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

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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

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

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

In this paper we establish several effective estimates on $H_t(x + iy)$, 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 $\Lambda \le 0.48$; we also obtain some new estimates controlling the asymptotic behavior of zeroes of $H_t(x + iy)$ as $x \to \infty$.

1. Introduction

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

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

where ξ denotes the Riemann xi function

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

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

It is a classical fact (see [21, 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)
$$\Phi(u) := \sum_{n=1}^{\infty} (2\pi^2 n^4 e^{9u} - 3\pi n^2 e^{5u}) \exp(-\pi n^2 e^{4u}).$$

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 [3] introduced the more general family of functions $H_t: \mathbb{C} \to \mathbb{C}$ for $t \in \mathbb{R}$ by the formula

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

As noted in [7, 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 $H_t(\overline{z}) = \overline{H_t(z)}$. De Bruijn showed that the zeroes of H_t are purely real for $t \ge 1/2$, and if H_t has purely real zeroes for some t, then $H_{t'}$ has purely real zeroes for all t' > t. Newman [12] strengthened this result by showing that there is an absolute constant $-\infty < \Lambda \le 1/2$, now known as the *De Bruijn-Newman constant*, with the property that H_t has purely real zeroes if and only if $t \ge \Lambda$. The Riemann hypothesis is then clearly equivalent to the upper bound $\Lambda \le 0$. Recently in [16] the complementary bound $\Lambda \ge 0$ was established, answering a conjecture of Newman [12]. Furthermore, Ki, Kim, and Lee [8] sharpened the upper bound $\Lambda \le 1/2$ of de Bruijn [3] slightly to $\Lambda < 1/2$.

2. Notation

Unless otherwise specified, log denotes the standard branch of the complex logarithm, thus the branch cut is on the negative real axis and imaginary part in $(-\pi, \pi]$. We then define the standard complex powers $z^w := \exp(w \log z)$, and in particular define the standard square root $\sqrt{z} := z^{1/2}$. We record the standard gaussian identity

(5)
$$\int_{\mathbb{R}} \exp\left(-(au^2 + bu + c)\right) du = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a} - c\right)$$

for any complex numbers a, b, c with Rea > 0.

To obtain effective estimates, it is convenient to use the notation $O_{\leq}(X)$ to denote any quantity that is bounded in magnitude by 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 $F : \mathbb{C} \to \mathbb{C}$ is meromorphic and is real-valued on \mathbb{R} then it is equal to its own reflection: $F = F^*$.

We use $x_+ := \max(x, 0)$ to denote the positive part of a real number x.

3. Applying the fundamental solution for the heat equation

We can write H_t in terms of H_0 using the fundamental solution to the heat equation. Namely, for any t > 0, we have from (5) 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

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

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

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

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

(6)
$$H_t(z) = \int_{\mathbb{R}} \frac{1}{8} \xi \left(\frac{1 + iz}{2} + \sqrt{t}v \right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

We now combine this formula with expansions of the Riemann ξ -function. From [21, (2.10.6)] we have the Riemann-Siegel formula

(7)
$$\frac{1}{8}\xi(s) = R_{0,0}(s) + R_{0,0}^*(1-s)$$

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

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

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

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

(9)
$$R_{0,N}(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{N \times N+1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}}$$

and $N \swarrow N+1$ 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 $v\to\pm\infty$ (indeed they grow like $\exp(O(|v|\log|v|))$, where the implied constants depend on t,z). From this and (6), (7) we conclude that

(10)
$$H_t(z) = \sum_{n=1}^{N} r_{t,n} \left(\frac{1+iz}{2} \right) + \sum_{n=1}^{N} r_{t,n}^* \left(\frac{1-iz}{2} \right) + R_{t,N} \left(\frac{1+iz}{2} \right) + R_{t,N}^* \left(\frac{1-iz}{2} \right)$$

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

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

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

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

(11)
$$r_{t,n}(s) = \exp\left(-\frac{t}{4}\alpha_n^2\right) \int_{\mathbb{R}} \exp\left(-\sqrt{t}v\alpha_n\right) r_{0,n}\left(s + \sqrt{t}v + \frac{t}{2}\alpha_n\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv$$

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

(12)
$$R_{t,N}(s) = \exp\left(-\frac{t}{4}\beta_N^2\right) \int_{\mathbb{R}} \exp\left(-\sqrt{t}\nu\beta_N\right) R_{0,N}\left(s + \sqrt{t}\nu + \frac{t}{2}\beta_N\right) \frac{1}{\sqrt{\pi}} e^{-\nu^2} d\nu$$

for any complex number β_N with 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 phases in $r_{0,n}$, $R_{0,N}$ close to stationary, in order to obtain good estimates and approximations for these terms.

4. Elementary estimates

We have the following elementary estimates:

Lemma 4.1 (Elementary estimates). Let x > 0.

(i) If a > 0 and $b \ge 0$ 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 $b, c \ge 0$ 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

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

(v) If z is a complex number with $|\text{Im}(z)| \ge 1$ or $\text{Re}z \ge 1$, 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 and $x \ge x_0 \ge \exp(b/a)$, then

$$\log^a x \le \frac{\log^a x_0}{x_0^b} x^b.$$

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 $0 \le t < x$.

