(20) \quad |\gamma| \leq e^{0.02y} \left(\frac{x}{4\pi}\right)^{-y/2}$$

$$(21) \quad \operatorname{Re} s_* \geq \frac{1+y}{2} + \frac{t}{4} \log \frac{x}{4\pi} - \frac{t}{2x^2} \left(1 - 3y + \frac{4y(1+y)}{x^2}\right)_+$$

$$(22) \quad |\kappa| \leq \frac{ty}{2(x-6)}$$

$$(23) \quad e_A + e_B \leq \sum_{n=1}^N (1 + |\gamma| N^{|\kappa|} n^y) \frac{b'_n}{n^{\operatorname{Re}(s_*)}} \left(\exp\left(\frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi n^2} + 0.626}{x - 6.66}\right) - 1 \right)$$

$$(24) \quad e_{C,0} \leq \left(\frac{x}{4\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16} \log^2 \frac{x}{4\pi} + \frac{1.24 \times (3^y + 3^{-y})}{N - 0.125} + \frac{3|\log \frac{x}{4\pi} + i\frac{\pi}{2}| + 10.44}{x - 8.52}\right)$$

This theorem will be proven in Section 6; see Figures 4, 5 for a numerical illustration of the approximation. The strategy is to express H_t as a convolution of H_0 with a gaussian heat kernel, then apply an effective Riemann-Siegel expansion to H_0 to rewrite H_t as the sum of various contour integrals; see Section 4 for details. One then uses the saddle point method to shift each such contour to a location that is suitable for effective estimation.

From (13) and the triangle inequality, we have a numerically verifiable criterion to establish non-vanishing of H_t at a given point:

¹See (71)-(74) for the precise definition of these quantities.

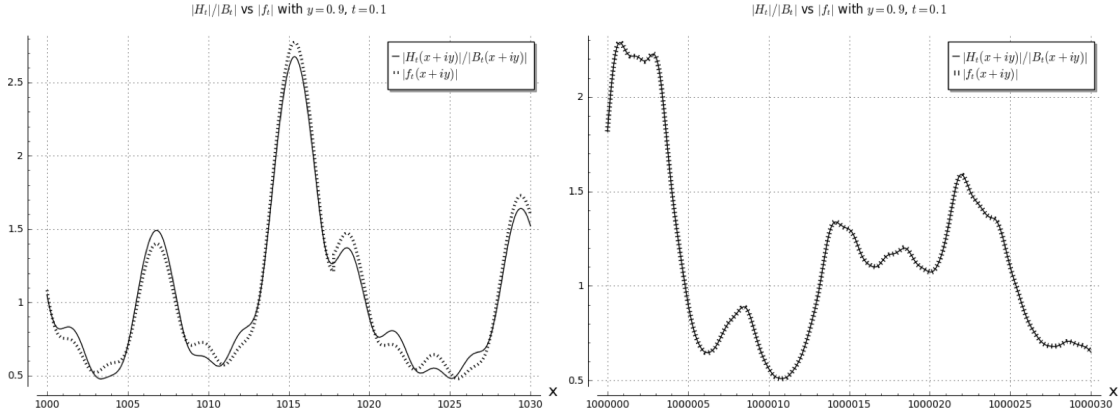


FIGURE 4. Comparison of $|f_t(x+iy)|$ and $|H_t(x+iy)|/|B_t(x+iy)|$ for $y = 0.9$, $t = 0.1$, $1000 \leq x \leq 1030$ (left) and when $10^6 \leq x \leq 10^6 + 30$ (right). The approximation improves as x gets larger.

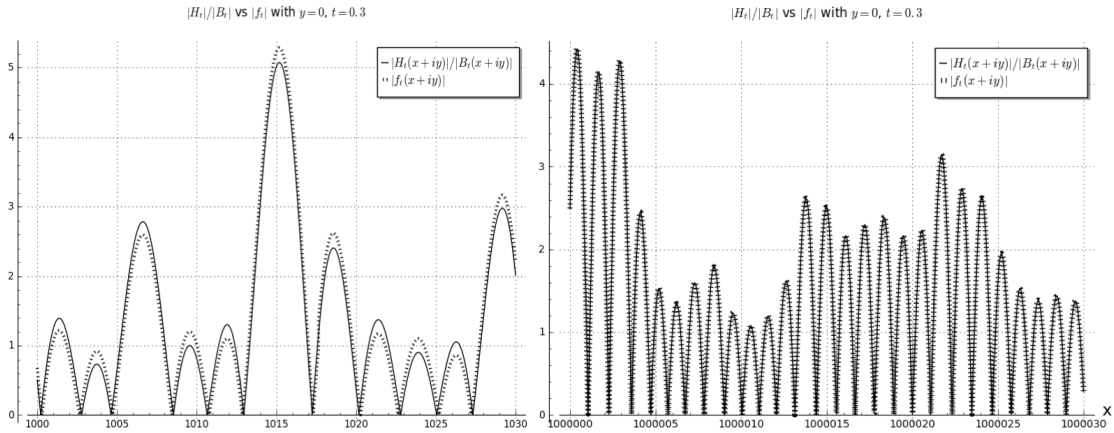


FIGURE 5. Comparison of $|f_t(x+iy)|$ and $|H_t(x+iy)|/|B_t(x+iy)|$ for $y = 0$, $t = 0.3$, $1000 \leq x \leq 1030$ (left), and when $10^6 \leq x \leq 10^6 + 30$ (right). Again notice the improving approximation with x .

Corollary 1.4 (Criterion for non-vanishing). *Let t, x, y lie in the region (5), and let $f_t, e_A, e_B, e_{C,0}$ be as in Theorem 1.3. If one has the inequality*

$$(25) \quad |f_t(x+iy)| > e_A + e_B + e_{C,0}$$

then $H_t(x+iy) \neq 0$.

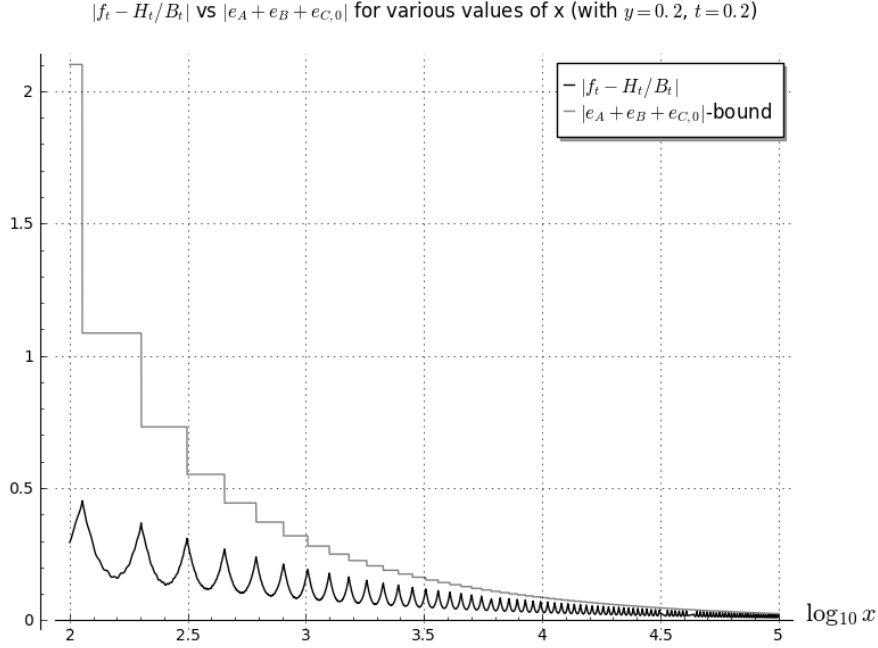


FIGURE 6. The error upper bound $|e_A + e_B + e_{C,0}|$ versus $|f_t - H_t/B_t|$ when $y = t = 0.2$ and $2 \leq \log_{10} x \leq 5$.

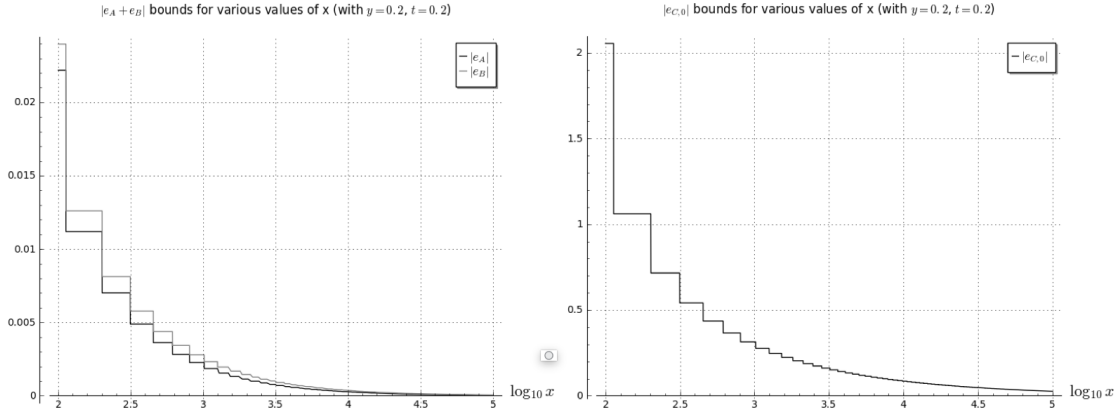


FIGURE 7. The individual error upper bounds $|e_A|$, $|e_B|$ and $|e_{C,0}|$ with $y = t = 0.2$ and $2 \leq \log_{10} x \leq 5$. The $e_{C,0}$ -term clearly dominates.

In the asymptotic limit $x \rightarrow \infty$, one easily sees that

$$\begin{aligned}
 e_A + e_B &= O\left(\frac{\log^2 x}{x}\right) \\
 e_{C,0} &= O\left(x^{-\frac{3+y}{4}} \exp\left(-\frac{t}{16} \log^2 x\right)\right) \\
 f_t(x + iy) &= 1 + O\left(x^{-\frac{t}{4}} \log^2\right),
 \end{aligned}$$

thus giving the crude asymptotic (12) in the region (5) at least. In practice, the $e_{C,0}$ term numerically dominates the $e_A + e_B$ term, although both errors will be quite small in the ranges of x under consideration; in particular, for the ranges needed to verify conditions (ii) and (iii) of Theorem 1.2, we can make $e_A + e_B$ and $e_{C,0}$ both significantly smaller than $|f_t(x + iy)|$. In the spirit of expanding the Riemann-Siegel approximation to higher order, we also obtain an even more accurate explicit approximation in which a correction term $-\frac{C_t}{B_t}$ is added to f_t , and the error term $e_{C,0}$ is replaced by a smaller quantity e_C ; see (69) and Figure 8.

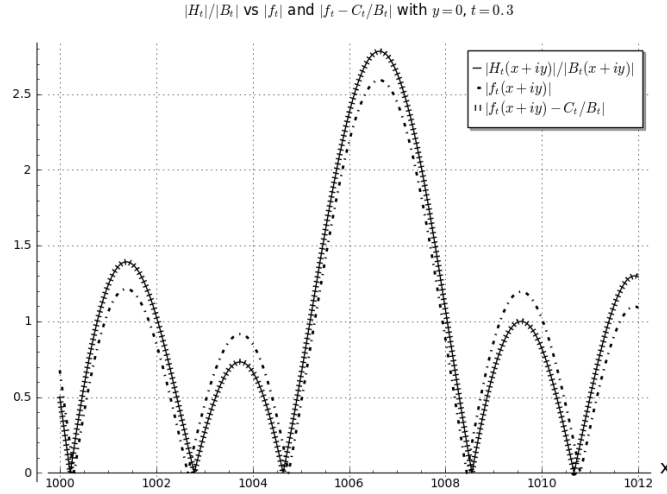


FIGURE 8. Comparison of $|f_t(x+iy)|$, $|f_t(x+iy) - \frac{C_t(x+iy)}{B_t(x+iy)}|$ and $|H_t(x+iy)|/|B_t(x+iy)|$ for $y = 0$, $t = 0.3$, $1000 \leq x \leq 1012$.

In addition to establishing upper bounds such as Theorem 1.1, one can use Theorem 1.3 and Corollary 1.4 (together with variants in slightly larger regions than (5), for instance if y is allowed to be as large as 10) to obtain asymptotic control on the zeroes of H_t , refining previous work of Ki, Kim, and Lee [9]. Indeed, in Section 10 we will establish

Theorem 1.5 (Distribution of zeroes of H_t). *Let $0 < t \leq 1/2$, let $C > 0$ be a sufficiently large absolute constant, and let $c > 0$ be a sufficiently small absolute constant. For $x \geq 4\pi$, define*

$$g(x, t) := \frac{x}{4\pi} \log \frac{x}{4\pi} - \frac{x}{4\pi} + \frac{11}{8} + \frac{t}{16} \log \frac{x}{4\pi}$$

and all $n \geq C$, let x_n be the unique real number greater than 4π such that

$$(26) \quad g(x_n, t) = n.$$

(This is well-defined since the $g(x, t)$ is increasing in x for $x \geq 4\pi$.)

- (i) *If $x \geq \exp(\frac{C}{t})$ and $H_t(x + iy) = 0$, then $y = 0$, and*

$$x = x_n + O(x^{-ct})$$

for some n .

- (ii) *Conversely, for each $n \geq \exp(\frac{C}{t})$ there is exactly one zero H_t in the disk $\{x + iy : |x + iy - x_n| \leq \frac{c}{\log x_n}\}$ (and by part (i), this zero will be real and lie within $O(x^{-ct})$ of x_n).*

(iii) If $X \geq \exp(\frac{C}{t})$, the number $N_t(X)$ of zeroes with real part between 0 and X (counting multiplicity) is

$$N_t(X) = g(X, t) + O(1).$$

(iv) For any $X \geq 0$, one has

$$N_t(X+1) - N_t(X) \leq O(\log(2+X))$$

and

$$N_t(X) = g(X, t) + O(\log(2+X)).$$

Here and in the sequel we use $X = O(Y)$ to denote the estimate $|X| \leq AY$ for some constant A that is absolute (in particular, A is independent of t and C).

Roughly speaking, these estimates tell us that the zeroes of H_t behaves (on macroscopic scales) like those of H_0 in the region $x = O(\exp(O(1/t)))$, and are very evenly spaced (and on the real axis) outside of this range. The factor $\frac{t}{16} \log \frac{x_n}{4\pi}$ in (26) indicates that as time t advances, the zeroes (or at least those with large values of x) will tend to move towards the origin at a speed of approximately $\frac{\pi}{4}$. Although we will not prove this here, the conclusions (i) and (iii) suggest that one in fact has an asymptotic of the form

$$N_t(X) = \left\lfloor g(X, t) + O(X^{-ct}) \right\rfloor$$

when $X \geq \exp(C/t)$; in particular (since the sawtooth function $x - \lfloor x \rfloor$ has average value $\frac{1}{2}$) one would have the heuristic approximation

$$N_t(X) \approx \frac{X}{4\pi} \log \frac{X}{4\pi} - \frac{X}{4\pi} + \frac{7}{8} + \frac{t}{16} \log \frac{X}{4\pi}$$

after performing some averaging in X , thus recovering the familiar $\frac{7}{8}$ term in the usual averaged asymptotics for $N_0(X)$.

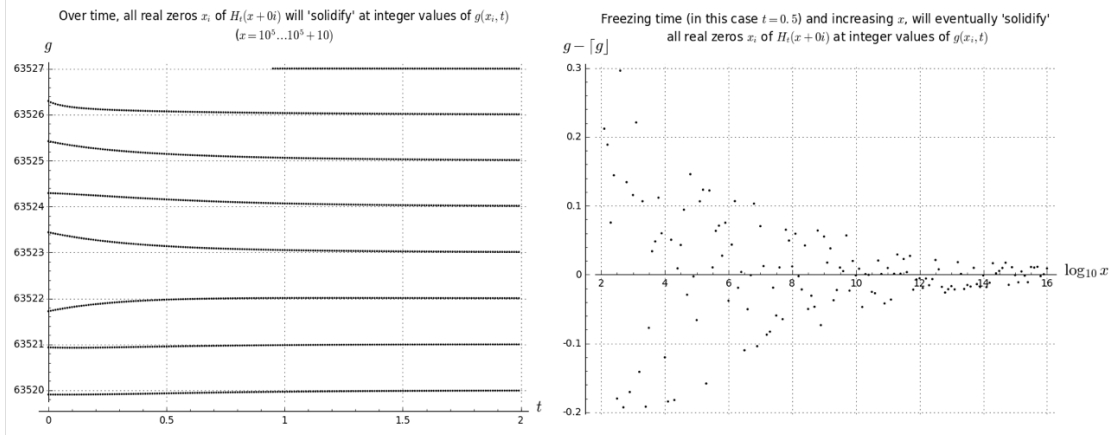


FIGURE 9. The real zeroes x_i of H_t will converge to integer values of $g(x_i, t)$ when t (left) and/or x (right) increases.

The results in Theorem 1.5 refine previous results of Ki, Kim, and Lee [9, Theorems 1.3, 1.4], which gave similar results but with constants that depended on t in a non-uniform (and ineffective) fashion, and error terms that were of shape $o(1)$ rather than $O(x^{-ct})$ in the limit

$x \rightarrow \infty$ (holding t fixed). The results may also be compared with those in [2], who (in our notation) show that assuming RH, the zeroes of H_0 are precisely the solutions x_n to the equation

$$\frac{1}{2\pi} \arg \left(-e^{2i\vartheta(x_n/2)} \frac{\zeta'(\frac{1-ix_n}{2})}{\zeta'(\frac{1+ix_n}{2})} \right) = n$$

for integer n , where $-\vartheta(t)$ is the phase of $\zeta(\frac{1}{2} + it)$ and one chooses a branch of the argument so that the left-hand side is $-\frac{1}{2}$ when $x_n = 0$.

Remark 1.6. *One can draw an analogy between the various potential behaviours of zeroes of H_t and the three classical states of matter. A “gaseous” state corresponds to the situation in which the zeroes of H_t are strictly complex. A “liquid” state corresponds to a situation in which the zeroes are real, but disordered (with highly unequal spacings between zeroes). A “solid” state corresponds to a situation in which the zeroes are real and arranged roughly in an arithmetic progression. Thus for instance the Riemann hypothesis and the GUE hypothesis assert (roughly speaking) that the zeroes of H_0 should exhibit liquid behaviour everywhere, while Theorem 1.5 asserts that the zeroes of H_t , $t > 0$ “solidify” in the region $x \geq \exp(C/t)$. Below this region we expect liquid behaviour. In general, as the parameter t increases, the zeroes appear to “cool” down, transitioning from gaseous to liquid to solid type states; see [20] for some formalisations of this intuition.*

1.1. About this project. This paper is part of the *Polymath project*, which was launched by Timothy Gowers in February 2009 as an experiment to see if research mathematics could be conducted by a massive online collaboration. The current project (which was administered by Terence Tao) is the fifteenth project in this series. Further information on the Polymath project can be found on the web site michaelnielsen.org/polymath1. Information about this specific project may be found at

michaelnielsen.org/polymath1/index.php?title=De.Bruijn-Newman.constant

and a full list of participants and their grant acknowledgments may be found at

michaelnielsen.org/polymath1/index.php?title=Polymath15.grant.acknowledgments

2. NOTATION

We use the standard branch Log of the logarithm to define the standard complex powers $z^w := \exp(w \text{Log} z)$, and in particular define the standard square root $\sqrt{z} := z^{1/2} = \exp(\frac{1}{2} \text{Log} z)$. We record the familiar gaussian identity

$$(27) \quad \int_{\mathbb{R}} \exp(-au^2 + bu + c) \, du = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a} - c\right)$$

for any complex numbers a, b, c with $\text{Re} a > 0$.

When using order of magnitude notation such as $O_{\leq}(X)$, any expression of the form $A = B$ using this notation should be interpreted as the assertion that any quantity of the form A is also of the form B , thus for instance $O_{\leq}(1) + O_{\leq}(1) = O_{\leq}(3)$. (In particular, the equality relation is no longer symmetric with this notation.)

If F is a meromorphic function, we use F' to denote its derivative. We also use F^* to denote the reflection $F^*(s) := \overline{F(\overline{s})}$ of F . Observe from analytic continuation that if $F : \Omega \rightarrow \mathbb{C}$ is holomorphic on a connected open domain $\Omega \subset \mathbb{C}$ containing an interval in \mathbb{R} , and is real-valued

on $\Omega \cap \mathbb{R}$, then it is equal to its own reflection: $F = F^*$ (since the holomorphic function $F - F^*$ has an uncountable number of zeroes).

3. DYNAMICS OF ZEROES

In this section we control the dynamics of the zeroes of H_t in order to establish Theorem 1.2. As H_t is even with functional equation $H_t = H_t^*$, the zeroes are symmetric around the origin and the real axis; from (4) and the positivity of Φ , we also see that $H_t(iy) > 0$ for all $y \in \mathbb{R}$, so there are no zeroes on the imaginary axis. From the super-exponential decay of Φ and (4) we see that the entire function H_t is of order 1; by Jensen's formula, this implies that the number of zeroes in a large disk $D(0, R)$ is at most $O(R^{1+o(1)})$ as $R \rightarrow \infty$.

We begin with the analysis of the dynamics of a single zero of H_t :

Proposition 3.1 (Dynamics of a single zero). *Let $t_0 \in \mathbb{R}$, and let $(z_k(t_0))_{k \in \mathbb{Z} \setminus \{0\}}$ be an enumeration of the zeroes of H_{t_0} in \mathbb{C} (counting multiplicity), with the symmetry condition $z_{-k}(t_0) = -z_k(t_0)$.*

- (i) *If $j \in \mathbb{Z} \setminus \{0\}$ is such that $z_j(t_0)$ is a simple zero of H_{t_0} , then there exists a neighbourhood U of $z_j(t_0)$, a neighbourhood I of t_0 in \mathbb{R} , and a smooth map $z_j : I \rightarrow U$ such that for every $t \in I$, $z_j(t)$ is the unique zero of H_t in U . Furthermore one has the equation*

$$(28) \quad \frac{\partial z_j}{\partial t}(t_0) = 2 \sum'_{k \neq j} \frac{1}{z_j(t_0) - z_k(t_0)}$$

where the sum is over those $k \in \mathbb{Z} \setminus \{0\}$ with $k \neq j$, and the prime means that the k and $-k$ terms are summed together (except for the $k = -j$ term, which is summed separately) in order to make the sum convergent.

- (ii) *If $j \in \mathbb{Z} \setminus \{0\}$ is such that $z_j(t_0)$ is a repeated zero of H_{t_0} of order $m \geq 2$, then there is a neighbourhood U of $z_j(t_0)$ such that for t sufficiently close to t_0 , there are precisely m zeroes of H_t in U , and they take the form*

$$z_j(t_0) + \sqrt{2}(t - t_0)^{1/2}x_j + O(|t - t_0|)$$

for $j = 1, \dots, m$ as $t \rightarrow t_0$, where $x_1 < \dots < x_m$ are the roots of the m^{th} Hermite polynomial

$$(29) \quad \text{He}_m(z) := (-1)^m \exp\left(\frac{z^2}{2}\right) \frac{d^m}{dz^m} \exp\left(-\frac{z^2}{2}\right)$$

$$(30) \quad = \sum_{0 \leq l \leq m/2} \frac{m!}{l!(m-2l)!} (-1)^l \frac{z^{m-2l}}{2^l}$$

and the implied constant in the $O()$ notation can depend on t_0 , j , and m .

The differential equation (28) was previously derived in [8, Lemma 2.4] in the case $t > \Lambda$ (in which all zeroes are real and simple); however, in our applications we also need to consider the regime $t < \Lambda$ in which the zeroes are permitted to be complex or repeated. The roots x_1, \dots, x_m can be given explicitly for small values of m as

$$x_1 = -1; \quad x_2 = +1$$

when $m = 2$,

$$x_1 = -\sqrt{3}; \quad x_2 = 0; \quad x_3 = +\sqrt{3}$$

when $m = 3$, and

$$x_1 = -\sqrt{3 + \sqrt{6}}; \quad x_2 = -\sqrt{3 - \sqrt{6}}; \quad x_3 = \sqrt{3 - \sqrt{6}}; \quad x_4 = \sqrt{3 + \sqrt{6}}$$

when $m = 4$. From (29) and iterating Rolle's theorem we see that all the roots x_1, \dots, x_m of He_m are real; from the Hermite equation $\left(\frac{d^2}{dz^2} - z\frac{d}{dz} + m\right)\text{He}_m(z) = 0$ and the Picard uniqueness theorem for ODE we see that the zeroes are all simple.

Proof. First suppose we are in the situation of (i). As $z_j(t_0)$ is simple, $\frac{\partial}{\partial z}H_t$ is non-zero at $z_j(t_0)$; since $H_t(z)$ is a smooth function of both t and z , we conclude from the implicit function theorem that there is a unique solution $z_j(t) \in U$ to the equation

$$H_t(z_j(t)) = 0$$

with $z_j(t)$ in a sufficiently small neighbourhood U of $z_j(t_0)$, if t is in a sufficiently small neighbourhood I of t_0 ; furthermore, $z_j(t)$ depends smoothly on t , and agrees with $z_j(t_0)$ when $t = t_0$. Differentiating the above equation at t_0 , we obtain

$$\frac{\partial H_t}{\partial t}\bigg|_{t=t_0}(z_j(t_0)) + \frac{\partial z_j}{\partial t}(t_0)H'_t(z_j(t_0)) = 0,$$

where the primes denote differentiation in the z variable. On the other hand, from (4) and differentiation under the integral sign (which can be justified using the rapid decrease of Φ) we have the backwards heat equation

$$(31) \quad \frac{\partial H_t}{\partial t} = -H_t''$$

for all $t \geq 0$. Inserting this into the previous equation, we conclude that

$$(32) \quad \frac{\partial z_j}{\partial t}(t_0) = \frac{H_t''}{H_t'}(z_j(t_0)),$$

noting that the denominator $H_t'(z_j(t_0))$ vanishes by the hypothesis that the zero at $z_j(t_0)$ is simple. Henceforth we omit the dependence on t_0 for brevity. From Taylor expansion of H_t , H_t' , and H_t'' around the simple zero z_j we see that

$$(33) \quad \frac{H_t''}{H_t'}(z_j) = 2 \lim_{z \rightarrow z_j} \left(\frac{H_t'}{H_t}(z) - \frac{1}{z - z_j} \right).$$

On the other hand, as H_t is even, non-zero at the origin, and entire of order 1, we see from the Hadamard factorization theorem that

$$H_t(z) = H_t(0) \prod_k' \left(1 - \frac{z}{z_k} \right),$$

where the prime indicates that the k and $-k$ factors are multiplied together. The product is locally uniformly convergent, so we may take logarithmic derivatives and conclude that

$$\frac{H_t'}{H_t}(z) = \sum_k' \frac{1}{z - z_k}.$$

Inserting this into (32), (33) and using the dominated convergence theorem (again using the growth in the number of zeroes to justify the interchange of summation and limits), we obtain the claim (i).

Now we prove (ii). We abbreviate $z_j(t_0)$ as z_j . By Taylor expansion we have

$$\frac{\partial^{2k} H_{t_0}}{\partial z^{2k}}(z) = m(m-1) \dots (m-2k+1) a_m (z - z_j)^{m-2k} + O(|z - z_j|^{\max(m-2k+1, 0)})$$

as $z \rightarrow z_j$ for any fixed integer $k \geq 0$ and some non-zero complex number $a_m = a_m(z_j, t_0)$ (with the implied constant in the $O()$ notation allowed to depend on k, z_j, t_0); applying the backwards heat equation (31) we thus have

$$\frac{\partial^k H_t}{\partial t^k} \Big|_{t=t_0}(z) = (-1)^k m(m-1) \dots (m-2k+1) a_m (z - z_j)^{m-2k} + O(|z - z_j|^{\max(m-2k+1, 0)}).$$

Performing Taylor expansion in time and using (30), we conclude that in the regime $z - z_j = O(|t - t_0|^{1/2})$, one has the bound

$$H_t(z) = a_m ((t - t_0)^{1/2})^m \left(\text{He}_m \left(\sqrt{2} \frac{z - z_j}{(t - t_0)^{1/2}} \right) + O(|t - t_0|^{1/2}) \right)$$

as $t \rightarrow t_0$, using (say) the standard branch of the square root. By the inverse function theorem (and the simple nature of the zeroes of He_m), we conclude that for t sufficiently close but not equal to t_0 , we have m zeroes of H_t of the form

$$z_j + (t - t_0)^{1/2} x_j + O(|t - t_0|).$$

By Rouché's theorem, if U is a sufficiently small neighborhood of z_j then these are the only zeroes of H_t in U for t sufficiently close to t_0 . The claim follows. \square

Next, we recall the following bound of de Bruijn:

Theorem 3.2. *Suppose that $t_0 \in \mathbb{R}$ and $y_0 > 0$ is such that there are no zeroes $H_{t_0}(x + iy) = 0$ with $x \in \mathbb{R}$ and $y > y_0$. Then for any $t > t_0$, there are no zeroes $H_t(x + iy) = 0$ with $x \in \mathbb{R}$ and $y > \max(y_0^2 - 2(t - t_0), 0)^{1/2}$. In particular one has $\Lambda \leq t_0 + \frac{1}{2}y_0^2$.*

Proof. See [4, Theorem 13]. \square

We are now ready to prove Theorem 1.2. The main step is to establish

Proposition 3.3 (Zero-free region criterion). *Suppose that $t_0, X > 0$ and $0 < y_0 \leq 1$ obey the following hypotheses:*

- (i) *There are no zeroes $H_0(x + iy) = 0$ with $0 \leq x \leq X$ and $\sqrt{y_0^2 + 2t_0} \leq y \leq 1$.*
- (ii) *There are no zeroes $H_{t_0}(x + iy) = 0$ with $x \geq X + \sqrt{1 - y_0^2}$ and $y_0 \leq y \leq \sqrt{1 - 2t_0}$.*
- (iii) *There are no zeroes $H_t(x + iy) = 0$ with $X \leq x \leq X + \sqrt{1 - y_0^2}$, $\sqrt{y_0^2 + 2(t_0 - t)} \leq y \leq \sqrt{1 - 2t}$, and $0 \leq t \leq t_0$.*

Then there are no zeroes $H_{t_0}(x + iy) = 0$ with $x \in \mathbb{R}$ and $y \geq y_0$.

Proof. It is well known that the Riemann ξ function has no zeroes outside of the strip $\{0 \leq \text{Re}(s) \leq 1\}$, hence there are no zeroes $H_0(x + iy) = 0$ with $y > 1$. By Theorem 3.2, we may thus remove the upper bound constraints $y \leq 1$, $y \leq \sqrt{1 - 2t_0}$, and $y \leq \sqrt{1 - 2t}$ from (i), (ii), and (iii) respectively.

By hypotheses (ii), (iii) and the symmetry properties of H_t , it suffices to show that for every $0 \leq t \leq t_0$, there are no zeroes $H_t(x + iy) = 0$ with $0 \leq x \leq X$ and $y \geq Y(t)$, where $Y(t) :=$

$\sqrt{y_0^2 + 2(t_0 - t)}$. By hypothesis (i), this is true at time $t = 0$. Suppose the claim failed for some time $0 < t \leq t_0$. Let $t_1 \in (0, t_0]$ be the minimal time in which this occurred (such a time exists because H_t varies continuously in t , and there are no zeroes $H_t(x + iy) = 0$ with (say) $y > 1$). From Rouché's theorem (or Proposition 3.1) we conclude that there is a zero $H_{t_1}(x + iy) = 0$ with $x + iy$ on the boundary of the region $\{x + iy : 0 \leq x \leq X, y \geq Y(t_1)\}$. The right side $x = X$ of this boundary is ruled out by hypothesis (ii), and (as mentioned at the start of the section) the left side $x = 0$ is ruled out by (4) and the positivity of Φ . Thus by the symmetry properties of H_{t_1} we must have

$$H_{t_1}(x + iY(t_1)) = 0$$

for some $0 < x < X$.

Suppose first that H_{t_1} has a repeated zero at $x + iy_0$. Using Proposition 3.1(ii) and observing (from the symmetry of H_{t_1}) that at least one of the roots x_1, \dots, x_m is positive, we then see that for $t < t_1$ sufficiently close to t_1 , H_t has a zero in the region $\{x + iy : 0 \leq x \leq X, y \geq Y(t)\}$, contradicting the minimality of t_1 . Thus the zero $x + iY(t_1)$ of H_{t_1} must be simple. In particular, by Proposition 3.1(i) we can write $x + iY(t_1) = z_j(t_1)$ for some smooth function z_j in a neighbourhood of t_1 obeying (28), such that $z_j(t)$ is a zero of H_t for all t close to t_1 . We will prove that

$$(34) \quad \operatorname{Im} \frac{\partial}{\partial t} z_j(t_1) < \frac{\partial}{\partial t} Y(t_1),$$

which implies that there is a zero of H_t in the region $\{x + iy : 0 \leq x \leq X, y \geq Y(t)\}$ for $t < t_1$ sufficiently close to t_1 , giving the required contradiction.

The right-hand side of (34) is

$$\frac{\partial}{\partial t} Y(t_1) = -\frac{1}{Y(t_1)}.$$

By Proposition 3.1(i), the left-hand side of (34) is

$$2 \sum'_{k \neq j} \frac{Y(t_1) - y_k}{(x - x_k)^2 + (Y(t_1) - y_k)^2}$$

where we write $z_k = x_k + iy_k$. Clearly any zero $x_k + iy_k$ with imaginary part y_k in $[-Y(t_1), Y(t_1)]$ gives a non-positive contribution to this sum, the contribution of the zero $x - iY(t_1)$ is $-\frac{1}{Y(t_1)}$, the contribution of the zero $-x + iY(t_1)$ vanishes, and the contribution of $-x - iY(t_1)$ is negative. Grouping the remaining zeroes with their complex conjugates, it then suffices to show that

$$\frac{Y(t_1) - y_k}{(x - x_k)^2 + (y_j - y_k)^2} + \frac{Y(t_1) + y_k}{(x - x_k)^2 + (Y(t_1) + y_k)^2} \leq 0$$

whenever $y_k > Y(t_1)$. Cross-multiplying and canceling like terms, this inequality eventually simplifies to

$$y_k^2 \leq (x - x_k)^2 + Y(t_1)^2.$$

But from the hypothesis (iii) and the assumption $y_k > Y(t_1)$, we have $|x_k| \geq X + \sqrt{1 - Y(t_1)^2}$, so $(x - x_k)^2 \geq 1 - Y(t_1)^2$. On the other hand from Theorem 3.2 one has $y_k < 1$, giving the required contradiction. \square

By combining Proposition 3.3 with Theorem 3.2, we obtain Theorem 1.2, noting from (1), (2) that condition (i) of Proposition 3.3 is equivalent to condition (i) of Theorem 3.2.

4. APPLYING THE FUNDAMENTAL SOLUTION FOR THE HEAT EQUATION

As discussed in the introduction, we will establish Theorem 1.3 by writing H_t in terms of H_0 using the fundamental solution to the heat equation. Namely, for any $t > 0$, we have from (27) that

$$e^{tu^2} = \int_{\mathbb{R}} e^{\pm 2\sqrt{t}vu} \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

for any complex u and either choice of sign \pm . Multiplying by $e^{\pm izu}$ and averaging, we conclude that

$$e^{tu^2} \cos(zu) = \int_{\mathbb{R}} \cos((z - 2i\sqrt{t}v)u) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

for any complex z, u . Multiplying by $\Phi(u)$ and using Fubini's theorem, we conclude the heat kernel representation

$$H_t(z) = \int_{\mathbb{R}} H_0(z - 2i\sqrt{t}v) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

for any complex z . Using (1), we thus have

$$(35) \quad H_t(z) = \int_{\mathbb{R}} \frac{1}{8} \xi \left(\frac{1+iz}{2} + \sqrt{t}v \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

Remark 4.1. We have found numerically that the formula (35) gives a fast and accurate means to compute $H_t(z)$ when z is of moderate size, e.g., if $z = x+iy$ with $|x| \leq 10^6$ and $|y| \leq 1$. However, we will not need to directly compute the right-hand side of (35) for our application to bounding Λ , as we will only need to control $H_t(x+iy)$ for large values of x , and we will shortly develop tractable approximations of Riemann-Siegel type that are more suitable for this regime.

We now combine this formula with expansions of the Riemann ξ -function. From [25, (2.10.6)] we have the Riemann-Siegel formula

$$(36) \quad \frac{1}{8} \xi(s) = R_{0,0}(s) + R_{0,0}^*(1-s)$$

for any complex s that is not an integer (in order to avoid the poles of the Gamma function), where $R_{0,0}(s)$ is the contour integral

$$R_{0,0}(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{0 \swarrow 1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}} dw$$

with $0 \swarrow 1$ any infinite line oriented in the direction $e^{5\pi i/4}$ that crosses the interval $[0, 1]$. From the residue theorem (and the gaussian decrease of $e^{i\pi w^2}$ along the $e^{\pi i/4}$ and $e^{5\pi i/4}$ directions) we may expand

$$R_{0,0}(s) = \sum_{n=1}^N r_{0,n}(s) + R_{0,N}(s)$$

for any non-negative integer N , where $r_{0,n}, R_{0,N}$ are the meromorphic functions

$$(37) \quad r_{0,n}(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) n^{-s},$$

$$(38) \quad R_{0,N}(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{N \swarrow N+1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}} dw$$

and $N \searrow N+1$ denotes any infinite line oriented in the direction $e^{5\pi i/4}$ that crosses the interval $[N, N+1]$. For any z that is not purely imaginary, we see from Stirling's approximation that the functions $r_{0,n}(\frac{1+iz}{2} + \sqrt{t}v)$ and $R_{0,N}(\frac{1+iz}{2} + \sqrt{t}v)$ grow slower than gaussian as $v \rightarrow \pm\infty$ (indeed they grow like $\exp(O(|v|\log|v|))$, where the implied constants depend on t, z). From this and (35), (36) we conclude that

$$(39) \quad H_t(z) = \sum_{n=1}^N r_{t,n} \left(\frac{1+iz}{2} \right) + \sum_{n=1}^N r_{t,n}^* \left(\frac{1-iz}{2} \right) + R_{t,N} \left(\frac{1+iz}{2} \right) + R_{t,N}^* \left(\frac{1-iz}{2} \right)$$

for any $t > 0$, any z that is not purely imaginary, and any non-negative integer N , where $r_{t,n}(s), R_{t,N}(s)$ are defined for non-real s by the formulae

$$r_{t,n}(s) := \int_{\mathbb{R}} r_{0,n}(s + \sqrt{t}v) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

$$R_{t,N}(s) := \int_{\mathbb{R}} R_{0,N}(s + \sqrt{t}v) \frac{1}{\sqrt{\pi}} e^{-v^2} dv;$$

these can be thought of as the evolutions of $r_{0,n}, R_{0,N}$ respectively under the forward heat equation.

The functions $r_{0,n}(s), R_{0,N}(s)$ grow slower than gaussian as long as the imaginary part of s is bounded and bounded away from zero. As a consequence, we may shift contours (replacing v by $v + \frac{\sqrt{t}}{2}\alpha_n$) and write

$$(40) \quad r_{t,n}(s) = \exp\left(-\frac{t}{4}\alpha_n^2\right) \int_{\mathbb{R}} \exp(-\sqrt{t}v\alpha_n) r_{0,n}\left(s + \sqrt{t}v + \frac{t}{2}\alpha_n\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

for any complex number α_n with $\text{Im}(s), \text{Im}(s + \frac{t}{2}\alpha_n)$ having the same sign. Similarly we may write

$$(41) \quad R_{t,N}(s) = \exp\left(-\frac{t}{4}\beta_N^2\right) \int_{\mathbb{R}} \exp(-\sqrt{t}v\beta_N) R_{0,N}\left(s + \sqrt{t}v + \frac{t}{2}\beta_N\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

for any complex number β_N with $\text{Im}(s), \text{Im}(s + \frac{t}{2}\beta_N)$ having the same sign. In the spirit of the saddle point method, we will select the parameters α_n, β_N later in the paper in order to make the integrands in (40), (41) close to stationary in phase at $v = 0$, in order to obtain good estimates and approximations for these terms.

5. ELEMENTARY ESTIMATES

In order to explicitly estimate various error terms arising in the proof of Theorem 1.3, we will need the following elementary estimates:

Lemma 5.1 (Elementary estimates). *Let $x > 0$.*

(i) *If $a > 0$ and $b \geq 0$ are such that $x > b/a$, then*

$$O_{\leq}\left(\frac{a}{x}\right) + O_{\leq}\left(\frac{b}{x^2}\right) = O_{\leq}\left(\frac{a}{x - b/a}\right).$$

More generally, if $a > 0$ and $b, c \geq 0$ are such that $x > b/a, \sqrt{c/a}$, then

$$O_{\leq}\left(\frac{a}{x}\right) + O_{\leq}\left(\frac{b}{x^2}\right) + O_{\leq}\left(\frac{c}{x^3}\right) = O_{\leq}\left(\frac{a}{x - \max(b/a, \sqrt{c/a})}\right).$$

(ii) If $x > 1$, then

$$\log\left(1 + O_{\leq}\left(\frac{1}{x}\right)\right) = O_{\leq}\left(\frac{1}{x-1}\right).$$

or equivalently

$$1 + O_{\leq}\left(\frac{1}{x}\right) = \exp\left(O_{\leq}\left(\frac{1}{x-1}\right)\right).$$

(iii) If $x > 1/2$, then

$$\exp\left(O_{\leq}\left(\frac{1}{x}\right)\right) = 1 + O_{\leq}\left(\frac{1}{x-0.5}\right).$$

(iv) We have

$$\exp(O_{\leq}(x)) = 1 + O_{\leq}(e^x - 1).$$

(v) If z is a complex number with $|\operatorname{Im}(z)| \geq 1$ or $\operatorname{Re} z \geq 1$, then

$$\Gamma(z) = \sqrt{2\pi} \exp\left(\left(z - \frac{1}{2}\right) \log z - z + O_{\leq}\left(\frac{1}{12(|z| - 0.33)}\right)\right).$$

(vi) If $a, b > 0, y \geq 0$ and $x \geq x_0 \geq \exp(a/b)$ and $x_0 > c \geq 0$, then

$$\frac{\log^a |x + iy|}{(x - c)^b} \leq \frac{\log^a |x_0 + iy|}{(x_0 - c)^b}.$$

Proof. Claim (i) follows from the geometric series formula

$$\frac{a}{x-t} = \frac{a}{x} + \frac{at}{x^2} + \frac{at^2}{x^3} + \dots$$

whenever $0 \leq t < x$.

For Claim (ii), we use the Taylor expansion of the logarithm to note that

$$\log\left(1 + O_{\leq}\left(\frac{1}{x}\right)\right) = O_{\leq}\left(\frac{1}{x} + \frac{1}{2x^2} + \frac{1}{3x^3} + \dots\right)$$

which on comparison with the geometric series formula

$$\frac{1}{x-1} = \frac{1}{x} + \frac{1}{x^2} + \frac{1}{x^3} + \dots$$

gives the claim. Similarly for Claim (iii), we may compare the Taylor expansion

$$\exp\left(O_{\leq}\left(\frac{1}{x}\right)\right) = 1 + O_{\leq}\left(\frac{1}{x} + \frac{1}{2!x^2} + \frac{1}{3!x^3} + \dots\right)$$

with the geometric series formula

$$\frac{1}{x-0.5} = \frac{1}{x} + \frac{1}{2x^2} + \frac{1}{2^2x^3} + \dots$$

and note that $k! \geq 2^k$ for all $k \geq 2$.

Claim (iv) follows from the trivial identity $e^x = 1 + (e^x - 1)$ and the elementary inequality $e^{-x} \geq 1 - (e^x - 1)$. For Claim (v), we may use the functional equation $\Gamma = \Gamma^*$ to assume that $\operatorname{Im}(z) \geq 0$. From the work of Boyd [3, (1.13), (3.1), (3.14), (3.15)] we have the effective Stirling approximation

$$\Gamma(z) = \sqrt{2\pi} \exp\left(\left(z - \frac{1}{2}\right) \log z - z\right) \left(1 + \frac{1}{12z} + R_2(z)\right)$$

where the remainder $R_2(z)$ obeys the bound

$$|R_2(z)| \leq (2\sqrt{2} + 1) \frac{C_2 \Gamma(2)}{(2\pi)^3 |z|^2}$$

for $\operatorname{Re}(z) \geq 0$ and

$$|R_2(z)| \leq (2\sqrt{2} + 1) \frac{C_2 \Gamma(2)}{(2\pi)^3 |z|^2 |1 - e^{2\pi iz}|}$$

for $\operatorname{Re}(z) \leq 0$, where C_2 is the constant

$$C_2 := \frac{1}{2}(1 + \zeta(2)) = \frac{1}{2} \left(1 + \frac{\pi^2}{6} \right).$$

In the latter case, we have $\operatorname{Im}(z) \geq 1$ by hypothesis, and hence $|1 - e^{2\pi iz}| \geq 1 - e^{-2\pi}$. We conclude that in all ranges of z of interest, we have

$$|R_2(z)| \leq (2\sqrt{2} + 1) \frac{C_2 \Gamma(2)}{(2\pi)^3 |z|^2 (1 - e^{-2\pi})} \leq \frac{0.0205}{|z|^2}$$

and hence by Claim (i)

$$\Gamma(z) = \sqrt{2\pi} \exp \left(\left(z - \frac{1}{2} \right) \log z - z \right) \left(1 + O_{\leq} \left(\frac{1}{12(|z| - 0.246)} \right) \right)$$

and the claim then follows by Claim (ii).

For Claim (vi), it suffices to show that the function $x \mapsto \frac{\log^a |x+iy|}{(x-c)^b}$ is non-increasing for $x \geq \exp(a/b)$. Since $\log |x+iy| = (\log x)(1 + \frac{\log(1+\frac{y^2}{x^2})}{2\log x})$ and the second factor is monotone decreasing in x , it suffices to show that $x \mapsto \frac{\log^a x}{(x-c)^b}$ is non-increasing in this region. Taking logarithms and differentiating, we wish to show that $\frac{a}{x \log x} - \frac{b}{x-c} \leq 0$. But this is clear since $\frac{b}{x-c} \geq \frac{b}{x}$ and $\log x \geq a/b$. \square

6. ESTIMATES FOR LARGE x

We can now begin the proof of Theorem 1.3. The strategy is to use the expansion (39), which turns out to be an effective approximation in the region (5), since we will be able to ensure that quantities such as $s + \sqrt{t}v + \frac{t}{2}\alpha_n$ or $s + \sqrt{t}v + \frac{t}{2}\beta_N$, with $s = \frac{1+i(x+iy)}{2}$, stay away from the real axis where the poles of Γ are located (and also where the error terms in the Riemann-Siegel approximation deteriorate).

Accordingly, we will need effective estimates on the functions $r_{t,n}, R_{t,N}$ appearing in Section 4. We will treat these two functions separately.

6.1. Estimation of $r_{t,n}$. We recall the function $\alpha(s)$ defined in (8). From differentiating (9) we see that

$$(42) \quad \alpha'(s) = -\frac{1}{2s^2} - \frac{1}{(s-1)^2} + \frac{1}{2s}$$

whenever $s \in \mathbb{C} \setminus (-\infty, 1]$. If $\text{Im}(s) > 3$, we conclude in particular the useful bound

$$(43) \quad \begin{aligned} \alpha'(s) &= O_{\leq} \left(\frac{1}{2\text{Im}(s)^2} \right) + O_{\leq} \left(\frac{1}{\text{Im}(s)^2} \right) + O_{\leq} \left(\frac{1}{2\text{Im}(s)} \right) \\ &= O_{\leq} \left(\frac{1}{2\text{Im}(s) - 6} \right) \end{aligned}$$

thanks to Lemma 5.1(i).