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

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

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

Claim (iv) follows from the trivial identity $e^x = 1 + (e^x - 1)$ and the elementary inequality $e^{-x} \ge 1 - (e^x - 1)$. For Claim (v), we may use the functional equation $\Gamma = \Gamma^*$ to assume that $\text{Im}(z) \ge 0$. We use equations (1.13), (3.14) and (3.15) of [2] to obtain the 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

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

for $Re(z) \ge 0$ and

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

for $Re(z) \le 0$, 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 $\text{Im}(z) \ge 1$ by hypothesis, and hence $|1 - e^{2\pi iz}| \ge 1 - e^{-2\pi}$. We conclude that in all ranges of z of interest, we have

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

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 $x \mapsto \frac{\log^a x}{x^b}$ is nonincreasing for $x \ge \exp(b/a)$. Taking logarithms and writing $y = \log x$, it suffices to show that $a \log y - by$ is non-increasing for $y \ge b/a$, but this is clear from taking a derivative.

5. Estimates for large x

The objective of this section is to obtain effective approximations for the expression $H_t(x+iy)$ in the region

(13)
$$0 < t \le \frac{1}{2}; \quad 0 \le y \le 1; \quad x \ge 200.$$

The bounds in this region are somewhat arbitrary; one could easily replace the constants $\frac{1}{2}$, 1, 200 here by other positive numbers, at the expense of altering many of the numerical constants in the effective estimates.

The strategy is to use the expansion (10), which turns out to be an effective approximation as long as x stays away from zero, so 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 3. We will treat these two functions separately.

5.1. **Estimation of** $r_{t,n}$. We will need the function

(14)
$$M_0(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \sqrt{2\pi} \exp\left(\left(\frac{s}{2} - \frac{1}{2}\right) \log \frac{s}{2} - \frac{s}{2}\right)$$

defined for all s away from the negative axis. Clearly this function is non-vanishing for all such s. We may compute the logarithmic derivative

(15)
$$\alpha \coloneqq \frac{M_0'}{M_0}$$

of this function as

(16)
$$\alpha(s) = \frac{1}{s} + \frac{1}{s-1} - \frac{1}{2}\log\pi + \frac{1}{2}\log\frac{s}{2} - \frac{1}{2s}$$
$$= \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2}\log\frac{s}{2\pi}.$$

We can also compute one further derivative:

(17)
$$\alpha'(s) = -\frac{1}{2s^2} - \frac{1}{(s-1)^2} + \frac{1}{2s}.$$

If Im(s) > 3, we conclude in particular that

(18)
$$\alpha'(s) = O_{\leq}\left(\frac{1}{2\operatorname{Im}(s)^{2}}\right) + O_{\leq}\left(\frac{1}{\operatorname{Im}(s)^{2}}\right) + O_{\leq}\left(\frac{1}{2\operatorname{Im}(s)}\right)$$
$$= O_{\leq}\left(\frac{1}{2(\operatorname{Im}(s) - 3)}\right)$$

thanks to Lemma 4.1(i). Finally, we introduce the more general functions

(19)
$$M_t(s) := \exp(\frac{t}{4}\alpha(s)^2)M_0(s)$$

for any $t \ge 0$, as well as the sequence

$$(20) b_n^t := \exp(\frac{t}{4}\log^2 n).$$

Proposition 5.1 (Estimate for $r_{t,n}$). Let σ be real, let T > 10, let n be a positive integer, and let $0 < t \le 1/2$. Then

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

where

(21)
$$\varepsilon_{t,n}(\sigma + iT) := \exp\left(\frac{\frac{t^2}{8}|\alpha(\sigma + iT) - \log n|^2 + \frac{t}{4} + \frac{1}{6}}{T - 3.33}\right) - 1,$$

Proof. From (8), (14) and Lemma 4.1(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 Im(s) > 2. Let α_n denote the quantity

(22)
$$\alpha_n := \alpha(\sigma + iT) - \log n;$$

this is the logarithmic derivative of $M(s)n^{-s}$ at $s = \sigma + iT$. From (11) we have

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

By (16) and the hypothesis $T \ge 10$, the imaginary part of α_n may be lower bounded by

$$\operatorname{Im}(\alpha_n) \ge -\frac{1}{2T} - \frac{1}{T} \ge -0.15;$$

since $t \le 1/2$, we conclude that $\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n$ has imaginary part at least T - 0.08. Thus

$$r_{t,n}(s) = \exp(-\frac{t}{4}\alpha_n^2) \int_{\mathbb{R}} \exp(-\sqrt{t}v\alpha_n) M_0 \left(\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n\right) \times \\ \times \exp\left(-\left(\sigma + iT + \sqrt{t}v + \frac{t}{2}\alpha_n\right) \log n + O_{\leq}\left(\frac{1}{6(T - 0.74)}\right)\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv.$$