We also recall the function M_t and the coefficients b_n^t from (10), (15) respectively. It turns out we have a good approximation

$$r_{t,n}(\sigma + iT) \approx M_t(\sigma + iT) \frac{b_n^t}{n^{\sigma + iT + \frac{t}{2}\alpha(\sigma + iT)}}.$$

More precisely, we have

Proposition 6.1 (Estimate for $r_{t,n}$). *Let σ be real, let $T > 10$, let n be a positive integer, and let $0 < t \leq 1/2$. Then*

$$r_{t,n}(\sigma + iT) = M_t(\sigma + iT) \frac{b_n^t}{n^{\sigma + iT + \frac{t}{2}\alpha(\sigma + iT)}} (1 + O_{\leq}(\varepsilon_{t,n}(\sigma + iT)))$$

where

$$(44) \quad \varepsilon_{t,n}(\sigma + iT) := \exp \left(\frac{\frac{t^2}{8} |\alpha(\sigma + iT) - \log n|^2 + \frac{t}{4} + \frac{1}{6}}{T - 3.33} \right) - 1.$$

Proof. From (37), (6) and Lemma 5.1(v) one has

$$r_{0,n}(s) = M_0(s) n^{-s} \exp \left(O_{\leq} \left(\frac{1}{6(|s| - 0.66)} \right) \right)$$

whenever $\text{Im}(s) > 2$. Let α_n denote the quantity

$$(45) \quad \alpha_n := \alpha(\sigma + iT) - \log n;$$

this is the logarithmic derivative of $M(s)n^{-s}$ at $s = \sigma + iT$. By (9) and the hypothesis $T \geq 10$, the imaginary part of α_n may be lower bounded by

$$(46) \quad \text{Im}(\alpha_n) \geq -\frac{1}{2T} - \frac{1}{T} \geq -0.15;$$

in particular, $\sigma + iT$ and $\sigma + iT + \frac{t}{2}\alpha_n$ have imaginary parts of the same sign. We can now apply (40) to obtain

$$\begin{aligned} r_{t,n}(\sigma + iT) &= \exp \left(-\frac{t}{4}\alpha_n^2 \right) \int_{\mathbb{R}} \exp(-\sqrt{t}v\alpha_n) M_0 \left(\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n \right) \times \\ &\quad \times \exp \left(- \left(\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n \right) \log n + O_{\leq} \left(\frac{1}{6(|\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n| - 0.66)} \right) \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv. \end{aligned}$$

From (46) we see that $\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n$ has imaginary part at least $T - 0.08$. Thus

$$O_{\leq} \left(\frac{1}{6(|\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n| - 0.66)} \right) = O_{\leq} \left(\frac{1}{6(T - 0.74)} \right) = O_{\leq} \left(\frac{1}{6(T - 3.08)} \right).$$

From (43) we have

$$\alpha'(s) = O_{\leq} \left(\frac{1}{2(T - 3.08)} \right)$$

for all s on the line segment between $\sigma + iT$ and $\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n$. Applying Taylor's theorem with remainder to the branch of the logarithm M_0 defined in (7), we conclude that

$$M_0(\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n) = M_0(\sigma + iT) \exp \left(\alpha(\sigma + iT) \left(\sqrt{t}v + \frac{t}{2}\alpha_n \right) + O_{\leq} \left(\frac{|\sqrt{t}v + \frac{t}{2}\alpha_n|^2}{4(T - 3.08)} \right) \right).$$

Combining these estimates, writing $\alpha(\sigma + iT) = \alpha_n + \log n$, estimating $|\sqrt{t}v + \frac{t}{2}\alpha_n|^2$ by $2tv^2 + \frac{t^2}{2}|\alpha_n|^2$, and simplifying, we conclude that

$$\begin{aligned} r_{t,n}(s) &= M_0(\sigma + iT) \exp \left(\frac{t}{4}\alpha_n^2 - (\sigma + iT) \log n \right) \times \\ &\quad \times \int_{\mathbb{R}} \exp \left(O_{\leq} \left(\frac{\frac{t}{2}v^2 + \frac{t^2}{8}|\alpha_n|^2 + \frac{1}{6}}{T - 3.08} \right) \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv. \end{aligned}$$

Using (45), (10), (15) we see that

$$M_0(\sigma + iT) \exp \left(\frac{t}{4}\alpha_n^2 - (\sigma + iT) \log n \right) = M_t(\sigma + iT) \frac{b_n^t}{n^{\sigma + iT + \frac{t}{2}\alpha(\sigma + iT)}}$$

and so it suffices to show that

$$\int_{\mathbb{R}} \exp \left(O_{\leq} \left(\frac{\frac{t}{2}v^2 + \frac{t^2}{8}|\alpha_n|^2 + \frac{1}{6}}{T - 3.08} \right) \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv = 1 + O \left(\exp \left(\frac{\frac{t^2}{8}|\alpha_n|^2 + \frac{t}{4} + \frac{1}{6}}{T - 3.33} \right) - 1 \right).$$

Since $\frac{1}{\sqrt{\pi}} e^{-v^2} dv$ integrates to one, it suffices by Lemma 5.1(iv) to show that

$$\int_{\mathbb{R}} \exp \left(\frac{tv^2 + \frac{t^2}{8}|\alpha_n|^2 + \frac{1}{6}}{2(T - 3.08)} \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv \leq \exp \left(\frac{\frac{t^2}{8}|\alpha_n|^2 + \frac{t}{4} + \frac{1}{6}}{T - 3.33} \right).$$

Since $\frac{1}{T-3.08} < \frac{1}{T-3.33}$, we can remove the $\frac{t^2}{8}|\alpha_n|^2 + \frac{1}{6}$ terms from both sides and reduce to showing that

$$(47) \quad \int_{\mathbb{R}} \exp \left(\frac{tv^2}{2(T - 3.08)} \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv \leq \exp \left(\frac{t}{4(T - 3.33)} \right).$$

Using (27), the left-hand side may be calculated exactly as

$$\left(1 - \frac{t}{2(T - 3.08)} \right)^{-1/2}.$$

Applying Lemma 5.1(ii) and using the hypotheses $t \leq 1/2$, $T \geq 10$, one has

$$1 - \frac{t}{2(T - 3.08)} = \exp \left(O_{\leq} \left(\frac{t}{2(T - 3.33)} \right) \right)$$

and the claim follows. \square

6.2. Estimation of $R_{t,N}$. We begin with the following estimates of Arias de Reyna [1] on the term $\int_{N \swarrow N+1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}}$ appearing in (38):

Proposition 6.2. *Let σ be real and $T' > 0$, and define the quantities*

$$(48) \quad s := \sigma + iT'$$

$$(49) \quad a := \sqrt{\frac{T'}{2\pi}}$$

$$(50) \quad N := \lfloor a \rfloor$$

$$(51) \quad p := 1 - 2(a - N)$$

$$(52) \quad U := \exp\left(-i\left(\frac{T'}{2} \log \frac{T'}{2\pi} - \frac{T'}{2} - \frac{\pi}{8}\right)\right).$$

Let K be a positive integer. Then we have the expansion

$$\int_{N \swarrow N+1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}} = (-1)^{N-1} U a^{-\sigma} \left(\sum_{k=0}^K \frac{C_k(p, \sigma)}{a^k} + RS_K(s) \right)$$

where $C_0(p, \sigma) = C_0(p)$ is independent of σ and is given explicitly by the formula

$$(53) \quad C_0(p) := \frac{e^{\pi i(\frac{p^2}{2} + \frac{3}{8})} - i\sqrt{2} \cos \frac{\pi p}{2}}{2 \cos(\pi p)}$$

(removing the singularities at $p = \pm 1/2$), while for $k \geq 1$ the $C_k(p, \sigma)$ are complex numbers obeying the bounds

$$(54) \quad |C_k(p, \sigma)| \leq \frac{\sqrt{2} 9^\sigma \Gamma(k/2)}{2\pi 2^k}$$

for $\sigma > 0$ and

$$(55) \quad |C_k(p, \sigma)| \leq \frac{2^{\frac{1}{2}-\sigma}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2}}$$

for $\sigma \leq 0$, while the error term $RS_K(s)$ is a complex number obeying the bounds

$$(56) \quad |RS_K(s)| \leq \frac{1}{7} 2^{3\sigma/2} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}}$$

for $\sigma \geq 0$, and

$$(57) \quad |RS_K(s)| \leq \frac{1}{2} \left(\frac{9}{10} \right)^{\lceil -\sigma \rceil} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}}$$

if $\sigma < 0$ and $K + \sigma \geq 2$.

Proof. This follows from [1, Theorems 3.1, 4.1, 4.2] combined with [1, (3.2), (5.2)]. The dependence of $C_k(p, \sigma)$, $k \geq 1$ on σ and the dependence of $RS_K(s)$ on s is suppressed in [1], but can be discerned from the definitions of these quantities (and the related quantities $g(\tau, z)$, $P_k(z) = P_k(z, \sigma)$, $Rg_K(\tau, z)$) in [1, (3.9), (3.10), (3.7), (3.6)]. \square

Note that p ranges in the interval $[-1, 1]$. One can show that

$$(58) \quad |C_0(p)| \leq \frac{1}{2}$$

for all $p \in [-1, 1]$; this follows for instance from the $n = 0$ case of [1, Theorem 6.1]. See also Figure 10.

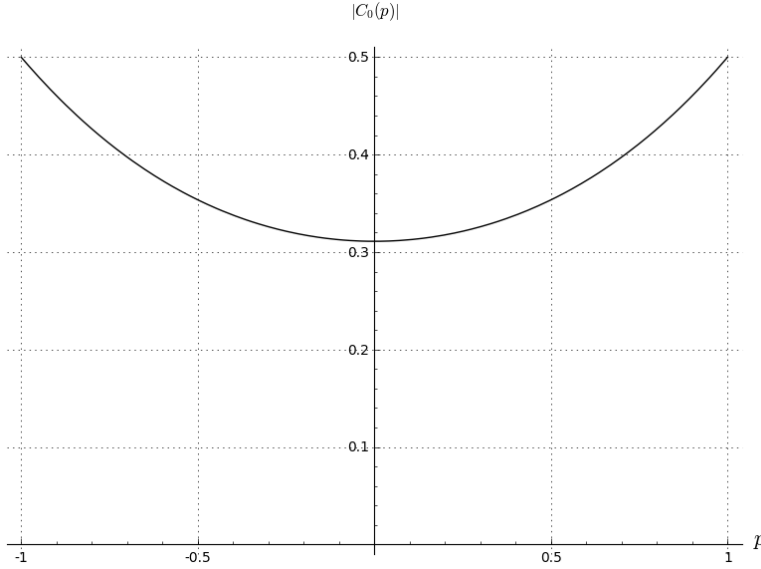


FIGURE 10. Plot of $|C_0(p)|$ for $-1 \leq p \leq 1$.

Informally, the above proposition (and (38), (6)) yield the approximation

$$\begin{aligned} R_{0,N}(s) &\approx \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) (-1)^{N-1} U a^{-\sigma} C_0(p) \\ &\approx (-1)^{N-1} U M_0(s) a^{-\sigma} C_0(p). \end{aligned}$$

If one writes $s = \sigma + iT$, then by using the approximation $\alpha(s) \approx \frac{1}{2} \log \frac{iT}{2\pi}$ for the log-derivative of M_0 , one can then obtain the approximate formula

$$R_{0,N}(s) \approx (-1)^{N-1} U e^{\pi i \sigma / 4} M_0(iT) C_p(p).$$

In fact we have the more general approximation

$$R_{t,N}(s) \approx (-1)^{N-1} U e^{\pi i \sigma / 4} \exp\left(\frac{t\pi^2}{64}\right) M_0(iT') C_p(p)$$

where $T' := T + \frac{\pi t}{8}$. More precisely, we have

Proposition 6.3 (Estimate for $R_{t,N}$). *Let $0 \leq \sigma \leq 1$, let $T \geq 100$, and let $0 < t \leq 1/2$. Set*

$$T' := T + \frac{\pi t}{8}$$

and then define $a, N, p, U, C_0(p)$ using (49), (50), (52), (53). Then

$$R_{i,N}(\sigma + iT) = (-1)^{N-1} U e^{\pi i \sigma / 4} \exp\left(\frac{i\pi^2}{64}\right) M_0(iT') (C_0(p) + O_{\leq}(\tilde{\varepsilon}(\sigma + iT)))$$

where

$$(59) \quad \tilde{\varepsilon}(\sigma + iT) := \left(\frac{0.397 \times 9^\sigma}{a - 0.125} + \frac{5}{3(T' - 3.33)} \right) \exp\left(\frac{3.49}{T' - 3.33}\right).$$

Proof. We apply (41) with $\beta_N := \pi i / 4$ to obtain

$$R_{i,N}(\sigma + iT) = \exp\left(\frac{i\pi^2}{64}\right) \int_{\mathbb{R}} \exp\left(-\frac{\sqrt{t}v\pi i}{4}\right) R_{0,N}(\sigma + iT' + \sqrt{t}v) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

From (38) we have

$$R_{0,N}(\sigma + iT' + \sqrt{t}v) = \frac{1}{8} \frac{s_v(s_v - 1)}{2} \pi^{-s_v/2} \Gamma\left(\frac{s_v}{2}\right) (-1)^{N-1} U a^{-\sigma - \sqrt{t}v} \left(\sum_{k=0}^{K_v} \frac{C_k(p, \sigma + \sqrt{t}v)}{a^k} + RS_{K_v}(s_v) \right)$$

for any positive integer K_v that we permit to depend (in a measurable fashion) on v , where $s_v := \sigma + iT' + \sqrt{t}v$. From (6) and Lemma 5.1(v) we thus have

$$R_{0,N}(\sigma + iT' + \sqrt{t}v) = M_0(s_v) \exp\left(O_{\leq}\left(\frac{1}{12(T' - 0.33)}\right)\right) (-1)^{N-1} U a^{-\sigma - \sqrt{t}v} \left(\sum_{k=0}^{K_v} \frac{C_k(p, \sigma + \sqrt{t}v)}{a^k} + RS_{K_v}(s_v) \right).$$

From (43) and Taylor expansion of the logarithm $\log M_0$ defined in (7), we have

$$M_0(s_v) = M_0(iT') \exp\left(\alpha(iT')(\sigma + \sqrt{t}v) + O_{\leq}\left(\frac{(\sigma + \sqrt{t}v)^2}{4(T' - 0.33)}\right)\right).$$

From (9), (49) one has

$$\alpha(iT') = O_{\leq}\left(\frac{1}{2T'}\right) + O_{\leq}\left(\frac{1}{T'}\right) + \frac{1}{2} \text{Log} \frac{iT'}{2\pi} = \log a + \frac{i\pi}{4} + O_{\leq}\left(\frac{3}{2T'}\right)$$

and hence (bounding $\frac{3}{2T'}$ by $\frac{6}{4(T' - 0.33)}$)

$$\alpha(iT')(\sigma + \sqrt{t}v) = (\sigma + \sqrt{t}v) \log a + \frac{\pi i \sigma}{4} + \frac{\sqrt{t}v \pi i}{4} + O_{\leq}\left(\frac{6|\sigma + \sqrt{t}v|}{4(T' - 0.33)}\right).$$

We conclude that

$$\begin{aligned} \exp\left(-\frac{\sqrt{t}v \pi i}{4}\right) R_{0,N}(\sigma + iT' + \sqrt{t}v) &= M_0(iT') \exp\left(O_{\leq}\left(\frac{(\sigma + \sqrt{t}v)^2 + 6|\sigma + \sqrt{t}v| + \frac{1}{3}}{4(T' - 0.33)}\right)\right) \times \\ &\quad \times (-1)^{N-1} U e^{\pi i \sigma / 4} \left(\sum_{k=0}^{K_v} \frac{C_k(p, \sigma + \sqrt{t}v)}{a^k} + RS_{K_v}(s_v) \right). \end{aligned}$$

Bounding $6|\sigma + \sqrt{t}v| \leq 3(\sigma + \sqrt{t}v)^2 + 3$, we have

$$\frac{(\sigma + \sqrt{t}v)^2 + 6|\sigma + \sqrt{t}v| + \frac{1}{3}}{4(T' - 0.33)} \leq \frac{(\sigma + \sqrt{t}v)^2 + \frac{5}{6}}{T' - 0.33}.$$

Putting all this together, we obtain

$$R_{t,N}(\sigma + iT) = (-1)^{N-1} U e^{\pi i \sigma / 4} \exp\left(\frac{t\pi^2}{64}\right) M_0(iT') \times \\ \times \int_{\mathbb{R}} \exp\left(O_{\leq}\left(\frac{(\sigma + \sqrt{t}v)^2 + \frac{5}{6}}{T' - 0.33}\right)\right) \left(\sum_{k=0}^{K_v} \frac{C_k(p, \sigma + \sqrt{t}v)}{a^k} + RS_{K_v}(s_v)\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

We separate the $k = 0$ term from the rest. By Lemma 5.1(iv) and the fact that $\frac{1}{\sqrt{\pi}} e^{-v^2}$ integrates to one, we can write the above expression as

$$(60) \quad R_{t,N}(\sigma + iT) = (-1)^{N-1} U e^{\pi i \sigma / 4} \exp\left(\frac{t\pi^2}{64}\right) M_0(iT') (C_0(p)(1 + O_{\leq}(\epsilon)) + O_{\leq}(\delta))$$

where

$$\epsilon := \int_{\mathbb{R}} \left(\exp\left(\frac{(\sigma + \sqrt{t}v)^2 + \frac{5}{6}}{T' - 0.33}\right) - 1 \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

and

$$\delta := \int_{\mathbb{R}} \exp\left(\frac{(\sigma + \sqrt{t}v)^2 + \frac{5}{6}}{T' - 0.33}\right) \left(\sum_{k=1}^{K_v} \frac{|C_k(p, \sigma + \sqrt{t}v)|}{a^k} + |RS_{K_v}(s_v)| \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

Bounding $(\sigma + \sqrt{t}v)^2 \leq 2\sigma^2 + 2tv^2$ and using (27) we obtain

$$\epsilon \leq \exp\left(\frac{2\sigma^2 + \frac{5}{6}}{T' - 0.33}\right) \left(1 - \frac{2t}{T' - 0.33}\right)^{-1/2} - 1.$$

Applying Lemma 5.1(ii) and using the hypotheses $t \leq 1/2$, $T \geq 100$, one has

$$1 - \frac{2t}{T' - 0.33} = \exp\left(O_{\leq}\left(\frac{2t}{T' - 3.33}\right)\right)$$

and hence

$$\epsilon \leq \exp\left(\frac{2\sigma^2 + t + \frac{5}{6}}{T' - 3.33}\right) - 1.$$

With $t \leq 1/2$ and $0 \leq \sigma \leq 1$, one has $2\sigma^2 + t + \frac{5}{6} \leq \frac{10}{3}$. By the mean value theorem we then have

$$(61) \quad \epsilon \leq \frac{10}{3(T' - 3.33)} \exp\left(\frac{10}{3(T' - 3.33)}\right).$$

Now we work on δ . Making the change of variables $u := \sigma + \sqrt{t}v$, we have

$$\delta = \int_{\mathbb{R}} \exp\left(\frac{u^2 + \frac{5}{6}}{T' - 0.33}\right) \left(\sum_{k=1}^{\tilde{K}_u} \frac{|C_k(p, u)|}{a^k} + |RS_{\tilde{K}_u}(u + iT')| \right) \frac{1}{\sqrt{\pi t}} e^{-(u-\sigma)^2/t} du,$$

where \tilde{K}_u is a positive integer parameter that can depend arbitrarily on u (as long as it is measurable, of course).

We choose \tilde{K}_u to equal 1 when $u \geq 0$ and $\max(\lfloor -\sigma \rfloor + 3, \lfloor \frac{T'}{\pi} \rfloor)$ when $u < 0$, so that Proposition 6.2 applies. The expression

$$\sum_{k=1}^{\tilde{K}_u} \frac{|C_k(p, u)|}{a^k} + |RS_{\tilde{K}_u}(u + iT')|$$

is then bounded by

$$(62) \quad \frac{\sqrt{2}}{2\pi} \frac{9^u \Gamma(1/2)}{2a} + \frac{1}{7} 2^{3u/2} \frac{\Gamma(1)}{(a/1.1)^2} \leq \frac{0.200 \times 9^u}{a} + \frac{0.173 \times 2^{3u/2}}{a^2}$$

for $u \geq 0$ and

$$(63) \quad \sum_{1 \leq k \leq \tilde{K}_u} \frac{2^{\frac{1}{2}-u}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2} a^k} + \frac{1}{2} (9/10)^{\lceil -u \rceil} \frac{\Gamma((\tilde{K}_u + 1)/2)}{(a/1.1)^{\tilde{K}_u+1}}$$

for $u < 0$. One can calculate that

$$\frac{2^{\frac{1}{2}}}{2\pi} \frac{1}{2\pi} \leq 0.036 \leq \frac{1}{2}$$

and

$$\frac{1}{((3-2\log 2)\pi)^{1/2}} \leq 0.445 \leq 1.1$$

and hence we can bound (63) by

$$0.0362^{-u} \sum_{1 \leq k \leq \frac{T'}{\pi}} (0.445)^k \frac{\Gamma(k/2)}{a^k} \frac{1}{2} 2^{-u} \sum_{\frac{T'}{\pi} \leq k \leq -u+4} \frac{\Gamma(k/2)}{(a/1.1)^k}.$$

For $u \geq 0$, we can estimate (62) by

$$0.2 \times 9^u \left(\frac{1}{a} + \frac{0.865}{a^2} \right) \leq \frac{0.2 \times 9^u}{a - 0.865}$$

thanks to Lemma 5.1(i). For $u < 0$, we observe that if $k \leq 2a^2 = \frac{T'}{\pi}$ then

$$\frac{\Gamma(k+2/2)}{a^{k+2}} = \frac{k}{2a^2} \frac{\Gamma(k/2)}{a^k} \leq \frac{\Gamma(k/2)}{a^k}$$

and hence by the geometric series formula

$$\sum_{2 \leq k \leq \frac{T'}{\pi}, k \text{ even}} (0.445)^k \frac{\Gamma(k/2)}{a^k} \leq \frac{(0.445)^2}{1 - (0.445)^2} \frac{\Gamma(2/2)}{a} \leq \frac{0.247}{a^2}$$

and similarly

$$\sum_{3 \leq k \leq \frac{T'}{\pi}, k \text{ odd}} (0.445)^k \frac{\Gamma(k/2)}{a^k} \leq \frac{(0.445)^3}{1 - (0.445)^2} \frac{\Gamma(3/2)}{(a/1.1)^3} \leq \frac{0.098}{a^3}$$

and hence we can bound (63) by

$$0.0362^{-u} \left(\frac{0.445 \sqrt{\pi}}{a} + \frac{0.247}{a^2} + \frac{0.098}{a^3} \right) + \frac{1}{2} 2^{-u} \sum_{\frac{T'}{\pi} \leq k \leq -u+4} \frac{\Gamma(k/2)}{(a/1.1)^k}.$$

By Lemma 5.1(i) we have

$$0.036 \left(\frac{0.445 \sqrt{\pi}}{a} + \frac{0.247}{a^2} + \frac{0.098}{a^3} \right) \leq \frac{0.029}{a - 0.353}$$

and thus we can bound (63) by

$$\frac{0.029 \times 2^{-u}}{a - 0.353} + \frac{1}{2} 2^{-u} \sum_{\frac{T'}{\pi} \leq k \leq -u+4} (1.1)^k \frac{\Gamma(k/2)}{a^k}.$$

Putting this together, we conclude that

$$\sum_{k=1}^{\tilde{K}_u} \frac{|C_k(p, u)|}{a^k} + |RS_{\tilde{K}_u}(u + iT')| \leq \frac{0.2 \times 9^u}{a - 0.865} + \frac{0.029 \times 2^{-u}}{a - 0.353} + \frac{2^{-u}}{2} \sum_{\frac{T'}{\pi} \leq k \leq -u+4} (1.1)^k \frac{\Gamma(k/2)}{a^k}$$

for all u (positive or negative). We conclude that $\delta \leq \delta_1 + \delta_2 + \delta_3$, where

$$\begin{aligned} \delta_1 &:= \int_{\mathbb{R}} \exp\left(\frac{u^2 + \frac{5}{6}}{T' - 0.33}\right) \frac{0.2 \times 9^u}{a - 0.865} \frac{1}{\sqrt{\pi t}} e^{-(u-\sigma)^2/t} du \\ \delta_2 &:= \int_{\mathbb{R}} \exp\left(\frac{u^2 + \frac{5}{6}}{T' - 0.33}\right) \frac{0.029 \times 2^{-u}}{a - 1.25} \frac{1}{\sqrt{\pi t}} e^{-(u-\sigma)^2/t} du \\ (64) \quad \delta_3 &:= \int_{\mathbb{R}} \exp\left(\frac{u^2 + \frac{5}{6}}{T' - 0.33}\right) \frac{2^{-u}}{2} \sum_{\frac{T'}{\pi} \leq k \leq -u+4} (1.1)^k \frac{\Gamma(k/2)}{a^k} \frac{1}{\sqrt{\pi t}} e^{-(u-\sigma)^2/t} du. \end{aligned}$$