From (18) 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 $\sigma + iT + \sqrt{tv} + \frac{t}{2}\alpha_n$. Applying Taylor's theorem with remainder to a branch of the complex logarithm of M_0 , we conclude that

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

Inserting this estimate, writing $\alpha(\sigma + iT) = \alpha_n + \log n$, estimating $\frac{1}{6(T-0.74)}$ by $\frac{1}{6(T-3.08)}$ and $|\sqrt{t}v + \frac{t}{2}\alpha_n|^2$ by $2tv^2 + \frac{t^2}{2}|\alpha_n|^2$, and simplifying, we conclude that

$$r_{t,n}(s) = M_0(\sigma + iT) \exp\left(\frac{t}{4}\alpha_n^2 - (\sigma + iT)\log n\right) \times$$

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

Using (22), (19), (20) 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, and $\frac{1}{T-3.08} \le \frac{1}{T-3.33}$, it suffices by Lemma 4.1(iv) to show that

(23)
$$\int_{\mathbb{R}} \exp\left(\frac{tv^2}{2(T-3.08)}\right) \frac{1}{\sqrt{\pi}} e^{-v^2} dv \le \exp\left(\frac{t}{4(T-3.33)}\right).$$

Using (5), the left-hand side may be calculated exactly as

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

Applying Lemma 4.1(ii) and using the hypotheses $t \le 1/2$, $T \ge 10$, 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.

5.2. **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 (9):

Proposition 5.2. Let σ be real and T' > 0, and define the quantities

$$(24) s := \sigma + iT'$$

$$a \coloneqq \sqrt{\frac{T'}{2\pi}}$$

$$(26) N := \lfloor a \rfloor$$

$$p := 1 - 2(a - N)$$

(28)
$$U := \exp\left(-i\left(\frac{T'}{2}\log\frac{T'}{2\pi} - \frac{T'}{2} - \frac{\pi}{8}\right)\right).$$

Let K be a positive integer. Then we have an 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

(29)
$$C_0(p) := \frac{e^{\pi i(\frac{p^2}{2} + \frac{3}{8})} - i\sqrt{2}\cos\frac{\pi p}{2}}{2\cos(\pi p)}$$

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

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

for $\sigma > 0$ and

(31)
$$|C_k(p,\sigma)| \le \frac{2^{\frac{1}{2}-\sigma}}{2\pi} \frac{\Gamma(k/2)}{2\pi ((3-2\log 2)\pi)^{k/2}}$$

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

(32)
$$|RS_K(s)| \le \frac{1}{7} 2^{3\sigma/2} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}}$$

for $\sigma \geq 0$, and

(33)
$$|RS_K(s)| \le \frac{1}{2} \left(\frac{9}{10}\right)^{\lceil -\sigma \rceil} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}}$$

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

Proof. This follows from [1, Theorems 3.1, 4.1, 4.2] combined with [1, (3.2), (5.2)]. The dependence of $C_k(p,\sigma), k \ge 1$ 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)].

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

$$|C_0(p)| \le \frac{1}{2}$$

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

Proposition 5.3 (Estimate for $R_{t,N}$). Let $0 \le \sigma \le 1$, let $T \ge 100$, and let $0 < t \le 1/2$. Set

$$T' \coloneqq T + \frac{\pi t}{8}$$

and then define $a, N, p, U, C_0(p)$ using (25), (26), (28), (29). Then

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

where

(35)
$$\tilde{\varepsilon}(\sigma + iT) := \left(\frac{0.397 \times 9^{\sigma}}{a - 0.125} + \frac{5}{3(T' - 3.33)}\right) \exp\left(\frac{3.49}{T' - 3.33}\right).$$

Proof. We apply (12) with $\beta_N := \pi i/4$ to obtain

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

From (9) we have

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

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 (14) and Lemma 4.1(v) we thus have

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

From (18) and Taylor expansion of a logarithm of M, 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 (16), (25) one has

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

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

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

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

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

Putting all this together, we obtain

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

We separate the k=0 term from the rest. By Lemma 4.1(iv) and the fact that $\frac{1}{\sqrt{\pi}}e^{-v^2}$ integrates to one, we can write the above expression as

(36)
$$R_{t,N}(\sigma + iT) = (-1)^{N-1} U e^{\pi i \sigma/4} \exp\left(\frac{t\pi^2}{64}\right) M_0(iT') \left(C_0(p)(1 + O_{\leq}(\epsilon)) + O_{\leq}(\delta)\right)$$

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 $(\sigma + \sqrt{t}v)^2 \le 2\sigma^2 + 2tv^2$ and using (5) we obtain

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

Applying Lemma 4.1(ii) and using the hypotheses $t \le 1/2$, $T \ge 100$, one has

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

and hence

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

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

(37)
$$\epsilon \le \frac{10}{3(T'-3.33)} \exp\left(\frac{10}{3(T'-3.33)}\right).$$

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 $u \ge 0$ and $\max(\lfloor -\sigma \rfloor + 3, \lfloor \frac{T'}{\pi} \rfloor)$ when u < 0, so that Proposition 5.2 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

(38)
$$\frac{\sqrt{2}}{2\pi} \frac{9^{u} \Gamma(1/2)}{2a} + \frac{1}{7} 2^{3u/2} \frac{\Gamma(1)}{(a/1.1)^{2}} \le \frac{0.200 \times 9^{u}}{a} + \frac{0.173 \times 2^{3u/2}}{a^{2}}$$

for $u \ge 0$ and

(39)
$$\sum_{1 \le k \le \tilde{K}_u} \frac{2^{\frac{1}{2} - u}}{2\pi} \frac{\Gamma(k/2)}{2\pi ((3 - 2\log 2)\pi)^{k/2} a^k} + \frac{1}{2} (9/10)^{\lceil -u \rceil} \frac{\Gamma((\tilde{K}_u + 1)/2)}{(a/1.1)^{\tilde{K}_u + 1}}$$

for u < 0. One can calculate that

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

and

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

and hence we can bound (39) by

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

For $u \ge 0$, we can estimate (38) by

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

thanks to Lemma 4.1(i). For u < 0, we observe that if $k \le 2a^2 = \frac{T'}{\pi}$ then

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

and hence by the geometric series formula

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

and similarly

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

and hence we can bound (39) by

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

By Lemma 4.1(i) we have

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

and thus we can bound (39) by

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

Putting this together, we conclude that

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

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

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

$$\delta_{2} := \int_{\mathbb{R}} \exp\left(\frac{u^{2} + \frac{5}{6}}{T' - 0.33}\right) \frac{0.029 \times 2^{-u}}{a - 1.25} \frac{1}{\sqrt{\pi t}} e^{-(u - \sigma)^{2}/t} du$$

$$\delta_{3} := \int_{\mathbb{R}} \exp\left(\frac{u^{2} + \frac{5}{6}}{T' - 0.33}\right) \frac{2^{-u}}{2} \sum_{\frac{T'}{2} \leq k \leq -u + 4} (1.1)^{k} \frac{\Gamma(k/2)}{a^{k}} \frac{1}{\sqrt{\pi t}} e^{-(u - \sigma)^{2}/t} du.$$

$$(40)$$

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 (5)

(41)
$$\delta_1 = \frac{0.2 \times 9^{\sigma}}{a - 0.865} \exp\left(\frac{\sigma^2 + \frac{5}{6}}{T' - 0.33} + \frac{t(\log 3 + \frac{\sigma}{T' - 0.33})^2}{1 - \frac{t}{T' - 0.33}}\right) \left(1 - \frac{t}{T' - 0.33}\right)^{-1/2}.$$

One can write

(42)
$$\frac{1}{1 - \frac{t}{T' - 0.33}} = 1 + \frac{t}{T' - 0.33 - t} \le 1 + \frac{t}{T' - 0.83}$$

while by Lemma 4.1(ii) we have

(43)
$$1 - \frac{t}{T' - 0.33} = \exp\left(O_{\leq}\left(\frac{t}{T' - 0.33 - t}\right)\right) = \exp\left(O_{\leq}\left(\frac{t}{T' - 0.83}\right)\right).$$

We conclude that

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

From Lemma 4.1(i) and the hypothesis $0 \le \sigma \le 1$, we have

$$\left(\log 3 + \frac{\sigma}{T' - 0.33}\right)^2 \le (\log^2 3) \left(1 + \frac{2\sigma/\log 3}{T' - 0.33 - \frac{\sigma}{2\log 3}}\right)$$
$$\le (\log^2 3) \left(1 + \frac{2\sigma/\log 3}{T' - 0.83}\right)$$

and therefore by a further application of Lemma 4.1(i)

$$\left(\log 3 + \frac{\sigma}{T' - 0.33}\right)^{2} \left(1 + \frac{t}{T' - 0.83}\right) \le \log^{2} 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - \frac{2\sigma t/\log 3}{2\sigma/\log 3 + t}}\right)$$

$$\le \log^{2} 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - t}\right)$$

$$\le \log^{2} 3 \left(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 1.33}\right)$$

and thus

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

By repeating the proof of (41), we have

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

We can bound $(-\log \sqrt{2} + \frac{\sigma}{T'-0.33})^2$ by $\log^2 \sqrt{2}$. Using (42), (43) we thus have

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

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

$$0.2 \exp(t \log^2 3) \le 0.366$$

$$0.029 \exp(t \log^2 \sqrt{2}) \le 0.031$$

$$\frac{5 + 3t + 6\sigma^2}{6} \le \frac{5 + 3t + 6\sigma^2 + 12t\sigma \log 3 + 6t^2 \log^2 3}{6} \le 3.49$$

and hence

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

and

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

Now we turn to δ_3 , which will end up being extremely small compared to δ_1 or δ_2 . By (40) and the Fubini-Tonelli theorem, we have

$$\delta_3 = \frac{1}{2\sqrt{\pi t}} \sum_{k \ge \frac{T'}{22\pi}} (1.1)^k \frac{\Gamma(k/2)}{a^k} \int_{-\infty}^{4-k} \exp\left(\frac{u^2 + \frac{5}{6}}{T' - 0.33} - \frac{(u - \sigma)^2}{t} - u \log 2\right) du.$$