For δ_1 , we translate u by σ to obtain

$$\delta_1 = \frac{0.2 \times 9^\sigma}{a - 0.865} \int_{\mathbb{R}} \exp\left(\frac{u^2 + 2\sigma u + \sigma^2 + \frac{5}{6}}{T' - 0.33} + 2u \log 3\right) \frac{1}{\sqrt{\pi t}} e^{-u^2/t} du$$

and hence by (27)

$$(65) \quad \delta_1 = \frac{0.2 \times 9^\sigma}{a - 0.865} \exp\left(\frac{\sigma^2 + \frac{5}{6}}{T' - 0.33} + \frac{t(\log 3 + \frac{\sigma}{T' - 0.33})^2}{1 - \frac{t}{T' - 0.33}}\right) \left(1 - \frac{t}{T' - 0.33}\right)^{-1/2}.$$

One can write

$$(66) \quad \frac{1}{1 - \frac{t}{T' - 0.33}} = 1 + \frac{t}{T' - 0.33 - t} \leq 1 + \frac{t}{T' - 0.83}$$

while by Lemma 5.1(ii) we have

$$(67) \quad 1 - \frac{t}{T' - 0.33} = \exp\left(O_{\leq}\left(\frac{t}{T' - 0.33 - t}\right)\right) = \exp\left(O_{\leq}\left(\frac{t}{T' - 0.83}\right)\right).$$

We conclude that

$$\delta_1 \leq \frac{0.2 \times 9^\sigma}{a - 0.865} \exp\left(\frac{5 + 3t + 6\sigma^2}{6(T' - 0.83)} + t\left(\log 3 + \frac{\sigma}{T' - 0.33}\right)^2 \left(1 + \frac{t}{T' - 0.83}\right)\right).$$

From Lemma 5.1(i) and the hypothesis $0 \leq \sigma \leq 1$, we have

$$\begin{aligned} \left(\log 3 + \frac{\sigma}{T' - 0.33}\right)^2 &\leq (\log^2 3) \left(1 + \frac{2\sigma/\log 3}{T' - 0.33 - \frac{\sigma}{2\log 3}}\right) \\ &\leq (\log^2 3) \left(1 + \frac{2\sigma/\log 3}{T' - 0.83}\right) \end{aligned}$$

and therefore by a further application of Lemma 5.1(i)

$$\begin{aligned} \left(\log 3 + \frac{\sigma}{T' - 0.33} \right)^2 \left(1 + \frac{t}{T' - 0.83} \right) &\leq \log^2 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - \frac{2\sigma t / \log 3}{2\sigma / \log 3 + t}} \right) \\ &\leq \log^2 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - t} \right) \\ &\leq \log^2 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 1.33} \right) \end{aligned}$$

and thus

$$\delta_1 \leq \frac{0.2 \times 9^\sigma \exp(t \log^2 3)}{a - 0.865} \exp \left(\frac{5 + 3t + 6\sigma^2 + 12t\sigma \log 3 + 6t^2 \log^2 3}{6(T' - 1.33)} \right).$$

By repeating the proof of (65), we have

$$\delta_2 = \frac{0.029 \times 2^{-\sigma}}{a - 0.353} \exp \left(\frac{\sigma^2 + \frac{5}{6}}{T' - 0.33} + \frac{t(-\log \sqrt{2} + \frac{\sigma}{T' - 0.33})^2}{1 - \frac{t}{T' - 0.33}} \right) \left(1 - \frac{t}{T' - 0.33} \right)^{-1/2}.$$

We can bound $(-\log \sqrt{2} + \frac{\sigma}{T' - 0.33})^2$ by $\log^2 \sqrt{2}$. Using (66), (67) we thus have

$$\delta_2 \leq \frac{0.029 \times 2^{-\sigma} \exp(t \log^2 \sqrt{2})}{a - 0.353} \exp \left(\frac{5 + 3t + 6\sigma^2}{6(T' - 1.33)} \right).$$

With $t \leq 1/2$ and $0 \leq \sigma \leq 1$ one has

$$\begin{aligned} 0.2 \exp(t \log^2 3) &\leq 0.366 \\ 0.029 \exp(t \log^2 \sqrt{2}) &\leq 0.031 \\ \frac{5 + 3t + 6\sigma^2}{6} &\leq \frac{5 + 3t + 6\sigma^2 + 12t\sigma \log 3 + 6t^2 \log^2 3}{6} \leq 3.49 \end{aligned}$$

and hence

$$\delta_1 \leq \frac{0.366 \times 9^\sigma}{a - 0.865} \exp \left(\frac{3.49}{T' - 1.33} \right)$$

and

$$\delta_2 \leq \frac{0.031 \times 2^{-\sigma}}{a - 0.353} \exp \left(\frac{3.49}{T' - 1.33} \right).$$

Now we turn to δ_3 , which will end up being extremely small compared to δ_1 or δ_2 . By (64) and the Fubini-Tonelli theorem, we have

$$\delta_3 = \frac{1}{2\sqrt{\pi t}} \sum_{k \geq \frac{T'}{2.2\pi}} (1.1)^k \frac{\Gamma(k/2)}{a^k} \int_{-\infty}^{4-k} \exp \left(\frac{u^2 + \frac{5}{6}}{T' - 0.33} - \frac{(u - \sigma)^2}{t} - u \log 2 \right) du.$$

Since $u \leq 4 - k$, $k \geq \frac{T'}{2.2\pi}$, and $T' \geq T \geq 100$, we have $k \geq 14$ and $u \leq -10$; since $\sigma \geq 0$, we may thus lower bound $(u - \sigma)^2/t$ by u^2/t . Since $t \leq 1/2$, we can upper bound $\frac{u^2 + \frac{5}{6}}{T' - 0.33} - \frac{u^2}{t}$ by (say)

$-\frac{u^2}{2t}$, thus

$$\delta_3 \leq \frac{1}{2\sqrt{\pi t}} \sum_{k \geq \frac{T'}{2.2\pi}} (1.1)^k \frac{\Gamma(k/2)}{a^k} \int_{-\infty}^{4-k} e^{-\frac{u^2}{2t} - u \log 2} du.$$

We can bound $e^{-\frac{u^2}{2t}} \leq e^{\frac{(k-4)u}{2t}}$, in the range of integration and thus

$$\int_{-\infty}^{4-k} e^{-\frac{u^2}{2t} - u \log 2} du \leq \frac{1}{\frac{k-4}{2t} - \log 2} e^{-\frac{(k-4)^2}{2t} + (k-4) \log 2} \leq \frac{1}{\frac{k-4}{2t} - \log 2} e^{-(k-4)^2 + (k-4) \log 2},$$

bounding

$$\frac{k-4}{2t} - \log 2 = \frac{k-4-2t \log 2}{2t} \geq \frac{k-6}{2t}$$

we conclude that

$$\delta_3 \leq \frac{\sqrt{t}}{\sqrt{\pi}} \sum_{k \geq \frac{T'}{2.2\pi}} (1.1)^k \frac{\Gamma(k/2)}{(k-6)a^k} e^{-(k-4)^2 + (k-4) \log 2}.$$

For $k \geq 14$ one can easily verify that $(1.1)^k \Gamma(k/2) e^{-(k-4)^2 + (k-4) \log 2} \leq 10^{-30}$; discarding the $\frac{\sqrt{t}}{\sqrt{\pi}}$ and $\frac{1}{k-6}$ factors we thus have

$$\delta_3 \leq \sum_{k \geq 14} \frac{10^{-30}}{a^k} \leq \frac{2 \times 10^{-30}}{a^{14}}$$

(say). Since

$$\frac{0.031 \times 2^{-\sigma}}{a - 0.353} + \frac{2 \times 10^{-30}}{a^{14}} \leq \frac{0.031 \times 2^{-\sigma}}{a - 0.865}$$

we thus have

$$\delta \leq \delta_1 + \delta_2 + \delta_3 \leq \frac{0.366 \times 9^\sigma + 0.031 \times 2^{-\sigma}}{a - 0.865} \exp\left(\frac{3.49}{T' - 1.33}\right).$$

Inserting this and (61), (58) into (60), and crudely bounding $2^{-\sigma}$ by 9^σ , we obtain the claim. \square

6.3. Combining the estimates. Combining Propositions 6.1, 6.3 with (39) and the triangle inequality (and noting that $M_0 = M_0^*$, $M_t = M_t^*$ and $\alpha = \alpha^*$, and that U has magnitude 1), we conclude the following “ $A + B - C$ approximation to H_t ”:

Corollary 6.4 ($A + B - C$ approximation). *Let t, x, y obey (5). Set*

$$(68) \quad T' := \frac{x}{2} + \frac{\pi t}{8}$$

and then define $a, N, p, U, C_0(p)$ using (49), (50), (52), (53). Define the quantities

$$\begin{aligned} s_+ &= s_+(x + iy) := \frac{1 + y - ix}{2} \\ s_- &= s_-(x + iy) := \frac{1 - y + ix}{2} \\ A_t(x + iy) &:= M_t(s_-) \sum_{n=1}^N \frac{b_n^t}{n^{s_- + \frac{1}{2}\alpha(s_-)}} \\ B_t(x + iy) &:= M_t(s_+) \sum_{n=1}^N \frac{b_n^t}{n^{s_+ + \frac{1}{2}\alpha(s_+)}} \\ C_t(x + iy) &:= 2e^{-\pi i y/8} (-1)^N \exp\left(\frac{t\pi^2}{64}\right) \operatorname{Re}(M_0(iT')C_0(p)Ue^{\pi i/8}) \end{aligned}$$

where M_0, b_n^t were defined in (10), (15). Then

$$H_t(x + iy) = A_t(x + iy) + B_t(x + iy) - C_t(x + iy) + O_{\leq}(E_A(x + iy) + E_B(x + iy) + E_C(x + iy))$$

where

$$\begin{aligned} E_A(x + iy) &:= |M_t(s_-)| \sum_{n=1}^N \frac{b_n^t}{n^{\frac{1-y}{2} + \frac{1}{2}\operatorname{Re}\alpha(s_-)}} \varepsilon_{t,n}(s_-) \\ E_B(x + iy) &:= |M_t(s_+)| \sum_{n=1}^N \frac{b_n^t}{n^{\frac{1+y}{2} + \frac{1}{2}\operatorname{Re}\alpha(s_+)}} \varepsilon_{t,n}(s_+) \\ E_C(x + iy) &:= \exp\left(\frac{t\pi^2}{64}\right) |M_0(iT')| (\tilde{\varepsilon}(s_-) + \tilde{\varepsilon}(s_+)) \end{aligned}$$

and $\varepsilon_{t,n}, \tilde{\varepsilon}$ were defined in (44), (59).

In our applications, we will just use the cruder “ $A + B$ ” approximation that is immediate from the above corollary and (58):

Corollary 6.5 ($A + B$ approximation). *With the notation and hypotheses as in Corollary 6.4, we have*

$$H_t(x + iy) = A_t(x + iy) + B_t(x + iy) + O_{\leq}(E_A(x + iy) + E_B(x + iy) + E_{C,0}(x + iy))$$

where

$$E_{C,0}(x + iy) := \exp\left(\frac{t\pi^2}{64}\right) |M_0(iT')| (1 + \tilde{\varepsilon}(s_-) + \tilde{\varepsilon}(s_+)).$$

We can now prove Theorem 1.3. Dividing by the expression B_t from (11), and using (14), we conclude that

$$(69) \quad \frac{H_t(x + iy)}{B_t(x + iy)} = f_t(x + iy) - \frac{C_t(x + iy)}{B_t(x + iy)} + O_{\leq}(e_A + e_B + e_C)$$

and

$$(70) \quad \frac{H_t(x + iy)}{B_t(x + iy)} = f_t(x + iy) + O_{\leq}(e_A + e_B + e_{C,0})$$

where

$$(71) \quad e_A := e_A(x + iy) := |\gamma| \sum_{n=1}^N n^y \frac{b_n^t}{n^{\operatorname{Re}(s) + \operatorname{Re}(\kappa)}} \varepsilon_{t,n}(s_-)$$

$$(72) \quad e_B := e_B(x + iy) := \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s)}} \varepsilon_{t,n}(s_+)$$

$$(73) \quad e_C := e_C(x + iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right) |M_0(iT')|}{|M_t(s_+)|} (\tilde{\varepsilon}(s_-) + \tilde{\varepsilon}(s_+)).$$

$$(74) \quad e_{C,0} := e_{C,0}(x + iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right) |M_0(iT')|}{|M_t(s_+)|} (1 + \tilde{\varepsilon}(s_-) + \tilde{\varepsilon}(s_+)),$$

and where γ, s_*, κ were defined in (16), (17), (18). Note also from (68), (49), (50) that N is given by (19).

To conclude the proof of Theorem 1.3 it thus suffices to obtain the following estimates.

Proposition 6.6 (Estimates). *Let the notation and hypotheses be as above.*

(i) *One has*

$$|\gamma| \leq e^{0.02y} \left(\frac{x}{4\pi}\right)^{-y/2}$$

(ii) *One has*

$$\operatorname{Re} s_* \geq \frac{1+y}{2} + \frac{t}{4} \log \frac{x}{4\pi} - \frac{(1-3y + \frac{4y(1+y)}{x^2})_+ t}{2x^2}.$$

(iii) *One has*

$$\kappa = O_{\leq} \left(\frac{ty}{2(x-6)} \right).$$

(iv) *One has*

$$e_A \leq |\gamma| N^{|k|} \sum_{n=1}^N n^y \frac{b_n^t}{n^{\operatorname{Re}(s_*)}} \left(\exp \left(\frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi n^2} + 0.626}{\frac{x}{2} - 6.66} \right) - 1 \right).$$

(v) *One has*

$$e_B \leq \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s_*)}} \left(\exp \left(\frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi n^2} + 0.626}{x - 6.66} \right) - 1 \right).$$

(vi) *One has*

$$e_C \leq \left(\frac{x}{4\pi}\right)^{-\frac{1+y}{4}} \exp \left(-\frac{t}{16} \log^2 \frac{x}{4\pi} + \frac{3|\log \frac{x}{4\pi} + i\frac{\pi}{2}| + 3.58}{x - 8.52} \right) \left(\frac{1.24 \times (3^y + 3^{-y})}{N - 0.125} + \frac{6.92}{x - 6.66} \right).$$

and

$$e_{C,0} \leq \left(\frac{x}{4\pi}\right)^{-\frac{1+y}{4}} \exp \left(-\frac{t}{16} \log^2 \frac{x}{4\pi} + \frac{3|\log \frac{x}{4\pi} + i\frac{\pi}{2}| + 3.58}{x - 8.52} \right) \left(1 + \frac{1.24 \times (3^y + 3^{-y})}{N - 0.125} + \frac{6.92}{x - 6.66} \right).$$

Note that to obtain the bound (24) from Proposition 6.6(vi) we may simply use the inequality $1 + u \leq \exp(u)$ for any $u \in \mathbb{R}$, and then bound $\frac{1}{x-6.66} \leq \frac{1}{x-8.52}$.

Proof. From the mean value theorem (and noting that $M_t = M_t^*$, so that $\left| M_t \left(\frac{1+y-ix}{2} \right) \right| = \left| M_t \left(\frac{1+y+ix}{2} \right) \right|$), we have

$$\log |\gamma| = -y \frac{d}{d\sigma} \log \left| M_t \left(\sigma + \frac{ix}{2} \right) \right|$$

for some $\frac{1-y}{2} \leq \sigma \leq \frac{1+y}{2}$. From (8), (10) we have

$$\frac{d}{d\sigma} \log \left| M_t \left(\sigma + \frac{ix}{2} \right) \right| = \operatorname{Re} \left(\frac{t}{2} \alpha \left(\sigma + \frac{ix}{2} \right) \alpha' \left(\sigma + \frac{ix}{2} \right) + \alpha \left(\sigma + \frac{ix}{2} \right) \right).$$

From (43) one has

$$(75) \quad \alpha' \left(\sigma + \frac{ix}{2} \right) = O_{\leq} \left(\frac{1}{x-6} \right)$$

and from Taylor expansion we also have

$$\alpha \left(\sigma + \frac{ix}{2} \right) = \alpha \left(\frac{ix}{2} \right) + O_{\leq} \left(\frac{\sigma}{x-6} \right);$$

from (9) one has

$$\alpha \left(\frac{ix}{2} \right) = O_{\leq} \left(\frac{1}{x} \right) + O_{\leq} \left(\frac{1}{x} \right) + \frac{1}{2} \operatorname{Log} \frac{ix}{4\pi} = \frac{1}{2} \log \frac{x}{4\pi} + i \frac{\pi}{4} + O_{\leq} \left(\frac{2}{x} \right)$$

and hence

$$(76) \quad \alpha \left(\sigma + \frac{ix}{2} \right) = \frac{1}{2} \log \frac{x}{4\pi} + i \frac{\pi}{4} + O_{\leq} \left(\frac{2+\sigma}{x-6} \right).$$

Inserting these bounds, we conclude that

$$\log |\gamma| = -y \operatorname{Re} \left(\left(\frac{1}{2} \log \frac{x}{4\pi} + i \frac{\pi}{4} + O_{\leq} \left(\frac{2+\sigma}{x-6} \right) \right) \left(1 + O_{\leq} \left(\frac{t}{2(x-6)} \right) \right) \right).$$

Expanding this out, we have

$$\log |\gamma| = -y \left(\frac{1}{2} \log \frac{x}{4\pi} + O_{\leq} \left(\frac{2+\sigma + \frac{t}{4} \log \frac{x}{4\pi} + \frac{t\pi}{8} + \frac{t(2+\sigma)}{2(x-6)}}{x-6} \right) \right).$$

In the region (5), which implies that $0 \leq \sigma \leq 1$, we have

$$2 + \sigma + \frac{t\pi}{8} + \frac{t(2+\sigma)}{2(x-6)} \leq 3.21$$

and thus

$$\log |\gamma| \leq -\frac{y}{2} \log \frac{x}{4\pi} + y \frac{\frac{t}{4} \log \frac{x}{4\pi} + 3.21}{x-6}.$$

The function $x \mapsto \frac{\log \frac{x}{4\pi}}{x-6}$ is decreasing for $x \geq 200$ thanks to Lemma 5.1(vi), hence

$$y \frac{\frac{t}{4} \log \frac{x}{4\pi} + 3.21}{x-6} \leq y \frac{\frac{t}{4} \log \frac{200}{4\pi} + 3.21}{200-6} \leq 0.02y.$$

Claim (i) follows. We remark that one can improve the $e^{0.02y}$ factor here by Taylor expanding α to second order rather than first order, but we will not need to do so here.

To prove claim (ii), it suffices by (48) to show that

$$\operatorname{Re} \alpha(s_+) \geq \frac{1}{2} \log \frac{x}{4\pi} - \frac{(1-3y)_+}{x^2} - \frac{4y(1+y)}{x^4}.$$

By (9) one has

$$\operatorname{Re} \alpha(s_+) = \frac{1+y}{(1+y)^2+x^2} - \frac{2(1-y)}{(1-y)^2+x^2} + \frac{1}{2} \log \frac{\sqrt{(1+y)^2+x^2}}{4\pi}.$$

We bound $\sqrt{(1+y)^2+x^2} \geq x$ and calculate

$$\begin{aligned} \frac{1+y}{(1+y)^2+x^2} - \frac{2(1-y)}{(1-y)^2+x^2} &= -\frac{1-3y}{(1+y)^2+x^2} - \frac{4y(1+y)}{((1+y)^2+x^2)((1-y)^2+x^2)} \\ &\geq -\frac{1-3y+\frac{4y(1+y)}{x^2}}{(1+y)^2+x^2}. \end{aligned}$$

Lower bounding the numerator by its nonnegative part and then lower bounding $(1+y)^2+x^2$ by x^2 , we obtain the claim.

Claim (iii) is immediate from (75) and the fundamental theorem of calculus. Now we turn to (iv), (v). From (76) one has

$$\alpha\left(\frac{1 \pm y + ix}{2}\right) - \log n = \frac{1}{2} \log \frac{x}{4\pi n^2} + i\frac{\pi}{4} + O_{\leq}\left(\frac{3}{x-6}\right)$$

for either choice of sign \pm . In particular, we have

$$(77) \quad \left| \alpha\left(\frac{1 \pm y + ix}{2}\right) - \log n \right|^2 = \frac{1}{4} \log^2 \frac{x}{4\pi n^2} + \frac{\pi^2}{16} + O_{\leq}\left(\frac{3|\log \frac{x}{4\pi n^2} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2}\right).$$

For any $1 \leq n \leq N$, we have

$$1 \leq n^2 \leq N^2 \leq a^2 = \frac{x + \frac{\pi t}{16}}{4\pi};$$

in the region (5), the right-hand side is certainly bounded by $(\frac{x}{4\pi})^2$, so that

$$\frac{4\pi}{x} \leq \frac{x}{4\pi n^2} \leq \frac{x}{4\pi}$$

and hence

$$\left| \log \frac{x}{4\pi n^2} + i\frac{\pi}{2} \right| \leq \left| \log \frac{x}{4\pi} + i\frac{\pi}{2} \right|.$$

In the region (5) we have $x \geq 200$, we see from Lemma 5.1(vi) (after squaring) that $\frac{|\log \frac{x}{4\pi} + i\frac{\pi}{2}|}{x-6}$ is decreasing in x . Thus

$$\begin{aligned} \frac{\pi^2}{16} + \frac{3|\log \frac{x}{4\pi n^2} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2} &\leq \frac{\pi^2}{16} + \frac{3|\log \frac{200}{4\pi} + i\frac{\pi}{2}|}{200-6} + \frac{9}{(200-6)^2} \\ &\leq 0.667. \end{aligned}$$

Similarly, in (5) we also have

$$\frac{t^2}{8} \times 0.667 + \frac{t}{4} + \frac{1}{6} \leq 0.313.$$

We conclude from (44) that

$$\varepsilon_{t,n}\left(\frac{1 \pm y + ix}{2}\right) \leq \exp\left(\frac{\frac{t^2}{32} \log^2 \frac{x}{4\pi n^2} + 0.313}{T - 3.33}\right) - 1.$$

Inserting this bound into (71), (72), we obtain claims (iv), (v).

Now we establish (vi). From (10) we have

$$\frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(s_+)|} = \exp\left(\frac{t\pi^2}{64} - \frac{t}{4}\operatorname{Re}\alpha(s_+)^2\right)\frac{|M_0(iT')|}{|M_0(s_+)|}.$$

Note that $\frac{1+y+ix}{2} = iT' + \frac{1+y}{2} - \frac{\pi it}{8}$. From (43) we see that $|\alpha'(s)| \leq \frac{1}{x-6}$ for any s on the line segment between iT' and $\frac{1+y+ix}{2}$. From Taylor's theorem with remainder applied to a branch of $\log M_0$, and noting that $|M_0(s_+)| = |M_0(\frac{1+y+ix}{2})|$, we conclude that

$$\frac{|M_0(iT')|}{|M_0(s_+)|} = \exp\left(\operatorname{Re}\left(\left(-\frac{1+y}{2} + \frac{\pi it}{8}\right)\alpha(iT')\right) + O_{\leq}\left(\frac{|\frac{1+y}{2} + \frac{\pi it}{8}|^2}{2(x-6)}\right)\right).$$

For $0 \leq y \leq 1$ and $0 < t \leq \frac{1}{2}$ we have

$$\frac{|\frac{1+y}{2} + \frac{\pi it}{8}|^2}{2} \leq 0.52$$

and from (9) one has

$$\alpha(iT') = O_{\leq}\left(\frac{1}{2T'}\right) + O_{\leq}\left(\frac{1}{T'}\right) + \frac{1}{2}\operatorname{Log}\frac{iT'}{2\pi} = \frac{1}{2}\log\frac{T'}{2\pi} + \frac{i\pi}{4} + O_{\leq}\left(\frac{3}{2T'}\right)$$

and hence

$$\frac{|M_0(iT')|}{|M_0(s_+)|} = \exp\left(-\frac{1+y}{4}\log\frac{T'}{2\pi} - \frac{t\pi^2}{32} + O_{\leq}\left(\frac{3|\frac{1+y}{2} + \frac{\pi it}{8}|}{2T'} + \frac{0.52}{x-6}\right)\right).$$

Bounding $\frac{1}{2T'} \leq \frac{1}{x-6}$ and $|\frac{1+y}{2} + \frac{\pi it}{8}| \leq 1.02$, this becomes

$$\frac{|M_0(iT')|}{|M_0(s_+)|} = \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t\pi^2}{32} + O_{\leq}\left(\frac{3.58}{x-6}\right)\right)$$

and hence

$$\frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} = \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t\pi^2}{64} - \frac{t}{4}\operatorname{Re}\alpha\left(\frac{1+y+ix}{2}\right)^2 + O_{\leq}\left(\frac{3.58}{x-6}\right)\right).$$

By repeating the proof of (77) we have

$$\operatorname{Re}\alpha\left(\frac{1 \pm y + ix}{2}\right)^2 = \frac{1}{4}\log^2\frac{x}{4\pi} - \frac{\pi^2}{16} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2}\right).$$

As before, in the region (5) we have

$$\frac{3|\log\frac{x}{4\pi} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2} \leq \frac{3|\log\frac{x}{4\pi} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2}$$

and thus

$$\begin{aligned} \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(s_+)|} &= \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi} + i\frac{\pi}{2}| + 3.58}{x-6} + \frac{9}{(x-6)^2}\right)\right) \\ &= \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi} + i\frac{\pi}{2}| + 3.58}{x-8.52}\right)\right) \end{aligned}$$

thanks to Lemma 5.1(i). Finally, since $T' \geq \frac{x}{2} \geq 100$ in (5), one has

$$\exp\left(\frac{3.49}{T' - 3.33}\right) \leq 1.037$$

and hence by (59)

$$\tilde{\varepsilon}\left(\frac{1 \pm y + ix}{2}\right) \leq \frac{1.24 \times 3^{\pm y}}{a - 0.125} + \frac{1.73}{T' - 3.33}.$$

Hence

$$\tilde{\varepsilon}(s_+) + \tilde{\varepsilon}(s_-) \leq \frac{1.24 \times (3^y + 3^{-y})}{a - 0.125} + \frac{3.46}{T' - 3.33}$$

giving the claim (substituting $T' = x/2$ and $a \geq N$). \square

7. BOUNDING DIRICHLET SERIES

In view of Corollary 1.4, it is of interest to obtain lower bounds for the quantity $f_t(x + iy)$ defined in (14) for x, y, t in the region (5). By the triangle inequality (and the trivial identity $|z| = |\bar{z}|$), we obtain the lower bound

$$|f_t(x + iy)| \geq \left(\left| \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} \right| - |\gamma| \left| \sum_{n=1}^N n^y \frac{b_n^t}{n^{s_* + \bar{k}}} \right| \right)_+.$$

It is thus of interest to obtain lower bounds for differences

$$(78) \quad \Delta := \left(\left| \sum_{n=1}^N \frac{\beta_n}{n^s} \right| - \left| \sum_{n=1}^N \frac{\alpha_n}{n^s} \right| \right)_+$$

of magnitudes of Dirichlet series for various coefficients β_n, α_n . Our tools for this will be as follows.