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

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

$$\delta_3 \le \frac{1}{2\sqrt{\pi t}} \sum_{k \ge \frac{T'}{22s}} (1.1)^k \frac{\Gamma(k/2)}{a^k} \int_{-\infty}^{4-k} e^{-\frac{u^2}{2t} - u \log 2} du.$$

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

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

bounding

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

we conclude that

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

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

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

(say). Since

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

we thus have

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

Inserting this and (37), (34) into (36), and crudely bounding $2^{-\sigma}$ by 9^{σ} , we obtain the claim. \Box

5.3. Combining the estimates. Combining Propositions 5.1, 5.3 with (10) 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 5.4 (A + B - C approximation). Let t, x, y obey (13). Set

$$T' := \frac{x}{2} + \frac{\pi t}{8}$$

and then define $a, N, p, U, C_0(p)$ using (25), (26), (28), (29). Define the quantities

$$A(x+iy) := M_t(\frac{1-y+ix}{2}) \sum_{n=1}^{N} \frac{b_n^t}{n^{\frac{1-y+ix}{2} + \frac{t}{2}\alpha(\frac{1-y+ix}{2})}}$$

$$B(x+iy) := M_t(\frac{1+y-ix}{2}) \sum_{n=1}^{N} \frac{b_n^t}{n^{\frac{1+y-ix}{2} + \frac{t}{2}\alpha(\frac{1+y-ix}{2})}}$$

$$C(x+iy) := 2e^{-\pi iy/8}(-1)^N \exp\left(\frac{t\pi^2}{64}\right) \operatorname{Re}(M_0(iT')C_0(p)Ue^{\pi i/8})$$

where M_0, b_n^t were defined in (19), (20). Then

$$H_t(x+iy) = A(x+iy) + B(x+iy) - C(x+iy) + O_{<}(E_A(x+iy) + E_B(x+iy) + E_C(x+iy))$$

where

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

and $\varepsilon_{t,n}$, $\tilde{\varepsilon}$ were defined in (21), (35).

In many cases one can use the cruder "A + B" approximation that is immediate from the above corollary and (34):

Corollary 5.5 (A + B approximation). With the notation and hypotheses as in Corollary 5.4, we have

$$H_t(x+iy) = A(x+iy) + B(x+iy) + O_{\leq}(E_A(x+iy) + E_B(x+iy) + E_{C_0}(x+iy))$$

where

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

It will be convenient to normalize by the first term

(44)
$$B_0(x+iy) := M_t(\frac{1+y-ix}{2})$$

of B(x + iy). This expression is non-zero, and we conclude (under the hypotheses of Corollary 5.5) that of B(x + iy). This expression is non-zero, and we conclude (under the hypotheses of Corollary 5.5) that

(45)
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{S_n}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{S_n}+\kappa}} + \frac{C(x+iy)}{B_0(x+iy)} + O_{\leq}(e_A + e_B + e_C)$$

and

(46)
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{s_*}+\kappa}} + O_{\leq} (e_A + e_B + e_{C,0})$$

where

(47)
$$\gamma \coloneqq \gamma(x+iy) \coloneqq \frac{M_t(\frac{1-y+ix}{2})}{M_t(\frac{1+y-ix}{2})}$$

(48)
$$s_* = s_*(x+iy) := \frac{1+y-ix}{2} + \frac{t}{2}\alpha(\frac{1+y-ix}{2})$$

(49)
$$\kappa := \kappa(x+iy) := \frac{t}{2} \left(\alpha(\frac{1-y+ix}{2}) - \alpha(\frac{1+y+ix}{2}) \right)$$

(50)
$$e_A := e_A(x+iy) := |\gamma| \sum_{n=1}^N n^y \frac{b_n^t}{n^{\operatorname{Re}(s) + \operatorname{Re}(\kappa)}} \varepsilon_{t,n}(\frac{1-y+ix}{2})$$

(51)
$$e_B := e_B(x+iy) := \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s)}} \varepsilon_{t,n} (\frac{1+y+ix}{2})$$

(52)
$$e_C := e_{C,0}(x+iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} (\tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2})).$$

(53)
$$e_{C,0} := e_{C,0}(x+iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} (1 + \tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2})).$$

It will be convenient to bound these quantities by expressions that depend on N rather than x. Observe that

$$N = \lfloor \sqrt{\frac{T'}{2\pi}} \rfloor = \lfloor \frac{x}{4\pi} + \frac{t}{16} \rfloor$$

and hence

$$(54) x_N \le x < x_{N+1}$$

where

$$(55) x_N \coloneqq 4\pi N^2 - \frac{\pi t}{4}.$$

Similarly one has

$$2\pi N^2 \le T' < 2\pi (N+1)^2.$$

Proposition 5.6 (Estimates). Let the notation and hypotheses be as in Corollary 5.4, and let γ , κ , e_A , e_B , $e_{C,0}$, e_C be defined by (47)-(53).

(i) One has

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

(ii) One has

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

(iii) One has

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

(iv) One has

$$e_A \le e^{0.02y} \left(\frac{x}{4\pi}\right)^{-y/2} \sum_{n=1}^{N} n^{y + \frac{ty}{2(x-6)}} \frac{b_n^t}{n^{\text{Re}(s_*)}} \left(\exp\left(\frac{\frac{t^2}{32} \log^2 \frac{x}{4\pi n^2} + 0.313}{T - 3.33}\right) - 1 \right).$$

(v) One has

$$e_B \le \sum_{n=1}^{N} \frac{b_n^t}{n^{\text{Re}(s_*)}} \left(\exp\left(\frac{\frac{t^2}{32} \log^2 \frac{x}{4\pi n^2} + 0.313}{T - 3.33}\right) - 1 \right).$$

(vi) One has

$$e_C \le \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + \frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}| + 3.58}{x - 8.52}\right) \left(\frac{1.24 \times (3^y + 3^{-y})}{a - 0.125} + \frac{3.46}{T' - 3.33}\right).$$

$$e_{C,0} \le \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + \frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}| + 3.58}{x - 8.52}\right) \left(1 + \frac{1.24 \times (3^y + 3^{-y})}{a - 0.125} + \frac{3.46}{T' - 3.33}\right).$$

Proof. From the mean value theorem we have

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

for some $\frac{1-y}{2} \le \sigma \le \frac{1+y}{2}$. From (15), (19) 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 (18) one has

(56)
$$\alpha'\left(\sigma + \frac{ix}{2}\right) = O_{\leq}\left(\frac{1}{x - 6}\right)$$

and from Taylor expansion we also have

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

from (16) one has

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

and hence

(57)
$$\alpha(\sigma + \frac{ix}{2}) = \frac{1}{2}\log\frac{x}{4\pi} + i\frac{\pi}{4} + O_{\leq}\left(\frac{2+\sigma}{x-6}\right).$$

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

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

In the region (13), which implies that $0 \le \sigma \le 1$, we have

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

and thus

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

The function $x \mapsto \frac{\log \frac{x}{4\pi}}{x-6}$ is decreasing for $x \ge 200$, hence

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

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 (24) to show that

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

By (16) one has

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

Bounding $\frac{1}{(1-y)^2+x^2} \ge \frac{1}{(1+y)^2+x^2}$ and $\sqrt{(1+y)^2+x^2} \ge x$, we conclude that

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

For $1 - 3y \ge 0$ we simply discard the second term on the right-hand side; otherwise we bound $\frac{1}{(1-y)^2 + x^2} \le \frac{1}{x^2}$, and the claim follows.

Claim (iii) is immediate from (56) and the fundamental theorem of calculus. Now we turn to (iv), (v). From (57) one has

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

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

$$(58) \qquad |\alpha(\frac{1\pm y+ix}{2})-\log n|^2=\frac{1}{4}\log^2\frac{x}{4\pi n^2}+\frac{\pi^2}{16}+O_{\leq}\left(\frac{3|\log\frac{x}{4\pi n^2}+i\frac{\pi}{2}|}{x-6}+\frac{9}{(x-6)^2}\right).$$

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

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

in the region (13), the right-hand side is certainly bounded by $(\frac{x}{4\pi})^2$, so that

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

and hence

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

In the region (13) we have $x \ge 200$, one can check that $\frac{|\log \frac{x}{4\pi} + i\frac{\pi}{2}|}{x-6}$ is decreasing in x. Thus

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

Similarly, in (13) we also have

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

We conclude from (21) that

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

Inserting this bound into (50), (51) and using claims (i), (ii), we obtain claims (iv), (v). Now we establish (vi). From (19) we have

$$\frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} = \exp\left(\frac{t\pi^2}{64} - \frac{t}{4}\mathrm{Re}\alpha\left(\frac{1+y+ix}{2}\right)^2\right) \frac{|M_0(iT')|}{|M_0\left(\frac{1+y+ix}{2}\right)|}.$$

Note that $\frac{1+y+ix}{2} = iT' + \frac{1+y}{2} - \frac{\pi it}{8}$. From (18) we see that $|\alpha'(s)| \le \frac{1}{x-6}$ 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 $\log M_0$, we conclude that

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

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

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

and from (16) one has

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

and hence

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

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

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

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 (58) we have

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

As before, in the region (13) we have

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

and thus

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

$$= \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}| + 3.58}{x - 8.52}\right)\right)$$

thanks to Lemma 4.1(i). Finally, since $T' \ge \frac{x}{2} \ge 100$ in (13), one has

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

and hence by (35)

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

Hence

$$\tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2}) \leq \frac{1.24 \times (3^y + 3^{-y})}{a - 0.125} + \frac{3.46}{T' - 3.33}$$

giving the claim.