Lemma 7.1. *Let N be a natural number, let $s = \sigma + iT$ be a complex number for some real σ, T , and let α_n, β_n be complex numbers for $n = 1, \dots, N$ with $\beta_1 = 1$. Let Δ denote the quantity (78).*

(i) *(Triangle inequality) We have*

$$\Delta \geq 1 - \alpha_1 - \sum_{n=2}^N \frac{|\alpha_n| + |\beta_n|}{n^\sigma}.$$

(ii) *(Refined triangle inequality) If the α_n, β_n are all real and $0 \leq \alpha_1 < 1$, then we have*

$$\Delta \geq 1 - \alpha_1 - \sum_{n=2}^N \frac{\max(|\beta_n - \alpha_n|, \frac{1-\alpha_1}{1+\alpha_1} |\beta_n + \alpha_n|)}{n^\sigma}.$$

(iii) *(Dirichlet mollifier) If $\lambda_1, \dots, \lambda_D$ are complex numbers, not all zero, then*

$$\Delta \geq \frac{\tilde{\Delta}}{\sum_{d=1}^D \frac{|\lambda_d|}{d^\sigma}}$$

where

$$\tilde{\Delta} := \left(\left| \sum_{n=1}^{DN} \frac{\tilde{\beta}_n}{n^s} \right| - \left| \sum_{n=1}^{DN} \frac{\tilde{\alpha}_n}{n^s} \right| \right)_+$$

and $\tilde{\alpha}_n, \tilde{\beta}_n$ are the Dirichlet convolutions of α_n, β_n with the λ_d :

$$\begin{aligned}\tilde{\alpha}_n &:= \sum_{1 \leq d \leq D: d|n} \lambda_d \alpha_{n/d} \\ \tilde{\beta}_n &:= \sum_{1 \leq d \leq D: d|n} \lambda_d \beta_{n/d}.\end{aligned}$$

Proof. The claim (i) is immediate from the triangle inequality.

Now we prove (ii). We may assume that the right-hand side is positive, as the claim is trivial otherwise. By a continuity argument (replacing β_n, α_n for $n \geq 2$ by $t\beta_n, t\alpha_n$ with t increasing continuously from zero to one, noting that this only increases the right-hand side of the inequality) it suffices to verify the claim when Δ is positive. In this case, we may write

$$\Delta = \left| \sum_{n=1}^N \frac{\beta_n - e^{i\theta} \alpha_n}{n^s} \right|$$

for some phase θ . By the triangle inequality, we then have

$$\Delta \geq |1 - e^{i\theta} \alpha_1| - \sum_{n=2}^N \frac{|\beta_n - e^{i\theta} \alpha_n|}{n^\sigma}.$$

We factor out $|1 - e^{i\theta} \alpha_1|$, which is at least $1 - \alpha_1$, to obtain the lower bound

$$\Delta \geq (1 - \alpha_1) \left(1 - \sum_{n=2}^N \frac{|\beta_n - e^{i\theta} \alpha_n| / |1 - e^{i\theta} \alpha_1|}{n^\sigma} \right).$$

By the cosine rule, we have

$$\left(|\beta_n - e^{i\theta} \alpha_n| / |1 - e^{i\theta} \alpha_1| \right)^2 = \frac{\beta_n^2 + \alpha_n^2 - 2\alpha_n \beta_n \cos \theta}{1 + \alpha_1^2 - 2\alpha_1 \cos \theta}.$$

This is a fractional linear function of $\cos \theta$ with no poles in the range $[-1, 1]$ of $\cos \theta$. Thus this function is monotone on this range and attains its maximum at either $\cos \theta = +1$ or $\cos \theta = -1$. We conclude that

$$\frac{|\beta_n - e^{i\theta} \alpha_n|}{|1 - e^{i\theta} \alpha_1|} \leq \max\left(\frac{|\beta_n - \alpha_n|}{1 - \alpha_1}, \frac{|\beta_n + \alpha_n|}{1 + \alpha_1}\right)$$

and the claim follows.

For claim (iii), we recall the well-known relationship

$$\begin{aligned}\sum_{n=1}^{DN} \frac{\tilde{\alpha}_n}{n^s} &= \left(\sum_{d=1}^D \frac{\lambda_d}{d^s} \right) \left(\sum_{n=1}^N \frac{\alpha_n}{n^s} \right) \\ \sum_{n=1}^{DN} \frac{\tilde{\beta}_n}{n^s} &= \left(\sum_{d=1}^D \frac{\lambda_d}{d^s} \right) \left(\sum_{n=1}^N \frac{\beta_n}{n^s} \right)\end{aligned}$$

between Dirichlet convolution and Dirichlet series, which implies that

$$\tilde{\Delta} = \left| \sum_{d=1}^D \frac{\lambda_d}{d^s} \right| \Delta.$$

Since $\tilde{\Delta}, \Delta$ are non-negative and

$$\left| \sum_{d=1}^D \frac{\lambda_d}{d^s} \right| \leq \sum_{d=1}^D \frac{|\lambda_d|}{d^\sigma},$$

the claim follows. \square

Returning to the estimation of $f_t(x + iy)$, we conclude from Lemma 7.1(i) with s replaced by s_* , β_n replaced by b_n^t , and α_n replaced by $|\gamma|n^{y-\bar{k}}b_n^t$ that

$$(79) \quad |f_t(x + iy)| \geq 2 - \sum_{n=1}^N \frac{b_n^t}{n^\sigma} - |\gamma| \sum_{n=1}^N \frac{b_n^t}{n^{\sigma-y-|k|}},$$

where $\sigma := \operatorname{Re} s_*$. This rather crude bound will suffice when x is very large, particularly when combined with the estimates in Proposition 6.6. For smaller values of x , we would like to use parts (ii) and (iii) of Lemma 7.1. A technical difficulty arises because the quantity $|\gamma|n^{y-\bar{k}}b_n^t$ quantity need not be real, so that Lemma 7.1(ii) is not directly available. However, by writing

$$n^{-\bar{k}} = 1 + O_\leq(n^{|k|} - 1)$$

we see from the triangle inequality that

$$|f_t(x + iy)| \geq \left(\left| \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} \right| - \left| \sum_{n=1}^N \frac{|\gamma|b_n^t n^y}{n^{s_*}} \right| \right)_+ - |\gamma| \sum_{n=1}^N \frac{b_n^t(n^{|k|} - 1)}{n^{\sigma-y}}.$$

Assuming for now that $|\gamma| < 1$ (which in practice will follow from Proposition 6.6(i)), we can then apply Lemma 7.1(iii) follows by Lemma 7.1(ii) to conclude that

$$(80) \quad |f_t(x + iy)| \geq \frac{1 - \tilde{\alpha}_1 - \sum_{n=2}^N \frac{\max(|\tilde{\beta}_n - \tilde{\alpha}_n|, \frac{1-\tilde{\alpha}_1}{1+\tilde{\alpha}_1}|\tilde{\beta}_n + \tilde{\alpha}_n|)}{n^\sigma}}{\sum_{d=1}^D \frac{|\lambda_d|}{d^\sigma}} - |\gamma| \sum_{n=1}^N \frac{b_n^t(n^{|k|} - 1)}{n^{\sigma-y}}$$

for any real numbers $\lambda_1, \dots, \lambda_D$ with $\lambda_1 = 1$, where

$$\begin{aligned} \tilde{\alpha}_n &:= \sum_{1 \leq d \leq D: d|n} \lambda_d b_{n/d}^t |\gamma| n^y \\ \tilde{\beta}_n &:= \sum_{1 \leq d \leq D: d|n} \lambda_d b_{n/d}^t. \end{aligned}$$

In practice, it has proven convenient to use this estimate with Dirichlet mollifiers $\sum_{d=1}^D \frac{\lambda_d}{d^s}$ that are partial Euler products of the form

$$(81) \quad \sum_{d=1}^D \frac{\lambda_d}{d^s} = \prod_{p \leq P} \left(1 - \frac{b_p^t}{p^s} \right)$$

for some small prime P , where the product is over primes p up to P . For instance, if $P = 3$, then we would take $D = 6$, $\lambda_1 = 1$, $\lambda_2 = -b_2^t$, $\lambda_3 = -b_3^t$, $\lambda_6 = b_2^t b_3^t$, and all other λ_d vanishing. This choice achieves a substantial amount of cancellation in the $\tilde{\beta}_n$ coefficients, which we have found to make the lower bound in (80) favorable. (For instance, it makes $\tilde{\beta}_p$ vanish for all primes $p \leq P$.) In the literature one also sees other choices of mollifier than this Euler product used, for instance to control the extreme values of Dirichlet polynomials; however our numerical experimentations with alternative mollifiers to (81) turned out to give inferior results for our application.

The above calculations also suggest that the quantity $f_i(x + iy)$ oscillates in inverse proportion to the Euler product (81). Thus, to minimise the relative size of the right-hand side of (25) with respect to the left-hand side, it would therefore seem to be advantageous to try to work as much as possible in regions where this product is small, which heuristically corresponds to $\frac{x}{4\pi} \log p$ being close to an integer for $p \leq P$ (so that p^s has argument close to zero). In our subsequent arguments, we will erect a barrier for x in the vicinity of 6×10^{10} (this number being largely dictated by the numerical verifications of the Riemann hypothesis in the literature); we will in fact place the barrier at

$$X := 6 \times 10^{10} + 83952 - 0.5$$

noting that the fractional parts $\{\frac{X}{4\pi} \log p\}$ for $p \leq 11$ are somewhat close to zero:

$$\begin{aligned} \left\{ \frac{X}{4\pi} \log 2 \right\} &= 0.0275 \dots \\ \left\{ \frac{X}{4\pi} \log 3 \right\} &= 0.0437 \dots \\ \left\{ \frac{X}{4\pi} \log 5 \right\} &= 0.0640 \dots \\ \left\{ \frac{X}{4\pi} \log 7 \right\} &= 0.0774 \dots \\ \left\{ \frac{X}{4\pi} \log 11 \right\} &= 0.0954 \dots \end{aligned}$$

We found this shift by the following somewhat *ad hoc* procedure. We first introduced the quantity

$$\text{eulerprod}(x, p_n) := \left| \prod_{p \leq p_n} \frac{1}{1 - \frac{1}{p^{1-ix/2}}} \right|,$$

which is the exponent corresponding to $y = 1$ (where the minimum value of $|f_i(x + iy)|$ in the barrier region is expected to occur). We numerically located candidate integers $1 \leq q \leq 10^5$ for which the quantity

$$\min_{x=6 \times 10^{10} - q \in \{-0.5, 0, 0.5\}} |\text{eulerprod}(x, 29)|$$

exceeded a threshold (we chose 4), to obtain seven candidates for q : 1046, 22402, 24198, 52806, 77752, 83952, and 99108. Among these candidates, we selected the value of q which maximised the quantity

$$\min_{x=6 \times 10^{10} - q \in \{-0.5, 0, 0.5\}} |f_0(x + i)|,$$

namely $q = 83952$ (this quantity being ≈ 4.32 for this value of q).

8. ESTIMATING A SUM

In order to use the bound (79) for very large values of N , the following estimate will be used.

Lemma 8.1. *Let $N \geq N_0 \geq 1$ be natural numbers, and let $\sigma, t > 0$ be such that*

$$\sigma > \frac{t}{2} \log N.$$

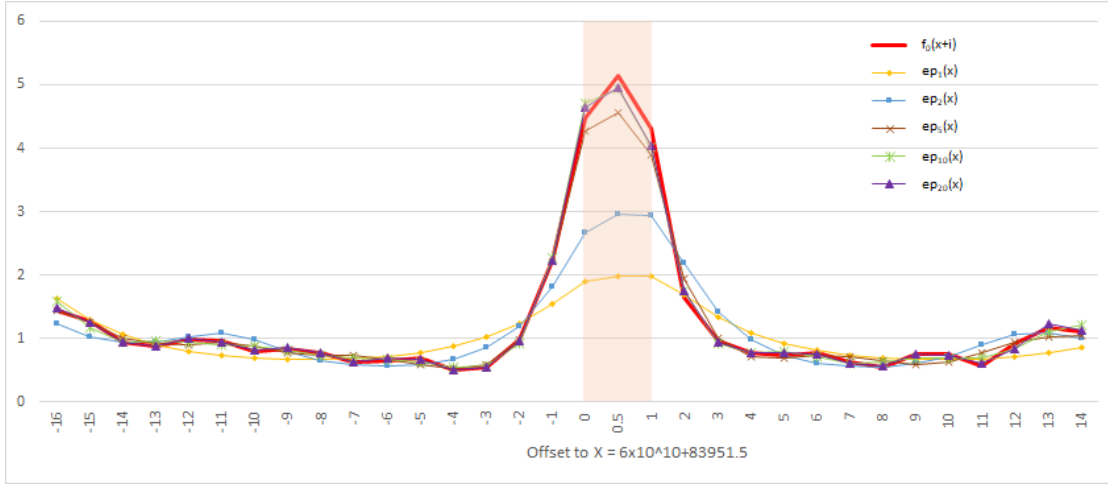


FIGURE 11. Improving approximation of $\text{ep}_n(x)$ w.r.t. $|f_0(x+iy)|$ as n is increased, where $\text{ep}_n(x) = \text{eulerprod}(x, p_n)$, shown near $X = 6 \times 10^{10} + 83951.5$, which was chosen as a barrier location.

Then

$$\sum_{n=1}^N \frac{b_n^t}{n^\sigma} \leq \sum_{n=1}^{N_0} \frac{b_n^t}{n^\sigma} + \max(N_0^{1-\sigma} b_{N_0}^t, N^{1-\sigma} b_N^t) \log \frac{N}{N_0}.$$

Proof. From the identity

$$\frac{b_n^t}{n^\sigma} = \frac{\exp\left(\frac{t}{4}(\log N - \log n)^2 - \frac{t}{4}(\log N)^2\right)}{n^{\sigma - \frac{t}{2} \log N}}$$

we see that the summands $\frac{b_n^t}{n^\sigma}$ are decreasing for $1 \leq n \leq N$, hence by the integral test one has

$$(82) \quad \sum_{n=1}^N \frac{b_n^t}{n^\sigma} \leq \sum_{n=1}^{N_0} \frac{b_n^t}{n^\sigma} + \int_{N_0}^N \frac{b_a^t}{a^\sigma} da.$$

Making the change of variables $a = e^u$, the right-hand side becomes

$$\sum_{n=1}^{N_0} \frac{b_n^t}{n^\sigma} \exp((1-\sigma)u + \frac{t}{4}u^2) du.$$

The expression $(1-\sigma)u + \frac{t}{4}u^2$ is convex in u , and is thus bounded by the maximum of its values at the endpoints $u = \log N_0, \log N$; thus

$$\exp((1-\sigma)u + \frac{t}{4}u^2) \leq N_0^{1-\sigma} b_{N_0}^t, N^{1-\sigma} b_N^t.$$

The claim follows. □

Remark 8.2. The right-hand side of (82) can be evaluated exactly as

$$\sum_{n=1}^{N_0} \frac{b_n^t}{n^\sigma} + \frac{\sqrt{\pi}}{\sqrt{t}} \exp\left(\frac{-(\sigma-1)^2}{t}\right) \left(\text{erfi}\left(\frac{\frac{t}{2} \log N - \sigma + 1}{\sqrt{t}}\right) - \text{erfi}\left(\frac{\frac{t}{2} \log N_0 - \sigma + 1}{\sqrt{t}}\right) \right).$$

In practice, this upper bound for $\sum_{n=1}^N \frac{b_n^t}{n^t}$ is slightly more accurate than the one in Lemma 8.1, and is a good approximation even for relatively small values of N_0 (e.g., $N_0 = 100$). However, the cruder bound above suffices for the numerical values of parameters needed to establish the bound $\Lambda \leq 0.22$.

8.1. Fast evaluation of multiple values of $f_t(s)$. Fix $t \geq 0$. For the verification of the barrier criterion (Theorem 1.2(iii)) using Corollary 1.4, we will need to evaluate the quantity $f_t(s)$ to reasonable accuracy for a large number of values of s in the vicinity of a fixed complex number $X + iy$. From (14) we have

$$(83) \quad f_t(s) = \sum_{n=1}^N \frac{n^b b_n^t}{n^{\frac{1+y-iX}{2}}} + \gamma(s) \sum_{n=1}^N \frac{n^a b_n^t}{n^{\frac{1-y+iX}{2}}},$$

where b_n^t is given by (15), $\gamma(s)$ is given by (16), N is given by (19) and

$$b = b(s) := \frac{1+y-iX}{2} - s_*$$

and

$$a = a(s) := \frac{1-y-iX}{2} - \overline{s_*} - \kappa$$

with s_*, κ defined by (17), (18). In practice the exponents a, b will be rather small, and N will be fixed (in our main verification we will in fact have $N = 69098$).

A naive computation of $f_t(s)$ for M values of s would take time $O(NM)$, which turns out to be somewhat impractical for the ranges of N, M we will need; indeed, for our main theorem, the total number of pairs (t, s) at which we need to perform the evaluation is 785052 (spread out over 152 values of t), and direct computation of all this data required 78.5 hours of computer time, which was still feasible at this order of magnitude of X but would not scale to significantly higher magnitudes. However, one can significantly speed up the computation (to about 0.025 hours) to extremely high accuracy by using Taylor series expansion to factorise the sums in (83) into combinations of sums that do not depend on s and thus can be computed in advance.

We turn to the details. To make the Taylor series converge² faster, we recenter the sum in n , writing

$$\sum_{n=1}^N F(n) = \sum_{h=-\lfloor N/2 \rfloor + 1}^{\lfloor (N+1)/2 \rfloor} F(n_0 + h)$$

for any function F , where $n_0 := \lfloor N/2 \rfloor$. We thus have

$$f_t(s) = B(b) + \gamma(s)A(n_0, a)$$

where

$$B(b) := \sum_{h=-\lfloor N/2 \rfloor + 1}^{\lfloor (N+1)/2 \rfloor} \frac{(n_0 + h)^b b_{n_0+h}^t}{(n_0 + h)^{\frac{1+y-iX}{2}}}$$

and

$$A(a) := \sum_{h=-\lfloor N/2 \rfloor + 1}^{\lfloor (N+1)/2 \rfloor} \frac{(n_0 + h)^a b_{n_0+h}^t}{(n_0 + h)^{\frac{1-y+iX}{2}}}.$$

²One can obtain even faster speedups here by splitting the summation range $\sum_{n=1}^N$ into shorter intervals and using a Taylor expansion for each interval, although ultimately we did not need to exploit this.

We discuss the fast computation of $B(b)$ for multiple values of b ; the discussion for $A(a)$ is analogous. We can write the numerator $(n_0 + h)^b b_{n_0+h}^t$ as

$$\exp(b \log(n_0 + h) + \frac{t}{4} \log^2(n_0 + h));$$

writing $\log(n_0 + h) = \log n_0 + \log(1 + \frac{h}{n_0})$, this becomes

$$n_0^{b + \frac{t}{4} \log n_0} \exp(\frac{t}{4} \log^2(1 + \frac{h}{n_0})) \exp((b + \frac{t}{2} \log n_0) \log(1 + \frac{h}{n_0})).$$

By Taylor expanding³ the exponentials, we can write this as

$$n_0^{b + \frac{t}{4} \log n_0} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{(\frac{t}{4} \log^2(1 + \frac{h}{n_0}))^i}{i!} \log^j(1 + \frac{h}{n_0}) \frac{(b + \frac{t}{2} \log n_0)^j}{j!}$$

and thus the expression $B(b)$ can be written as

$$B(b) = n_0^{b + \frac{t}{4} \log n_0} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} B_{i,j} \frac{(b + \frac{t}{2} \log n_0)^j}{j!}$$

where

$$B_{i,j} := \sum_{h=-\lfloor N/2 \rfloor + 1}^{\lfloor (N+1)/2 \rfloor} \frac{(\frac{t}{4} \log^2(1 + \frac{h}{n_0}))^i}{i!} \frac{\log^j(1 + \frac{h}{n_0})}{(n_0 + h)^{\frac{1+y-iX}{2}}}.$$

If we truncate the i, j summations at some cutoff E , we obtain the approximation

$$B(b) \approx n_0^{b + \frac{t}{4} \log n_0} \sum_{i=0}^{E-1} \sum_{j=0}^{E-1} B_{i,j}(n_0) \frac{(b + \frac{t}{2} \log n_0)^j}{j!}.$$

The quantities $B_{i,j}, i, j = 0, \dots, E-1$ may be evaluated in time $O(NE^2)$, and then the sums $B(b)$ for M values of b may be evaluated in time $O(ME^2)$, leading to a total computation time of $O((N + M)E^2)$ which can be significantly faster than $O(NM)$ even for relatively large values of E . We took $E = 50$, which is more than adequate to obtain extremely high accuracy for $f_t(s)$; see ???. The code for implementing this may be found in the file

`dbn_upper_bound/pari/barrier_multieval_t_agnostic.txt`

in the github repository [19].

9. A NEW UPPER BOUND FOR THE DE BRUIJN-NEWMAN CONSTANT

In this section we prove Theorem 1.1. As stated in the introduction, it suffices to verify the conditions (i), (ii), (iii) of Theorem 1.2 $t_0 := 0.2$, $X := X_0 - 0.5$, and $y_0 := 0.2$, where $X_0 := 6 \times 10^{10} + 83952$.

Claim (i) is immediate from the result of Platt [17] that all the non-trivial zeroes of ζ with imaginary part between 0 and 3.06×10^{10} lie on the critical line $\{\text{Re}(s) = 1/2\}$. For the remaining claims (ii), (iii), we need to verify that $H_t(x + iy) \neq 0$ for two regions of (x, y, t) :

(ii) $x \geq X_0 - 0.5 + \sqrt{0.96}$, $0.2 \leq y \leq \sqrt{0.6}$, and $t = 0.2$.

(iii) $X_0 - 0.5 \leq x \leq X_0 - 0.5 + \sqrt{0.96}$, $\sqrt{0.04 + 2(0.2 - t)} \leq y \leq \sqrt{0.6}$, and $0 \leq t \leq 0.2$.

³It is also possible to proceed by just performing Taylor expansion on the second exponential and leaving the first exponential untouched; this turns out to lead to a comparable numerical run time.

Both of these regions lie in (5). Enlarging the regions slightly, and applying Corollary 1.4, it thus suffices to establish the following claim:

Proposition 9.1. *Let (x, y, t) lie in one of the following regions:*

- (ii) (Asymptotic zero free region) $x \geq X_0$, $0.2 \leq y \leq \sqrt{0.6}$, and $t = 0.2$.
- (iii) (Barrier) $X_0 - 0.5 \leq x \leq X_0 + 0.5$, $0.2 \leq y \leq \sqrt{0.6}$, and $0 \leq t \leq 0.2$.

Define

$$f_t(x + iy) := \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{s_*} + \kappa}}$$

$$b_n^t := \exp\left(\frac{t}{4} \log^2 n\right),$$

$$N := \left\lfloor \sqrt{\frac{x}{4\pi} + \frac{t}{16}} \right\rfloor \leq \left(\frac{x}{4\pi} \left(1 + \frac{\pi t}{4x}\right) \right)^{1/2},$$

so in particular

$$(84) \quad \log \frac{x}{4\pi} \geq 2 \log N - \log\left(1 + \frac{\pi t}{4x}\right),$$

and let $\kappa, s_*, \gamma, e_A, e_B, e_{C_0}$ be as in Theorem 1.3, and e_A, e_B, e_{C_0} . Then

$$(85) \quad |f_t(x + iy)| > e_A + e_B + e_{C,0}.$$

Note that if $x \geq X_0 - 0.5$ then $N \geq N_0 := 69098$, with $N = N_0$ when $X_0 - 0.5 \leq x \leq X_0 + 0.5$. We calculate a somewhat crude upper bound for the right-hand side of (85):

Lemma 9.2. *For (x, y, t) in either of the regions (ii), (iii) in Proposition 9.1, one has*

$$e_A + e_B + e_{C,0} \leq 1.25 \times 10^{-3}.$$

Proof. From Theorem 1.3 we have

$$(86) \quad e_A + e_B \leq (e^{\delta_1} - 1)(F_{N,t}(\operatorname{Re}(s_*)) + |\gamma|F_{N,t}(\operatorname{Re}(s_*) - y - |\kappa|))$$

where

$$(87) \quad F_{N,t}(\sigma) := \sum_{n=1}^N \frac{b_n^t}{n^\sigma}.$$

and

$$(88) \quad \delta_1 := \frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi} + 0.626}{x - 6.66}.$$

From Lemma 5.1(vi), the quantity δ_1 is monotone decreasing in x in the region (5). Thus we have

$$(89) \quad \delta_1 \leq \frac{\frac{(0.2)^2}{16} \log^2 \frac{X_0 - 0.5}{4\pi} + 0.626}{X_0 - 0.5 - 6.66}$$

whenever $x \geq X_0 - 0.5 \geq 200$ and $0 \leq t \leq 0.2$. Computing the right-hand side, we conclude that

$$\delta_1 \leq 3.12 \times 10^{-11}$$

and hence by Taylor expansion

$$e^{\delta_1} - 1 \leq 1.001\delta_1$$

(say). Also, from Theorem 1.3 and (87) we can bound

$$\begin{aligned} |\gamma|F_{N,t}(\operatorname{Re}(s_*) - y - |\kappa|) &\leq |\gamma|N^y N^{|\kappa|} F_{N,t}(\operatorname{Re}(s_*)) \\ &\leq \exp\left(0.02y + y(\log N - \frac{1}{2} \log \frac{x}{4\pi}) + \frac{ty}{2(x-6)} \log N\right) F_{N,t}(\operatorname{Re}(s_*)) \\ &\leq \exp\left(0.02y + (y + \frac{ty}{2(x-6)}) \frac{1}{2} \log(1 + \frac{\pi t}{4x}) + \frac{ty}{4(x-6)} \log \frac{x}{4\pi}\right) F_{N,t}(\operatorname{Re}(s_*)). \end{aligned}$$

For $0.2 \leq y \leq 1$, $0 \leq t \leq 0.2$, and $x \geq X_0 - 0.5$ we see from Lemma 5.1(vi) that

$$\frac{ty}{4(x-6)} \log \frac{x}{4\pi} \leq \frac{0.2}{4(X_0 - 0.5 - 6)} \log \frac{X_0 - 0.5}{4\pi} \leq 1.86 \times 10^{-11}$$

and

$$(y + \frac{ty}{2(x-6)}) \frac{1}{2} \log(1 + \frac{\pi t}{4x}) \leq (1 + \frac{0.2}{2(X_0 - 0.5 - 6)}) \frac{1}{2} \log(1 + \frac{0.2\pi}{4(X_0 - 0.5)}) \leq 1.31 \times 10^{-12}$$

and thus

$$(90) \quad |\gamma|F_{N,t}(\operatorname{Re}(s_*) - y - |\kappa|) \leq 1.021 F_{N,t}(\operatorname{Re}(s_*)).$$

Thus

$$e_A + e_B \leq 1.023 \delta_1 F_{N,t}(\operatorname{Re}(s_*)).$$

To estimate $\operatorname{Re}(s_*)$, we use Proposition 6.6(ii) or (22), together with the inequality

$$\frac{t}{2x^2} \left(1 - 3y + \frac{4y(1+y)}{x^2}\right)_+ \leq \frac{0.2}{2(X_0 - 0.5)^2} \left(1 - 3 \times 0.2 + \frac{8}{(X_0 - 0.5)^2}\right)_+ \leq 1.2 \times 10^{-23}$$

to obtain

$$\operatorname{Re}(s_*) \geq 0.6001 + \frac{t}{4} \log \frac{x}{4\pi}$$

(say). Since $F_{N,t}(\sigma)$ is non-increasing in σ , we conclude

$$e_A + e_B \leq 1.023 \delta_1 F_{N,t}(0.6001 + \frac{t}{4} \log \frac{x}{4\pi}).$$

Since

$$N = \left\lfloor \sqrt{\frac{x}{4\pi} + \frac{t}{16}} \right\rfloor,$$

$0 \leq t \leq 0.2$, and $x \geq X_0 - 0.5$, it is easy to see that

$$N \leq \frac{x}{4\pi}$$

and hence by (15)

$$\frac{b'_n}{n^{\frac{t}{4} \log \frac{x}{4\pi}}} \leq 1$$

for all $1 \leq n \leq N$. Therefore

$$F_{N,t}(0.6001 + \frac{t}{4} \log \frac{x}{4\pi}) \leq \sum_{n=1}^N \frac{1}{n^{0.6001}}$$

and hence by the integral test

$$F_{N,t}(0.6001 + \frac{t}{4} \log \frac{x}{4\pi}) \leq \int_1^{N+1} \frac{ds}{s^{0.6001}} = \frac{1}{0.3999} (N+1)^{0.3999}$$

so that (by (88))

$$e_A + e_B \leq 1.023 \frac{\frac{(0.2)^2}{16} \log^2 \frac{x}{4\pi} + 0.626}{x - 6.66} \frac{1}{0.3999} (N + 1)^{0.3999}.$$

We have

$$N + 1 \leq (1.001) \left(\frac{x - 6.66}{4\pi} \right)^{1/2}$$

(say), and hence

$$e_A + e_B \leq 0.7220 \frac{0.0025 \log^2 \frac{x}{4\pi} + 0.626}{(x - 6.66)^{0.79995}}$$

From Lemma 5.1(vi), the right-hand side is monotone decreasing in the region $x \geq X_0 - 0.5$, thus

$$\begin{aligned} e_A + e_B &\leq 0.7220 \frac{0.0025 \log^2 \frac{X_0 - 0.5}{4\pi} + 0.626}{(X_0 - 0.5 - 6.66)^{0.79995}} \\ &\leq 3.444 \times 10^{-9}. \end{aligned}$$

Meanwhile, from Proposition 6.6(vi) one has

$$e_{C,0} \leq \left(\frac{x}{4\pi} \right)^{-\frac{1+y}{4}} \exp \left(-\frac{t}{16} \log^2 \frac{x}{4\pi} + \frac{3|\log \frac{x}{4\pi} + i\frac{\pi}{2}| + 3.58}{x - 8.52} \right) \left(1 + \frac{1.24 \times (3^y + 3^{-y})}{N - 0.125} + \frac{6.92}{x - 6.66} \right).$$

From Lemma 5.1(vi), the quantity $\frac{\log^2 \frac{x}{4\pi} + \frac{\pi^2}{4}}{(x - 8.52)^2}$ is monotone decreasing in x in (5), hence $\frac{|\log \frac{x}{4\pi} + i\frac{\pi}{2}|}{x - 8.52}$ is also monotone decreasing. Also the expression is monotone decreasing in y . We conclude that

(91)

$$\begin{aligned} e_{C,0} &\leq \left(\frac{X_0 - 0.5}{4\pi} \right)^{-\frac{1+0.2}{4}} \exp \left(\frac{3|\log \frac{X_0 - 0.5}{4\pi} + i\frac{\pi}{2}| + 3.58}{X_0 - 0.5 - 8.52} \right) \left(1 + \frac{1.24 \times (3^{\sqrt{0.6}} + 3^{-\sqrt{0.6}})}{N_0 - 0.125} + \frac{6.92}{X_0 - 0.5 - 6.66} \right) \\ &\leq 1.249 \times 10^{-3} \end{aligned}$$

where we have discarded the negative term $-\frac{t}{16} \log^2 \frac{X_0 - 0.5}{4\pi}$. Combining the estimates, we obtain the claim. \square

It now suffices to establish the bound

$$(92) \quad |f_t(x + iy)| > 1.25 \times 10^{-3}$$

in the following regions:

- (i) When $6 \times 10^{10} + 83952 - 0.5 \leq x \leq 6 \times 10^{10} + 83952 + 0.5$, $0 \leq t \leq 0.2$, and $0.2 \leq y \leq 1$.
- (ii) When $x \geq 6 \times 10^{10} + 83952 - 0.5$, $69098 \leq N \leq 80000$, $t = 0.2$, and $0.2 \leq y \leq 1$.
- (iii) When $80000 \leq N \leq 1.5 \times 10^6$, $t = 0.2$, and $0.2 \leq y \leq 1$.
- (iv) When $N \geq 1.5 \times 10^6$, $t = 0.2$, and $0.2 \leq y \leq 1$.

We begin with claim (i). The function $f_t(x + iy)$ is holomorphic, so by Rouché's theorem, it suffices to show that for each time $0 \leq t \leq 0.2$, as $x + iy$ traverses the boundary ∂R of the rectangle

$$R := \{x + iy : 10^{10} + 83952 - 0.5 \leq x \leq 6 \times 10^{10} + 83952 + 0.5; 0.2 \leq y \leq 1\},$$

the function $f_t(x + iy)$ stays outside of the ball $B := \{z : |z| \leq 1.25 \times 10^{-3}\}$, and furthermore has a winding number of zero around the origin.

To verify this claim numerically for a given value of t , we subdivide each edge of ∂R into some number n of equally spaced mesh points, thus approximating ∂R by a discrete mesh $x_j + iy_j$, $j = 1, \dots, 4n$, with any two adjacent points on this mesh separated by a distance at most $1/n$. Using the techniques in Section 8.1, we evaluate $f_t(x_j + iy_j)$ numerically for each such value of j . The polygonal path connecting these points then winds around the origin with winding number

$$\frac{1}{2\pi} \sum_{j=1}^{4n} \arg(f_t(x_{j+1} + iy_{j+1})/f_t(x_j + iy_j))$$

which can be easily computed (and verified to be zero). To pass from this polygonal path to the true trajectory $f_t(\partial R)$ of $f_t(x + iy)$ on ∂R , we again use Rouché's theorem. If one has a derivative bound $|\frac{\partial}{\partial z} f_t(z)| \leq D_z$ on the boundary of the rectangle, the polygonal path and the true trajectory $f_t(\partial R)$ differ by a distance of at most $\frac{D_z}{2n}$, and the latter will have the same winding number around the origin (and stay outside of the ball B) as long as

$$|f_t(x_j + iy_j)| > 1.25 \times 10^{-3} + \frac{D_z}{2n}.$$

Furthermore, the same is true for nearby times $t \leq t'0.2$ to t , as long as one has the stronger bound

$$(93) \quad |f_t(x_j + iy_j)| > 1.25 \times 10^{-3} + \frac{D_z}{2n} + \frac{D_t|t' - t|}{2n}$$

and a bound of the form $|\frac{\partial}{\partial t} f_t(z)| \leq D_t$ for $t \leq \tilde{t} \leq 0.2$ and $z \in \partial R$.

This gives the following algorithm to verify (i) for the entire range $0 \leq t \leq 0.2$. We start with $t = 0$ and obtain bounds D_t, D_z for the derivatives of $f_t(z)$ in the indicated ranges. Because of the way the barrier location X was selected, we expect $|f_t(x + iy)|$ to stay well above 1 in magnitude. We thus choose n so that $\frac{D_z}{2n} \leq 1$, and evaluate $f_t(x_j + iy_j)$ at all the mesh points (in particular confirming that $|f_t(x_j + iy_j)|$ does stay well above 1). Using the minimum value of $|f_t(x_j + iy_j)|$, we can then use the condition (93) to establish the claim for times in the interval $[t, t')$ where $t' > t$ is chosen so that (93) holds (or $t' = 0.2$, if that is also possible); the most aggressive choice of t' would be one in which (93) held with equality, but in practice we can afford to take more conservative values of t' and still obtain good runtime performance. If $t' < 0.2$, we then repeat the process, replacing t by t' , until the entire range $0 \leq t \leq 0.2$ is verified.

To run this algorithm, we need bounds on D_t and D_z . This is achieved by the following lemma, which gives bounds which are somewhat complicated but which can be easily upper bounded numerically on ∂R :

Lemma 9.3. *In the region (5), and away from the jump discontinuities of N , we have*

$$\begin{aligned} \left| \frac{\partial f_t}{\partial z} \right| &\leq \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s_*)}} \left(\frac{\log n}{2} + \frac{t \log n}{4(x-6)} \right) \\ &\quad + |\gamma| N^{|k|} \sum_{n=1}^N \frac{b_n^t n^y}{n^{\operatorname{Re}(s_*)}} \left(\frac{t \log n}{4(x-6)} + \left(\log \frac{|1+y+ix|}{4\pi} + \pi + \frac{3}{x} \right) \left(\frac{1}{2} + \frac{t}{4(x-6)} \right) \right) \end{aligned}$$

and

$$\begin{aligned} \left| \frac{\partial f_t}{\partial t} \right| &\leq \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s_*)}} \left(\frac{1}{4} \log n \log \frac{x}{4\pi n} + \frac{\pi}{8} \log n + \frac{2 \log n}{x-6} \right) \\ &\quad + |\gamma| N^{|k|} \sum_{n=1}^N \frac{b_n^t n^y}{n^{\operatorname{Re}(s_*)}} \left(\frac{1}{4} \log n \log \frac{x}{4\pi n} + \frac{\pi}{8} \log n + \frac{2 \log n}{x-6} + \frac{1}{4} \left(\frac{\pi}{2} + \frac{8}{x-6} \right) \left(\log \frac{x}{4\pi} + \frac{8}{x-6} \right) \right). \end{aligned}$$

Proof. We begin with the first estimate. Write

$$s_{**} := \overline{s_*} - y + \kappa = \frac{1-y+ix}{2} + \frac{t}{2} \alpha \left(\frac{1-y+ix}{2} \right)$$

then

$$(94) \quad f_t = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N \frac{b_n^t}{n^{s_{**}}}.$$

One can check that s_* , s_{**} , γ are holomorphic functions of $x+iy$, hence by the Cauchy-Riemann equations

$$\left| \frac{\partial f_t}{\partial x} \right| = \left| \frac{\partial f_t}{\partial y} \right|.$$

By the product and chain rules, we may calculate

$$\frac{\partial f_t}{\partial x} = - \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} \frac{\partial s_*}{\partial x} \log n + \gamma \sum_{n=1}^N \frac{b_n^t}{n^{s_{**}}} \left(\frac{\partial}{\partial x} \log \gamma - \frac{\partial s_{**}}{\partial x} \log n \right).$$

From (17), (43) we have

$$\begin{aligned} \frac{\partial s_*}{\partial x} &= -\frac{i}{2} - \frac{it}{4} \alpha' \left(\frac{1-y+ix}{2} \right) \\ &= -\frac{i}{2} + O_{\leq} \left(\frac{t}{4(x-6)} \right). \end{aligned}$$

Similarly we have

$$\frac{\partial s_{**}}{\partial x} = \frac{i}{2} + O_{\leq} \left(\frac{t}{4(x-6)} \right).$$

Writing $s = \frac{1-y+ix}{2}$, we have from (16), (10) that

$$\log \gamma = \frac{t}{4} (\alpha(s)^2 - \alpha(1-s)^2) + \log M_0(s) - \log M_0(1-s)$$

and hence by (8)

$$\frac{\partial \gamma}{\partial x} = \frac{it}{4} (\alpha(s) \alpha'(s) + \alpha(1-s) \alpha'(1-s)) + \frac{i}{2} \alpha(s) + \frac{i}{2} \alpha(1-s).$$

From the triangle inequality and (43), we thus have

$$\left| \frac{\partial f_t}{\partial x} \right| \leq \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s_*)}} \left(\frac{\log n}{2} + \frac{t \log n}{4(x-6)} \right) + |\gamma| \sum_{n=1}^N \frac{b_n^t}{n^{\operatorname{Re}(s_{**})}} \left(\frac{t \log n}{4(x-6)} + \frac{|\alpha(s) + \alpha(1-s) - \log n|}{2} + \frac{t(|\alpha(s)| + |\alpha(1-s)|)}{4(x-6)} \right).$$

We have from (9) that

$$|\alpha(s)|, |\alpha(s) - \frac{1}{2} \log n| \leq \frac{1}{2} \log \frac{|1 - y + ix|}{4\pi} + \frac{\pi}{2} + \frac{3}{2x}$$

since $n \leq N \leq \frac{x}{4\pi} \leq \frac{|1-y+ix|}{4\pi}$. Similarly

$$|\alpha(1-s)|, |\alpha(1-s) - \frac{1}{2} \log n| \leq \frac{1}{2} \log \frac{|1 + y + ix|}{4\pi} + \frac{\pi}{2} + \frac{3}{2x}$$

and thus

$$|\alpha(s) + \alpha(1-s)|, |\alpha(s) + \alpha(1-s) - \log n| \leq \log \frac{|1 + y + ix|}{4\pi} + \pi + \frac{3}{x}.$$

Writing $\text{Re}(s_{**}) = \text{Re}(s_*) - y + \text{Re}(\kappa)$, we then have the first estimate.

Now we estimate the time derivative. Since

$$\begin{aligned} \frac{\partial}{\partial t} \log b_n^t &= \frac{1}{4} \log^2 n \\ \frac{\partial}{\partial t} s_* &= \frac{1}{2} \alpha\left(\frac{1+y-ix}{2}\right) \\ \frac{\partial}{\partial t} s_{**} &= \frac{1}{2} \alpha\left(\frac{1-y+ix}{2}\right) \\ \frac{\partial}{\partial t} \log \gamma &= \frac{1}{4} \left(\alpha\left(\frac{1-y+ix}{2}\right)^2 - \alpha^2\left(\frac{1+y-ix}{2}\right) \right) \end{aligned}$$

we see from differentiating (94) that, we obtain

$$\frac{\partial f_t}{\partial t} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} \left(\frac{\log^2 n}{4} - \frac{\alpha\left(\frac{1+y-ix}{2}\right)}{2} \log n \right) + \gamma \sum_{n=1}^N \frac{b_n^t}{n^{s_{**}}} \left(\frac{\log^2 n}{4} - \frac{\alpha\left(\frac{1-y+ix}{2}\right)}{2} \log n + \frac{1}{4} \left(\alpha\left(\frac{1-y+ix}{2}\right)^2 - \alpha^2\left(\frac{1+y-ix}{2}\right) \right) \right).$$

From (43), (9) we have

$$\begin{aligned} \alpha\left(\frac{1 \pm y + ix}{2}\right) &= \alpha\left(\frac{ix}{2}\right) + O_{\leq}\left(\frac{1}{x-6}\right) \\ &= \frac{1}{2} \log \frac{x}{4\pi} + \frac{\pi i}{4} + O_{\leq}\left(\frac{4}{x-6}\right) \end{aligned}$$

and hence (since $\alpha = \alpha^*$)

$$\alpha\left(\frac{1 \pm y - ix}{2}\right) = \frac{1}{2} \log \frac{x}{4\pi} - \frac{\pi i}{4} + O_{\leq}\left(\frac{4}{x-6}\right)$$

so in particular (recalling that $s_+ = \frac{1+y-ix}{2}$ and $s_- = \frac{1-y+ix}{2}$)

$$\alpha(s_-) - \alpha(s_+) = \frac{\pi i}{2} + O_{\leq}\left(\frac{8}{x-6}\right)$$

and

$$\alpha(s_-) + \alpha(s_+) = \log \frac{x}{4\pi} + O_{\leq}\left(\frac{8}{x-6}\right)$$

so that

$$|\alpha(s_-)^2 - \alpha(s_+)^2| \leq \left(\frac{\pi}{2} + \frac{8}{x-6} \right) \left(\log \frac{x}{4\pi} + \frac{8}{x-6} \right).$$

We conclude from the triangle inequality that

$$\left| \frac{\partial f_t}{\partial t} \right| \leq \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s_*)}} \left(\frac{1}{4} \log n \log \frac{x}{4\pi n} + \frac{\pi}{8} \log n + \frac{2 \log n}{x-6} \right) \\ + |\gamma| \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s_{**})}} \left(\frac{1}{4} \log n \log \frac{x}{4\pi n} + \frac{\pi}{8} \log n + \frac{2 \log n}{x-6} + \frac{1}{4} \left(\frac{\pi}{2} + \frac{8}{x-6} \right) \left(\log \frac{x}{4\pi} + \frac{8}{x-6} \right) \right)$$

giving the second claim. \square

The next few graphs summarize the numerical output of the algorithm for the following Barrier parameters: $x = 6 \times 10^{10} + 83925 \pm 0.5$, $y = 0.2 \dots 1$, $t = 0 \dots 0.2$.

The first step in the Barrier verification process was to precalculate a 'stored sum' of Taylor expansion terms that allows for fast recreation of $f_t(x + iy)$ during the execution of the algorithm. The number of Taylor terms required was determined through an iterative process targeted to achieve a 20 decimal accuracy. The following plot illustrates that the achieved accuracy for all rectangular mesh points at $t = 0$.