6. Bounding Dirichlet series

In view of the approximation (46), it is of interest to obtain lower bounds for the quantity

(59)
$$X := \left| \sum_{n=1}^{N} \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^{N} n^y \frac{b_n^t}{n^{\overline{s_*} + \kappa}} \right|$$

for x, y, t in the region (13). By the triangle inequality (and the trivial identity $|z| = |\overline{z}|$), we obtain the lower bound

$$X \ge \left(\left| \sum_{n=1}^{N} \frac{b_n^t}{n^{s_*}} \right| - |\gamma| \left| \sum_{n=1}^{N} n^{y} \frac{b_n^t}{n^{s_* + \overline{k}}} \right| \right)_{+}.$$

It is thus of interest to obtain lower bounds for differences

(60)
$$\Delta := \left(\left| \sum_{n=1}^{N} \frac{\beta_n}{n^s} \right| - \left| \sum_{n=1}^{N} \frac{\alpha_n}{n^s} \right| \right)$$

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

Lemma 6.1. 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, ..., N with $\beta_1 = 1$. Let Δ denote the quantity (60).

(i) (Triangle inequality) We have

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

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

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

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

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

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 :

$$\begin{split} \tilde{\alpha}_n &\coloneqq \sum_{1 \leq d \leq D: d \mid n} \lambda_d \alpha_{n/d} \\ \tilde{\beta}_n &\coloneqq \sum_{1 \leq d \leq D: d \mid n} \lambda_d \beta_{n/d}. \end{split}$$

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 $n \ge 2$ 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

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

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

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

By the cosine rule, we have

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

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

$$\frac{|\beta_n - e^{i\theta}a_n|}{|1 - e^{i\theta}a_1|} \le \max(\frac{|\beta_n - \alpha_n|}{1 - \alpha_1}, \frac{|\beta_n + \alpha_n|}{1 + \alpha_1})$$

and the claim follows.

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

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

between Dirichlet convolution and Dirichlet series, which implies that

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

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

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

the claim follows.

Returning to the estimation of (59), we conclude from Lemma 6.1(i) with s replaced by s_* , β_n replaced by b_n^t , and α_n replaced by $|\gamma|n^{\gamma-\overline{k}}b_n^t$ that

(61)
$$X \ge 1 - |\gamma| - \sum_{n=2}^{N} \frac{b_n^t}{n^{\sigma}} (1 + |\gamma| n^{y - \operatorname{Re}(\kappa)}),$$

where $\sigma := \text{Re } s_*$. This rather crude bound will suffice when x is very large, particularly when combined with the estimates in Proposition 5.6. For smaller values of x, we would like to use parts (ii) and (iii) of Lemma 6.1. A technical difficulty arises because the quantity $|\lambda| n^{\nu - \bar{k}} b_n^t$ quantity need not be real, so that Lemma 6.1(ii) is not directly available. However, by writing

$$n^{-\overline{\kappa}} = 1 + O_{\leq}(n^{|\kappa|} - 1)$$

we see from the triangle inequality that

$$X \ge \left(\left| \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} \right| - \left| \sum_{n=1}^N \frac{|\gamma| b_n^t n^y}{n^{s_*}} \right| \right)_+ - |\gamma| \sum_{n=1}^N \frac{b_n^t (n^{|\kappa|} - 1)}{n^{\sigma - y}}.$$

Assuming for now that $|\gamma| < 1$ (which in practice will follow from Proposition 5.6(i)), we can then apply Lemma 6.1(iii) follows by Lemma 6.1(ii) to conclude that

(62)
$$X \ge \frac{1 - \tilde{\alpha}_1 - \sum_{n=2}^{N} \frac{\max(\tilde{\beta}_n - \tilde{\alpha}_n, \frac{1 - \tilde{\alpha}_1}{1 + \tilde{\alpha}_1} | \tilde{\beta}_n + \tilde{\alpha}_n|)}{n^{\sigma}} - |\gamma| \sum_{n=1}^{N} \frac{b_n^t (n^{|\kappa|} - 1)}{n^{\sigma - y}}$$

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

$$\tilde{\alpha}_n := \sum_{1 \le d \le D: d \mid n} \lambda_d b_{n/d}^t |\gamma| n^y$$

$$\tilde{\beta}_n := \sum_{1 \le d \le D: d \mid n} \lambda_d b_{n/d}^t.$$

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

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

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, $\lambda_1=1$, $\lambda_2=-b_2^t$, $\lambda_3=-b_3^t$, $\lambda_6=b_2^tb_3^t$, 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 (62) favorable. (For instance, it makes $\tilde{\beta}_p$ vanish for all primes $p \leq P$).