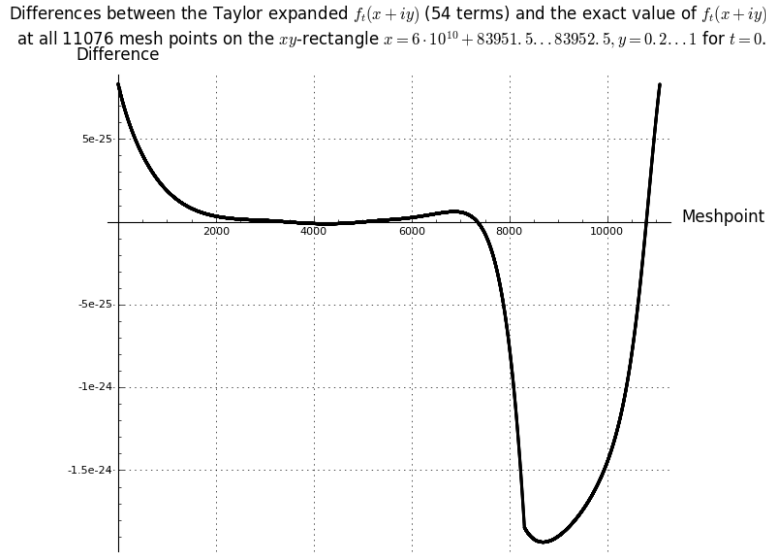
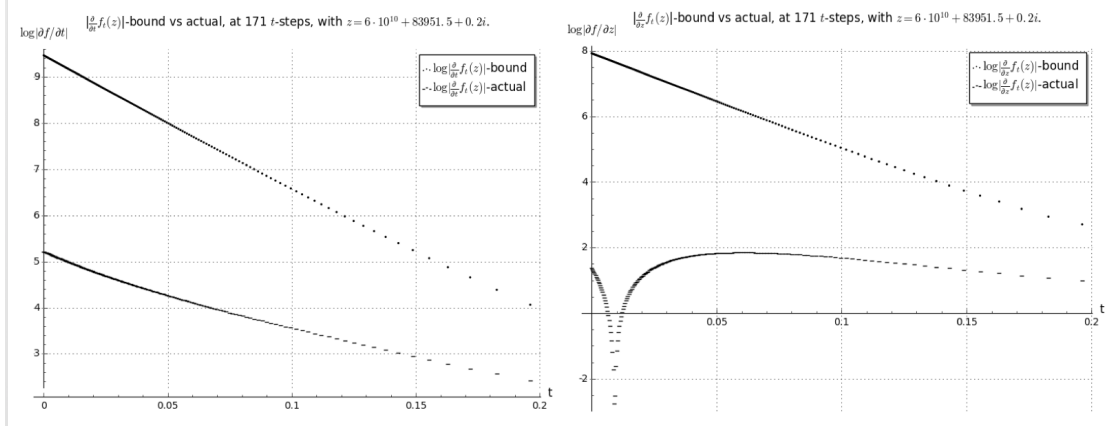
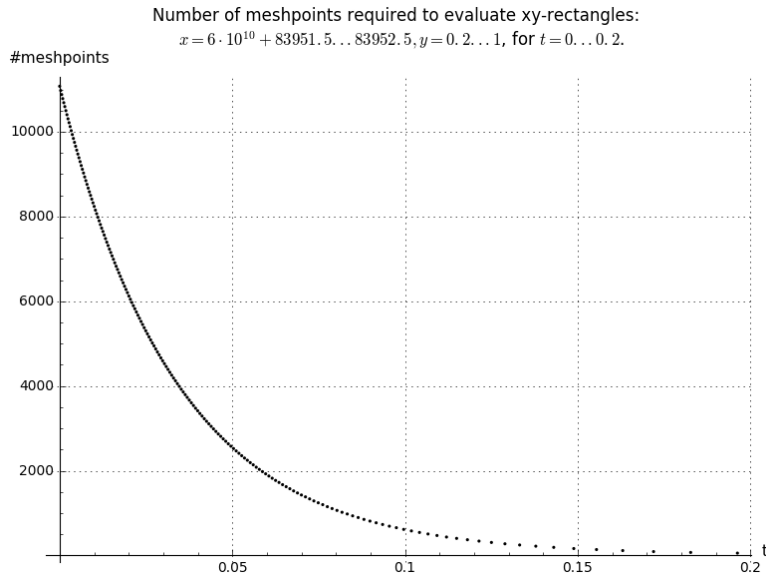


FIGURE 12. Achieved error term in the Taylor expansion at $t = 0$. Target was set at 20 decimal places accuracy.

The derivative bounds determine the number of mesh points required on each xy -rectangle and in the t -direction. The next two plots illustrate that these bounds have been chosen quite conservatively:

The number of rectangle mesh points varies with t ranging from 11076 at $t = 0$ to 56 at $t = 0.195$:

The overall winding number for the Barrier at this specific location came out at 0. The next graph shows the winding process at $t = 0$. Due to the choice of the Barrier location and the small Barrier width compared to the wave length of the x variable, little oscillation is expected to occur in each rectangle:

FIGURE 13. Derivative bounds versus their actual values at all required steps of t .FIGURE 14. The number of mesh points required per rectangle for each step of t .

Now we prove claim (ii).

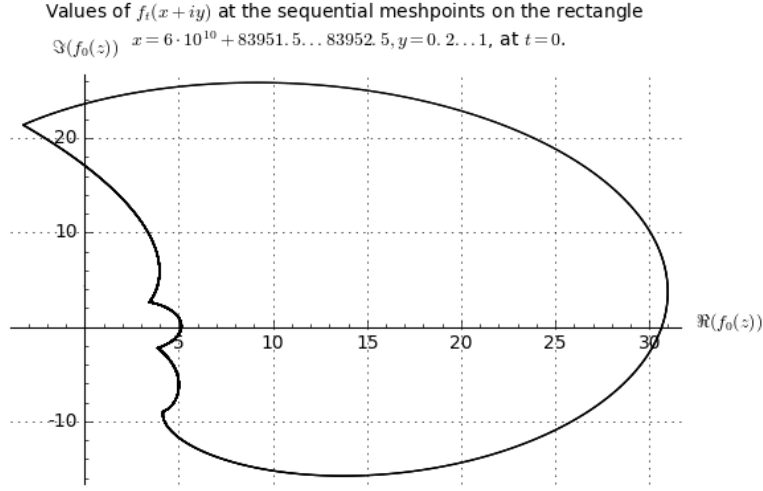
need to detail this more

For $N \in [69098, 80000]$, it was computationally verified that $|f_N| > 0.042$, since the Lemma bound (eqn 78) using the Euler 5 mollifier monotonically increased with N , from 0.04278 to 0.08011.

Now we prove claim (iii).

need to detail this more

We attempt here to find N dependent positive lower bounds for $|f_t(x + iy)|$ or corresponding mollified sums through an incremental approach,

FIGURE 15. Winding the rectangle at $t = 0$.

$$|f_{N+1}| \geq |f_N| - \sum (\text{additional terms corresponding to } N+1)$$

with the bound for $|f_{N_{min}}|$ computed similarly to (77) or (78).

If the incremental bound goes below a positive threshold at N , we reset N_{min} to N and restart the process, generating a sawtooth pattern.

For verifying the lower bounds for $[N_{min}, N_{max}]$, and with

$$\beta_{n,N} = \sum_{1 \leq d \leq D: d|n: n \leq dN} \lambda_d b_{n/d}^t,$$

$$\alpha_{n,N} = \sum_{1 \leq d \leq D: d|n: n \leq dN} \lambda_d a_{n/d}^t,$$

$$g(n, N, N_{max}) = \max\left(\frac{1-|\gamma|N_{max}}{1+|\gamma|N_{max}}|\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} - \alpha_{n,N}|, |\beta_{n,N} - |\frac{\gamma N_{max}}{\gamma_N}|\alpha_{n,N}|\right),$$

For the Triangle inequality bound,

$$|f_{N_{min}}| \geq \frac{1}{\sum_{d=1}^D \frac{|\lambda_d|}{d^{\sigma_{N_{min}}}}} (1 - |\gamma_{N_{min}}| - \sum_{n=2}^{DN_{min}} \frac{|\beta_{n,N_{min}}| + |\alpha_{n,N_{min}}|}{n^{\sigma_{N_{min}}}}) - |\gamma_{N_{min}}| \sum_{n=1}^{N_{min}} \frac{b_n^t (n^{|k|} - 1)}{n^{\sigma_{N_{min}} - \gamma}}$$

$$|f_{N+1}| \geq |f_N| - \frac{1}{\sum_{d=1}^D \frac{|\lambda_d|}{d^{\sigma_{N+1}}}} \sum_{1 \leq d \leq D: d|D} \left(\sum_{n=dN+1}^{dN+d} \frac{|\beta_{n,N+1}| + |\alpha_{n,N+1}|}{n^{\sigma_{N+1}}} \right) - |\gamma_{N+1}| \frac{b_{N+1}^t ((N+1)^{|k|} - 1)}{(N+1)^{\sigma_{N+1} - \gamma}}$$

For the Lemma inequality bound,

$$|f_{N_{min}}| \geq \frac{1}{\sum_{d=1}^D \frac{|\lambda_d|}{d^{\sigma_{N_{min}}}}} (1 - |\gamma_{N_{min}}| - \sum_{n=2}^{DN_{min}} \frac{g(n, N_{min}, N_{max})}{n^{\sigma_{N_{min}}}}) - |\gamma_{N_{min}}| \sum_{n=1}^{N_{min}} \frac{b_n^t (n^{|k|} - 1)}{n^{\sigma_{N_{min}} - \gamma}}$$

$$|f_{N+1}| \geq |f_N| - \frac{1}{\sum_{d=1}^D \frac{|\lambda_d|}{d^{\sigma_{N+1}}}} \sum_{1 \leq d \leq D: d|D} \left(\sum_{n=dN+1}^{dN+d} \frac{g(n, N_{\min}, N_{\max})}{n^{\sigma_{N+1}}} \right) - |\gamma_{N+1}| \frac{b_{N+1}^t ((N+1)^{|k|} - 1)}{(N+1)^{\sigma_{N+1}-y}}$$

Note: The incremental bounds work since,

1) $\beta_{n,N} = \beta_{n,N+1}$ and $\frac{\alpha_{n,N}}{\gamma_N} = \frac{\alpha_{n,N+1}}{\gamma_{N+1}}$ when $n \notin [dN, dN+d]$ for $d : d|D$

2) $g(n, N, N_{\max})$ can be seen to have the following properties with n fixed and N varying, resulting in it being constant or decreasing with increasing N ,

• $g(n, N, N_{\max}) = |\beta_{n,N} - \alpha_{n,N}|$ when $\beta_{n,N} \alpha_{n,N} \leq 0$

• $g(n, N, N_{\max}) = \max(\frac{1-|\gamma|N_{\max}}{1+|\gamma|N_{\max}} |\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} - \frac{\gamma N_{\max}}{\gamma_N} |\alpha_{n,N}|))$ when $\beta_{n,N} \alpha_{n,N} > 0$ and $|\beta_{n,N}| \geq |\alpha_{n,N}|$

• $g(n, N, N_{\max}) = \max(\frac{1-|\gamma|N_{\max}}{1+|\gamma|N_{\max}} |\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} - \alpha_{n,N}|, |\beta_{n,N} - \frac{\gamma N_{\max}}{\gamma_N} |\alpha_{n,N}|))$ when $\beta_{n,N} \alpha_{n,N} > 0$ and $|\alpha_{n,N}| > |\beta_{n,N}|$

Now, with $N_{\max} = 1.5 \text{million}$, $y = 0.2$, $t = 0.2$, Euler 5 mollifier, and threshold = 0.03 and starting with $N_{\min} = 80000$, and resetting N_{\min} whenever the incremental lemma bound goes below 0.03,

it was computationally verified that $|f_N| \geq 0.03$ for $N \in [80000, 1.5 \text{million}]$

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Finally, we prove claim (iv). In this regime we have

$$x \geq x_N := 4\pi N^2 - \frac{\pi t}{4};$$

in particular,

$$x \geq x_{1.5 \times 10^6} \geq 2.82 \times 10^{13}.$$

In view of (79), it suffices to show that

$$(95) \quad \sum_{n=1}^N \frac{b_n^{0.2}}{n^{\sigma}} + |\gamma| \sum_{n=1}^N \frac{b_n^{0.2}}{n^{\sigma-0.2-|k|}} < 2 - 1.25 \times 10^{-3}$$

where $\sigma := \text{Re}_{S_*}$. Our main tool here will be Lemma 8.1 (with $N_0 = 69098$). First observe from (22) that

$$|k| \leq \frac{0.2 \times 0.2}{2(2.82 \times 10^{13} - 6)} \leq 7.08 \times 10^{-16}$$

while from (20) one has

$$|\gamma| \leq 1.005 \left(\frac{x_N}{4\pi} \right)^{-0.1}$$

and from (21) one has

$$\begin{aligned}
\sigma &\geq 0.6 + \frac{0.2}{4} \log \frac{x_N}{4\pi} - \frac{0.2}{2x_{1.5*10^6}^2} \left(0.4 + \frac{0.96}{x_{1.5*10^6}^2} \right)_+ \\
&\geq 0.6 + 0.1 \log N + 0.05 \log \left(1 - \frac{t}{16(1.5 * 10^6)^2} \right) - \frac{0.2}{2x_{1.5*10^6}^2} \left(0.4 + \frac{0.96}{x_{1.5*10^6}^2} \right)_+ \\
&\geq 0.6 + 0.1 \log N - 5.1 \times 10^{-29}.
\end{aligned}$$

We can then apply Lemma 8.1 twice to bound the left-hand side of (95) by $A + B$, where

$$\begin{aligned}
A &:= \sum_{n=1}^{N_0} \frac{b_n^{0.2}}{n^{\sigma'}} + 1.005 \left(\frac{x_N}{4\pi} \right)^{-0.1} \sum_{n=1}^{N_0} \frac{b_n^{0.2}}{n^{\sigma''}}, \\
B &:= (\max(N_0^{1-\sigma'} b_{N_0}^{0.2}, N^{1-\sigma'} b_N^{0.2}) + 1.005 \left(\frac{x_N}{4\pi} \right)^{-0.1} \max(N_0^{1-\sigma''} b_{N_0}^{0.2}, N^{1-\sigma''} b_N^{0.2})) \log \frac{N}{N_0} \\
\sigma' &:= 0.6 + 0.1 \log N - 5.1 \times 10^{-29} \\
\sigma'' &:= 0.4 + 0.1 \log N - 7.09 \times 10^{-16}.
\end{aligned}$$

The quantity A is decreasing in N , so we may bound it by its value at $N = 1.5 \times 10^6$. Performing the sum numerically, we obtain

$$A \leq 1.88.$$

Finally, the quantity B can also be seen to be decreasing in N in the range $N \geq 1.5 \times 10^6$, and obeys the bound

$$B \leq 0.075.$$

The claim follows.

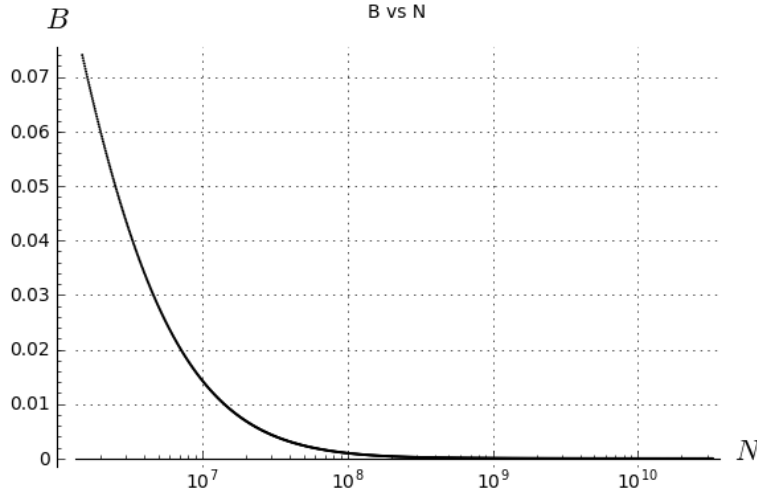


FIGURE 16. Plot of B vs N

10. ASYMPTOTIC RESULTS

In this section we use the effective estimates from Theorem 1.3 to obtain asymptotic information about the function H_t , which improves (and makes more effective) the results of Ki, Kim, and Lee [9], by establishing Theorem 1.5.

We begin with an asymptotic

Proposition 10.1. *Let $0 < t \leq 1/2$, $x \geq 200$, and $-10 \leq y \leq 10$.*

(i) *If $x \geq \exp(\frac{C}{t})$ for a sufficiently large absolute constant C , then*

$$H_t(x + iy) = (1 + O(x^{-ct}))M_t\left(\frac{1 + y - ix}{2}\right) + (1 + O(x^{-ct}))M_t\left(\frac{1 - y + ix}{2}\right)$$

for an absolute constant $c > 0$, where M_t is defined in (10).

(ii) *If instead we have $3 \leq y \leq 4$ and $x \geq C$ for a sufficiently large absolute constant C , then*

$$H_t(x + iy) = (1 + O_{\leq}(0.7))M_t\left(\frac{1 + y - ix}{2}\right).$$

(iii) *If $x = x_0 + O(1)$ for some $x_0 \geq 200$, then*

$$H_t(x + iy) = O(x_0^{O(1)}|M_t(\frac{1 + y - ix}{2})|) = O(x_0^{O(1)}|M_t(\frac{ix_0}{2})|).$$

Proof. We begin with (i). Since $H_t = H_t^*$ and $M_t = M_t^*$, we may assume without loss of generality that $y \geq 0$. Using (16), (11) we may write the desired estimate as

$$\frac{H_t(x + iy)}{B_0(x + iy)} = 1 + O(x^{-ct}) + \gamma.$$

We apply Theorem 1.3. (Strictly speaking, the estimates there required $y \leq 1$ rather than $y \leq 10$; however, as remarked at the beginning of Section 6, all the estimates in that section would continue to hold under this weaker hypothesis if one adjusted all the numerical constants appropriately.) This gives

$$(96) \quad \frac{H_t(x + iy)}{B_0(x + iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{s_* + \kappa}} + O_{\leq}(e_A + e_B + e_{C,0})$$

where

$$\begin{aligned} \gamma &= O(x^{-y/2}) \\ \kappa &= O(x^{-1}) \\ \operatorname{Re}(s_*) &\geq \frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi} - O(x^{-2}) \\ e_A &= O\left(x^{-y/2} \sum_{n=1}^N b_n^t n^{-\frac{1-y}{2} - \frac{t}{2} \log \frac{x}{4\pi} - O(x^{-1})} \frac{\log^2 x}{x}\right) \\ e_B &= O\left(\sum_{n=1}^N b_n^t n^{-\frac{1+y}{2} - \frac{t}{2} \log \frac{x}{4\pi} + O(x^{-1})} \frac{\log^2 x}{x}\right) \\ e_{C,0} &= O\left(x^{-\frac{1+y}{4}}\right) \end{aligned}$$

Since $N = O(x^{1/2})$, we have $x^{-y/2}n^y = O(1)$ and $n^{O(x^{-1})} = O(1)$ for all $1 \leq n \leq N$. We conclude that

$$\frac{H_t(x+iy)}{B_0(x+iy)} = 1 + \gamma + O\left(\frac{\log^2 x}{x} + \sum_{n=2}^N \frac{b_n^t}{n^{\frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi}}} + x^{-\frac{1+y}{4}}\right)$$

so it will suffice (for c small enough) to show that

$$\sum_{n=2}^N \frac{b_n^t}{n^{\frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi}}} = O(x^{-ct}).$$

By (15) we can write the left-hand side as

$$\sum_{n=2}^N \frac{1}{n^{\frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi\sqrt{n}}}} = O(x^{-ct}).$$

For $2 \leq n \leq N$, we have

$$\frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi\sqrt{n}} \geq ct \log x$$

for some absolute constant $c > 0$. By the integral test, the left-hand side is then bounded by

$$\frac{1}{2^{ct \log x}} + \int_2^\infty \frac{1}{u^{ct \log x}} du$$

which, for $x \geq \exp(C/t)$ and C large, is bounded by $O(2^{-ct \log x})$. The claim then follows after adjusting c appropriately.

Now we prove (ii). As before we have the expansion (96). We have

$$\begin{aligned} \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\frac{y}{2} + \kappa}} &= O\left(x^{-y/2} \sum_{n=1}^N \frac{b_n^t}{n^{-\frac{1-y}{2} + \frac{t}{2} \log \frac{x}{4\pi}}}\right) \\ &= O\left(x^{-y/2} \sum_{n=1}^N n^{\frac{y-1}{2}}\right) \\ &= O(x^{-\frac{y-1}{4}}); \end{aligned}$$

similar arguments give $e_A = O(\frac{\log^2 x}{x^{\frac{y-1}{4}}})$, while

$$\begin{aligned} e_B &= O\left(\frac{\log^2 x}{x} \sum_{n=1}^N b_n^t n^{-\frac{1+y}{2} - \frac{t}{2} \log \frac{x}{4\pi}}\right) \\ &= O\left(\frac{\log^2 x}{x} \sum_{n=1}^N n^{-2}\right) \\ &= O\left(\frac{\log^2 x}{x}\right). \end{aligned}$$

We conclude that

$$\begin{aligned}
\frac{H_t(x+yi)}{B_0(x+yi)} &= \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + O(x^{-\frac{y-1}{4}}) \\
&= 1 + O_{\leq} \left(\sum_{n=2}^N n^{-\frac{1+y}{2} - \frac{t}{2} \log \frac{x}{4\pi} - O(x^{-1})} \right) + O(x^{\frac{y-1}{4}}) \\
&= 1 + O_{\leq} \left(\sum_{n=2}^N n^{-2} \right) + O(x^{-1/2}) \\
&= 1 + O_{\leq} \left(\frac{\pi^2}{6} - 1 \right) + O(x^{-1/2}) \\
&= 1 + O_{\leq}(0.7)
\end{aligned}$$

as claimed, if $x \geq C$ for C large enough.

Finally we prove (iii). Again our starting point is (96). The right-hand side can be bounded crudely by $O(x^{O(1)}) = O(x_0^{O(1)})$, hence

$$H_t(x+iy) = O(x_0^{O(1)} |M_t(\frac{1+y+ix}{2})|).$$

However, from (10), (6), (9) it is not hard to see that the log-derivative of $M_t(s)$ is of size $O(\log x_0)$ in the region $s = \frac{ix_0}{2} + O(1)$. Thus

$$|M_t(\frac{1+y+ix}{2})| = O(x_0^{O(1)} |M_t(\frac{ix_0}{2})|),$$

giving the claim. \square

To understand the behavior of $M_t(x+iy)$ we make the following simple observations:

Lemma 10.2. *Let $0 < t \leq 1/2$, let $x_* > 0$ be sufficiently large, and let $x+iy = x_* + O(1)$. Then*

$$M_t(\frac{1+y+ix}{2}) = M_t(\frac{1+ix_*}{2}) \exp \left((i(x-x_*) + y) \left(\frac{1}{4} \log \frac{x_*}{4\pi} + \frac{\pi i}{8} \right) + O\left(\frac{\log x_*}{x_*}\right) \right).$$

Also, there is a continuous branch of $\arg M_t(\frac{1+ix_}{2})$ for all large real x_* such that*

$$\arg M_t\left(\frac{1+ix_*}{2}\right) = \frac{t\pi}{16} \log \frac{x_*}{4\pi} + \frac{7\pi}{8} + \frac{x_*}{4} \log \frac{x_*}{4\pi} - \frac{x_*}{4} + O\left(\frac{\log x_*}{x_*}\right).$$

Proof. By (10), (8), the log-derivative of M_t is given by

$$(97) \quad \frac{M'_t}{M_t} = \alpha + \frac{t}{2} \alpha \alpha'.$$

For $s = \frac{ix_*}{2} + O(1)$, we have from (9) that

$$(98) \quad \alpha(s) = \frac{1}{2} \log \frac{x_*}{4\pi} + \frac{\pi i}{4} + O\left(\frac{1}{x_*}\right)$$

and from this and (43) we conclude that

$$\frac{M'_t(s)}{M_t(s)} = \frac{1}{2} \log \frac{x_*}{4\pi} + \frac{\pi i}{4} + O\left(\frac{\log x_*}{x_*}\right)$$

whenever $s = \frac{ix_*}{2} + O(1)$. The first claim then follows by applying the fundamental theorem of calculus to a branch of $\log M_t$.

For the second claim, we calculate

$$\begin{aligned} \arg M_t \left(\frac{1+ix_*}{2} \right) &= \frac{t}{4} \operatorname{Im} \alpha \left(\frac{1+ix_*}{2} \right)^2 + \pi - \frac{x_*}{4} \log \pi + \operatorname{Im} \left(\frac{-1+ix_*}{4} \log \frac{1+ix_*}{4} - \frac{1+ix_*}{4} \right) \\ &= \frac{t}{4} \left(\frac{\pi}{4} \log \frac{x_*}{4\pi} + O\left(\frac{\log x_*}{x_*}\right) \right) + \pi - \frac{x_*}{4} \log \pi + \operatorname{Im} \left(\frac{-1+ix_*}{4} \left(\log \frac{x_*}{4} + \frac{i\pi}{2} - \frac{i}{x_*} + O\left(\frac{1}{x_*^2}\right) \right) \right) - \frac{x_*}{4} \\ &= \frac{t\pi}{16} \log \frac{x_*}{4\pi} + \pi + \frac{x_*}{4} \log \pi + \frac{x_*}{4} \log \frac{x_*}{4} - \frac{\pi}{8} + O\left(\frac{\log x_*}{x_*}\right) \\ &= \frac{t\pi}{16} \log \frac{x_*}{4\pi} + \frac{7\pi}{8} + \frac{x_*}{4} \log \frac{x_*}{4\pi} - \frac{x_*}{4} + O\left(\frac{\log x_*}{x_*}\right) \end{aligned}$$

as desired. \square

Now we can prove Theorem 1.5. We begin with (ii). Let $n \geq \exp(\frac{c}{t})$, and suppose that $x + iy = x_n + O(1)$. By Proposition 10.1(i) and Lemma 10.2 we have

$$\begin{aligned} (99) \quad H_t(x + iy) &= \overline{M_t \left(\frac{1+ix_n}{2} \right)} \exp \left((-i(x - x_n) + y) \left(\frac{1}{4} \log \frac{x_n}{4\pi} - \frac{\pi i}{8} \right) + O(x_n^{-ct}) \right) \\ &\quad + M_t \left(\frac{1+ix_n}{2} \right) \exp \left((i(x - x_n) - y) \left(\frac{1}{4} \log \frac{x_n}{4\pi} + \frac{\pi i}{8} \right) + O(x_n^{-ct}) \right). \end{aligned}$$

From Lemma 10.2 and (26) one has

$$\arg M_t \left(\frac{1+ix_n}{2} \right) = -\frac{\pi}{2} + O\left(\frac{\log x_n}{x_n}\right) \pmod{\pi}$$

and hence

$$(100) \quad \overline{M_t \left(\frac{1+ix_n}{2} \right)} = -\exp \left(O\left(\frac{\log x_n}{x_n}\right) \right) M_t \left(\frac{1+ix_n}{2} \right).$$

If we now make the further assumption $y = O\left(\frac{1}{\log x_n}\right)$, we can thus simplify the above approximation as

$$\begin{aligned} (101) \quad H_t(x + iy) &= -M_t \left(\frac{1+ix_n}{2} \right) e^{-\pi(x-x_n)/8} \exp \left((-i(x - x_n) + y) \frac{1}{4} \log \frac{x_n}{4\pi} + O(|y| \log x_n + x_n^{-ct}) \right) \\ &\quad + M_t \left(\frac{1+ix_n}{2} \right) e^{-\pi(x-x_n)/8} \exp \left((i(x - x_n) - y) \frac{1}{4} \log \frac{x_n}{4\pi} + O(|y| \log x_n + x_n^{-ct}) \right) \\ &= 2iM_t \left(\frac{1+ix_n}{2} \right) e^{-\pi(x-x_n)/8} \left(\sin \left(\frac{x + iy - x_n}{4} \log \frac{x_n}{4\pi} \right) + O(|y| \log x_n + x_n^{-ct}) \right). \end{aligned}$$

In particular, if $x + iy$ traverses the circle $\{x_n + \frac{c}{\log n} e^{i\theta} : 0 \leq \theta \leq 2\pi\}$ once anti-clockwise and c is small enough, the quantity $H_t(x + iy)$ will wind exactly once around the origin, and hence by the argument principle there is precisely one zero of H_t inside this circle. As the zeroes of H_t are symmetric around the real axis, this zero must be real. This proves (ii).

Now we prove (i). Suppose that $H_t(x + iy) = 0$ and $x \geq \exp(\frac{c}{t})$. We can assume $|y| \leq 1$ since it is known (e.g., from [4, Theorem 13]) that there are no zeroes with $|y| > 1$.

Let n be a natural number that minimises $|x - x_n|$, then $x = x_n + O\left(\frac{1}{\log x_n}\right)$ since the derivative of the left-hand side of (26) in x_n is comparable to $\log x_n$. From (99) we have

$$0 = \overline{M_t\left(\frac{1+ix_n}{2}\right)} \exp\left((-i(x-x_n)+y)\left(\frac{1}{4}\log\frac{x_n}{4\pi} - \frac{\pi i}{8}\right) + O(x_n^{-ct})\right) \\ + M_t\left(\frac{1+ix_n}{2}\right) \exp\left((i(x-x_n)-y)\left(\frac{1}{4}\log\frac{x_n}{4\pi} + \frac{\pi i}{8}\right) + O(x_n^{-ct})\right).$$

Thus both summands on the right-hand side have the same magnitude, which on taking logarithms and canceling like terms implies that

$$y\frac{1}{4}\log\frac{x_n}{4\pi} + O(x_n^{-ct}) = -y\frac{1}{4}\log\frac{x_n}{4\pi} + O(x_n^{-ct})$$

and hence $y = O\left(\frac{x_n^{-ct}}{\log x_n}\right)$. We can now apply (101) to conclude that

$$\sin\left(\frac{x+iy-x_n}{4}\log\frac{x_n}{4\pi}\right) + O(x_n^{-ct}) = 0$$

which (when combined with the hypothesis that $|x - x_n|$ is minimal) forces $x - x_n = O\left(\frac{x_n^{-ct}}{\log x_n}\right)$. This gives the claim.

Next, we prove (iii). In view of parts (i) and (ii), and adjusting C if necessary, we may assume that X takes the form $X = x_n + \frac{c}{\log x_n}$ for some $n \geq \exp(\frac{C}{t})$. By the argument principle, $N_t(X)$ is equal to $\frac{-1}{2\pi}$ times the variation in the argument of H_t on the boundary of the rectangle $\{x + iy : 0 \leq x \leq X; -3 \leq y \leq 3\}$ traversed clockwise, since there are no zeroes with imaginary part of magnitude greater than one. By compactness, the variation on the left edge $\{iy : -3 \leq y \leq 3\}$ is $O(1)$, and similarly for any fixed portion $\{x + 3i : 0 \leq y \leq C\}$ of the upper edge. From Proposition 10.1 (and (99)), we see that the variation of $H_t(x + iy)/M_t(\frac{1+y-ix}{2})$ on the remaining upper edge $\{x + 3i : C \leq x \leq X\}$ and on the top half $\{X + iy : 0 \leq y \leq 3\}$ of the right edge are both equal to $O(1)$. Since $H_t = H_t^*$, the variation on the lower half of the rectangle is equal to that of the upper half. We thus conclude that

$$N_t(X) = -\frac{1}{\pi} \arg M_t\left(\frac{1-iX}{2}\right) + O(1)$$

where we use a continuous branch of the argument of $M_t\left(\frac{1-iX}{2}\right)$ that is bounded at $3i$. The claim now follows from Lemma 10.2.

Finally, we prove (iv). From (4) and the rapid decrease of Φ it is easy to verify that the entire function H_t has order 1, while from the positivity of Φ we see that H_t has no zero at the origin. Thus by the Hadamard factorization theorem we have

$$H_t(z) = \exp(a + bz) \prod_n \left(1 - \frac{z}{z_n}\right) \exp\left(\frac{z}{z_n}\right)$$

for some complex numbers a, b , where z_n are the zeroes of H_t counting multiplicity; using the functional equation $H_t(z) = H_t(-z)$ we can index the zeros as $z_n = (z_n)_{n \in \mathbb{Z} \setminus \{0\}}$ with $z_{-n} = -z_n$, and conclude that $b = 0$, and

$$H_t(z) = \exp(a) \prod_{n>0} \left(1 - \frac{z^2}{z_n^2}\right).$$

Taking logarithmic derivatives, we conclude that

$$(102) \quad \frac{H'_t(z)}{H_t(z)} = \sum_{n>0} \left(\frac{1}{z - z_n} + \frac{1}{z + z_n} \right).$$

Setting $z = X + 4i$, we see from Proposition 10.1 and the generalized Cauchy integral formula that the logarithmic derivative of $H_t(x + iy)/M_t\left(\frac{1+y-ix}{2}\right)$ is equal to $O(1)$ at $X + 4i$ for all sufficiently large X , and hence for all X by symmetry and compactness. On the other hand, from Stirling's formula (or the logarithmic growth of the digamma function) one easily verifies that the logarithmic derivative of $M_t\left(\frac{1+y-ix}{2}\right)$ is equal to $O(\log(2 + X))$ at $X + 4i$. Hence $\frac{H'_t(X+4i)}{H_t(X+4i)} = O(\log(2 + X))$. Taking imaginary parts, we conclude that

$$\sum_{n>0} \frac{(4 - y_n)}{(X - x_n)^2 + (4 - y_n)^2} + \frac{(4 - y_n)}{(X + x_n)^2 + (4 + y_n)^2} = O(\log(2 + X))$$

where we write $z_n = x_n + iy_n$; equivalently one has

$$\sum_n \frac{(4 - y_n)}{(X - x_n)^2 + (4 - y_n)^2} = O(\log(2 + X))$$

where the sum now ranges over all zeroes, including any at the origin. Since $|y_n| \leq 1$, every zero in $[X, X + 1]$ makes a contribution of at least $\frac{1}{100}$ (say). As the summands are all positive, the first part of claim (iv) follows. To prove the second part, we may assume by compactness that $x \geq C$. Repeating the proof of (iii), and reduce to showing that the variation of $\arg H_t$ on the short vertical interval $\{X + iy : 0 \leq y \leq 3\}$ is $O(\log X)$. If we let θ be a phase such that $e^{i\theta} H_t(X + 3i)$ is real and positive, we see that this variation is at most $\pi(m + 1)$, where m is the number of zeroes of $\operatorname{Re} e^{i\theta} H_t(X + yi)$ for $0 \leq y \leq 3$, since every increment of π in $\arg e^{i\theta} H_t$ must be accompanied by at least one such zero. As $H_t = H_t^*$, this is also the number of zeroes of $e^{i\theta} H_t(X + yi) + e^{-i\theta} H_t(2X - (X + yi))$. On the other hand, from Proposition 10.1(ii), (iii) and Jensen's formula we see that the number of such zeroes is $O(\log X)$, and the claim follows.

Remark 10.3. *Theorem 1.5 gives good control on $H_t(x + iy)$ whenever $x \geq \exp(C/t)$. As a consequence (and assuming for sake of argument that the Riemann hypothesis holds), then for any $\Lambda_0 > 0$, the bound $\Lambda \leq \Lambda_0$ should be numerically verifiable in time $O(\exp(O(1/\Lambda_0)))$, by applying the arguments of previous sections with t and y set equal to small multiples of Λ_0 . We leave the details to the interested reader.*

Remark 10.4. *Our discussion here will be informal. In view of the results of [8], it is expected that the zeroes $z_j(t)$ of $H_t(x + iy)$ should evolve according to the system of ordinary differential equations*

$$\partial_t z_k(t) = 2 \sum'_{j \neq k} \frac{1}{z_k(t) - z_j(t)}$$

where the sum is evaluated in a suitable principal value sense, and one avoids those times where the zero $z_k(t)$ fails to be simple; see [8, Lemma 2.4] for a verification of this in the regime $t > \Lambda$. In view of the Riemann-von Mangoldt formula (as well as variants such Corollary 1.5, it is expected that the number of zeroes in any region of the form $\{x + iy : x + iy = x_* + O(1)\}$ for large x_* should be of the order of $\log x_*$. As a consequence, we expect a typical zero $z_k(t)$ to move with speed $O(\log |z_k(t)|)$, although one may occasionally move much faster than this if two zeroes are exceptionally close together, or less than this if the zeroes are close to being evenly

spaced. As a consequence, if the Riemann hypothesis fails and there is a zero $x + iy$ of H_0 with y comparable to 1, it should take time comparable to $\frac{1}{\log x}$ for this zero to move towards the real axis, leading to the heuristic lower bound $\Lambda \gg \frac{1}{\log x}$. Thus, in order to obtain an upper bound $\Lambda \leq \Lambda_0$, it will probably be necessary to verify that there are no zeroes $x + iy$ of H_0 with y comparable to 1 and $|x| \leq c \log \frac{1}{\Lambda}$ for some small absolute constant $c > 0$. This suggests that the time complexity bound in Remark 10.3 is likely to be best possible (unless one is able to prove the Riemann hypothesis, of course).

In [8, Lemma 2.1] it is also shown that the velocity of a given zero $z(t)$ is given by the formula

$$\partial_t z(t) = \frac{H'_t(z(t))}{H'_t(z(t))}$$

assuming that the zero is simple. By using the asymptotics in Proposition 10.1 and Corollary 1.5 together with the generalized Cauchy integral formula to then obtain asymptotics for H'_t and H''_t , it is possible to show that for the zeroes $x(t)$ that are real and larger than $\exp(C/t)$, and move leftwards with velocity

$$\partial_t x(t) = -\frac{\pi}{4} + O(x^{-ct});$$

we leave the details to the interested reader.

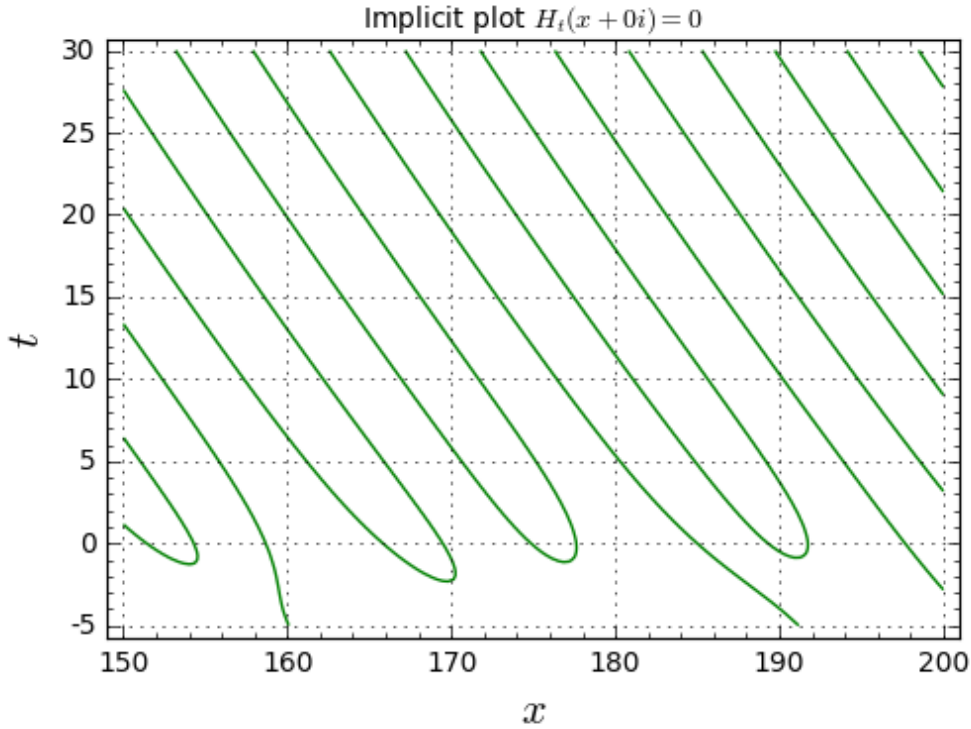


FIGURE 17. Real zeros moving up leftwards and getting ‘solidified’.

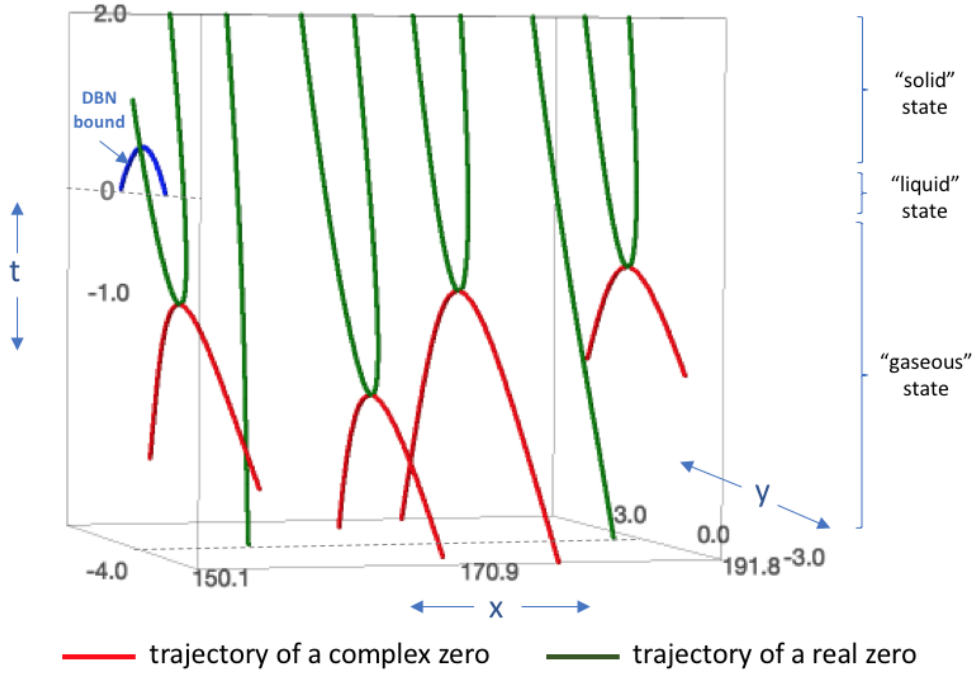


FIGURE 18. Actual trajectories of some real and complex zeros.

11. FURTHER NUMERICAL RESULTS

By Theorem 1.5, one can verify the second hypothesis of Theorem 1.2 when $X \geq \exp(C/t_0)$ for a large constant C . If we ignore for sake of discussion the third hypothesis of Theorem 1.2 (which turns out to be relatively easy to verify numerically in practice), this suggests that one can obtain a bound of the form $\Lambda \leq O(t_0)$ provided that one can verify the Riemann hypothesis up to a height $\exp(C/t_0)$. In other words, if one has numerically verified the Riemann hypothesis up to a large height T , this should soon lead to a bound of the form $\Lambda \leq O\left(\frac{1}{\log T}\right)$.

Aside from improving the implied constant in this bound, it does not seem easy to improve this sort of implication without a major breakthrough on the Riemann hypothesis (such as a massive expansion of the known zero-free regions for the zeta function inside the critical strip). We shall justify this claim heuristically as follows. Suppose that there was a counterexample to the Riemann hypothesis at a large height T , so that $H_0(2T + iy) = 0$ for some positive y , which for this discussion we will take to be comparable to 1. The Riemann von Mangoldt formula indicates that the number of zeroes of H_0 within a bounded distance of this zero should be comparable to $\log T$; the majority of these zeroes should obey the Riemann hypothesis and thus stay at roughly unit distance from our initial zero $2T + iy$. Proposition 3.1 then suggests that as time t advances, this zero should move at speed comparable to $\log T$. Thus one should not expect this zero to reach the real axis until a time comparable to $\frac{1}{\log T}$. This heuristic analysis therefore indicates that it is unlikely that one can significantly improve the bound $\Lambda \leq O\left(\frac{1}{\log T}\right)$ without being able to exclude significant violations of the Riemann hypothesis at height T .

In this section we collect some numerical results verifying the second two hypotheses of Theorem 1.2 for larger values of X , and smaller values of t_0 , than were considered in Section 9. This leads to improvements to the bound $\Lambda \leq 0.22$ conditional on the assumption that the Riemann Hypothesis can be numerically verified beyond the height $T \approx 1.2 \times 10^{11}$ used in Section 9. Our conclusions may be summarised as follows:

TABLE 1. Conditional Λ Results

X	t_0	y_0	Λ	Winding Number	N_a	Moll2 Bound
$2 \times 10^{12} + 129093$	0.198	0.15492	0.21	0	398942	0.0341
$5 \times 10^{12} + 194858$	0.186	0.16733	0.20	0	630783	0.0376
$2 \times 10^{13} + 131252$	0.180	0.14142	0.19	0	1261566	0.0349
$6 \times 10^{13} + 123375$	0.168	0.15492	0.18	0	2185096	0.0377
$3 \times 10^{14} + 188911$	0.161	0.13416	0.17	0	4886025	0.0369
$2 \times 10^{15} + 122014$	0.153	0.11832	0.16	0	12615662	0.0532
$7 \times 10^{15} + 68886$	0.139	0.14832	0.15	0	23601743	0.0350
$6 \times 10^{16} + 156984$	0.132	0.12649	0.14	0	69098829	0.0307
$6 \times 10^{17} + 88525$	0.122	0.12649	0.13	0	218509686	0.0347
$9 \times 10^{18} + 35785$	0.113	0.11832	0.12	0	846284375	0.0318
$2 \times 10^{20} + 66447$	0.102	0.12649	0.11	0	3989422804	0.0305
$9 \times 10^{21} + 70686$	0.093	0.11832	0.1	0	26761861742	0.0321

The computations for $X = 2 \times 10^{20} + 66447$ and $X = 9 \times 10^{21} + 70686$ in the above table were massive, and performed using a Boinc based grid computing setup, in which a few hundred volunteers participated. Their contributions can be tracked at <http://anthgrid.com/dbnupperbound>
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REFERENCES

- [1] J. Arias de Reyna, *High-precision computation of Riemann's zeta function by the Riemann-Siegel asymptotic formula, I*, Mathematics of Computation, **80** (2011), 995–1009.
- [2] J. Arias de Reyna, J. Van de Lune, *On the exact location of the non-trivial zeroes of Riemann's zeta function*, Acta Arith. **163** (2014), 215–245.
- [3] W. G. C. Boyd, *Gamma Function Asymptotics by an Extension of the Method of Steepest Descents*, Proceedings: Mathematical and Physical Sciences, Vol. 447, No. 1931 (Dec. 8, 1994), 609–630.
- [4] N. C. de Bruijn, *The roots of trigonometric integrals*, Duke J. Math. **17** (1950), 197–226.
- [5] G. Csordas, T. S. Norfolk, R. S. Varga, *A lower bound for the de Bruijn-Newman constant Λ* , Numer. Math. **52** (1988), 483–497.
- [6] G. Csordas, A. M. Odlyzko, W. Smith, R. S. Varga, *A new Lehmer pair of zeros and a new lower bound for the De Bruijn-Newman constant Λ* , Electronic Transactions on Numerical Analysis. **1** (1993), 104–111.
- [7] G. Csordas, A. Ruttan, R. S. Varga, *The Laguerre inequalities with applications to a problem associated with the Riemann hypothesis*, Numer. Algorithms, **1** (1991), 305–329.
- [8] G. Csordas, W. Smith, R. S. Varga, *Lehmer pairs of zeros, the de Bruijn-Newman constant Λ , and the Riemann hypothesis*, Constr. Approx. **10** (1994), no. 1, 107–129.
- [9] H. Ki, Y. O. Kim, and J. Lee, *On the de Bruijn-Newman constant*, Advances in Mathematics, **22** (2009), 281–306.
- [10] D. H. Lehmer, *On the roots of the Riemann zeta-function*, Acta Math. **95** (1956), 291–298.

- [11] H. L. Montgomery, *The pair correlation of zeros of the zeta function*, Analytic number theory (Proc. Sympos. Pure Math., Vol. XXIV, St. Louis Univ., St. Louis, Mo., 1972), 181–193. Amer. Math. Soc., Providence, R.I., 1973.
- [12] H. L. Montgomery, R. C. Vaughan, *Multiplicative number theory. I. Classical theory*. Cambridge Studies in Advanced Mathematics, 97. Cambridge University Press, Cambridge, 2007.
- [13] C. M. Newman, *Fourier transforms with only real zeroes*, Proc. Amer. Math. Soc. **61** (1976), 246–251.
- [14] T. S. Norfolk, A. Ruttan, R. S. Varga, *A lower bound for the de Bruijn-Newman constant ΛII* , in A. A. Gonchar and E. B. Saff, editors, *Progress in Approximation Theory*, 403–418. Springer-Verlag, 1992.
- [15] A. M. Odlyzko, *An improved bound for the de Bruijn-Newman constant*, Numerical Algorithms **25** (2000), 293–303.
- [16] T. K. Petersen, *Eulerian numbers*. With a foreword by Richard Stanley. Birkhäuser Advanced Texts: Basler Lehrbücher. Birkhäuser/Springer, New York, 2015.
- [17] D. J. Platt, *Isolating some non-trivial zeros of zeta*, Math. Comp. **86** (2017), 2449–2467.
- [18] G. Polya, *Über trigonometrische Integrale mit nur reellen Nullstellen*, J. Reine Angew. Math. **58** (1927), 6–18.
- [19] D. H. J. Polymath, github.com/km-git-acc/dbn_upper_bound
- [20] B. Rodgers, T. Tao, *The De Bruijn-Newman constant is nonnegative*, preprint. [arXiv:1801.05914](https://arxiv.org/abs/1801.05914)
- [21] Y. Saouter, X. Gourdon, P. Demichel, *An improved lower bound for the de Bruijn-Newman constant*, Mathematics of Computation. **80** (2011), 2281–2287.
- [22] J. Stopple, *Notes on Low discriminants and the generalized Newman conjecture*, Funct. Approx. Comment. Math., vol. 51, no. 1 (2014), 23–41.
- [23] J. Stopple, *Lehmer pairs revisited*, Exp. Math. **26** (2017), no. 1, 45–53.
- [24] H. J. J. te Riele, *A new lower bound for the de Bruijn-Newman constant*, Numer. Math., **58** (1991), 661–667.
- [25] E. C. Titchmarsh, *The Theory of the Riemann Zeta-function*, Second ed. (revised by D. R. Heath-Brown), Oxford University Press, Oxford, 1986.

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