7. Estimation for small x

We now turn to the problem of estimating $H_t(x + iy)$ (and its derivative) accurately when x is small (e.g., $x \le 200$). Here, the approximations based on the Riemann-Siegel formula (7) do not seem to be particularly efficient. Instead, we return to the original definition (4). From the functional equation $\Phi(-u) = -\Phi(u)$ we have

$$H_t(z) = \frac{1}{2} \int_{\mathbb{D}} e^{tu^2} \Phi(u) e^{izu} \ du$$

and hence on differentiation under the integral sign (which can be justified using for instance the Cauchy integral formula and Fubini's theorem) we have

$$H'_t(z) = \frac{i}{2} \int_{\mathbb{R}} e^{tu^2} u \Phi(u) e^{izu} du.$$

For any parameter $0 \le \theta < \pi/8$, we may shift the contour to $i\theta + \mathbb{R}$ and then use the even nature of Φ to reflect the left half of that contour around the origin to obtain the identities

$$H_{t}(z) = \frac{1}{2} \int_{i\theta}^{i\theta+\infty} e^{tu^{2}} \Phi(u) e^{izu} du + \frac{1}{2} \int_{i\theta-\infty}^{i\theta} e^{tu^{2}} \Phi(u) e^{izu} du$$

$$= \frac{1}{2} \int_{i\theta}^{i\theta+\infty} e^{tu^{2}} \Phi(u) e^{izu} du + \frac{1}{2} \int_{-i\theta}^{-i\theta+\infty} e^{tu^{2}} \Phi(u) e^{-izu} du$$

$$= \frac{1}{2} \int_{i\theta}^{i\theta+\infty} e^{tu^{2}} \Phi(u) e^{izu} du + \frac{1}{2} \int_{i\theta}^{i\theta+\infty} e^{tu^{2}} \Phi(u) e^{i\overline{z}u} du$$

and similarly

(64)
$$H'_t(z) = \frac{i}{2} \int_{i\theta}^{i\theta + \infty} e^{tu^2} \Phi(u) u e^{izu} du - \frac{i}{2} \overline{\int_{i\theta}^{i\theta + \infty} e^{tu^2} \Phi(u) u e^{i\overline{z}u} du}.$$

Since

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

we thus have for z = x + iy that

(65)

$$\begin{split} H_{t}(z) &= \frac{1}{2} \sum_{n=1}^{\infty} 2\pi^{2} n^{4} I_{t,\theta}(z - 9i, \pi n^{2}) - 3\pi n^{2} I_{t,\theta}(z - 5i, \pi n^{2}) + 2\pi^{2} n^{4} \overline{I_{t,\theta}(\overline{z} - 9i, \pi n^{2})} - 3\pi n^{2} \overline{I_{t,\theta}(\overline{z} - 5i, \pi n^{2})} \\ &= \frac{1}{2} \sum_{n=1}^{\infty} 2\pi^{2} n^{4} I_{t,\theta}(x - (9 - y)i, \pi n^{2}) - 3\pi n^{2} I_{t,\theta}(x - (5 - y)i, \pi n^{2}) \\ &+ 2\pi^{2} n^{4} \overline{I_{t,\theta}(x - (9 + y)i, \pi n^{2})} - 3\pi n^{2} \overline{I_{t,\theta}(x - (5 + y)i, \pi n^{2})} \end{split}$$

and similarly

(66)

$$H'_{t}(z) = \frac{i}{2} \sum_{n=1}^{\infty} 2\pi^{2} n^{4} J_{t,\theta}(z - 9i, \pi n^{2}) - 3\pi n^{2} J_{t,\theta}(z - 5i, \pi n^{2}) - 2\pi^{2} n^{4} \overline{J_{t,\theta}(\overline{z} - 9i, \pi n^{2})} + 3\pi n^{2} \overline{J_{t,\theta}(\overline{z} - 5i, \pi n^{2})}$$

$$= \frac{i}{2} \sum_{n=1}^{\infty} 2\pi^{2} n^{4} J_{t,\theta}(x - (9 - y)i, \pi n^{2}) - 3\pi n^{2} J_{t,\theta}(x - (5 - y)i, \pi n^{2})$$

$$- 2\pi^{2} n^{4} \overline{J_{t,\theta}(x - (9 + y)i, \pi n^{2})} + 3\pi n^{2} \overline{J_{t,\theta}(x - (5 + y)i, \pi n^{2})}$$

where $I_{t,\theta}(b,\beta)$, $J_{t,\theta}(b,\beta)$ denote the integrals

(67)
$$I_{t,\theta}(b,\beta) := \int_{i\theta}^{i\theta+\infty} \exp(tu^2 - \beta e^{4u} + ibu) du$$

(68)
$$J_{t,\theta}(b,\beta) := \int_{i\theta}^{i\theta+\infty} \exp(tu^2 - \beta e^{4u} + ibu)u \ du.$$

It is thus of interest to find good estimates for $I_{t,\theta}(b,\beta)$, $J_{t,\theta}(b,\beta)$ when $\beta = \pi n^2$ for some n, and b = x - ia for a = 9 + y, 9 - y, 5 + y, 5 - y. It will be convenient to split

$$I_{t,\theta}(b,\beta) = I_{t,\theta, < X}(b,\beta) + I_{t,\theta, > X}(b,\beta)$$

for any cutoff $X \ge 0$, where

$$I_{t,\theta,\leq X}(b,\beta) := \int_{i\theta}^{i\theta+X} \exp(tu^2 - \beta e^{4u} + ibu) du$$

and

$$I_{t,\theta,\geq X}(b,\beta) := \int_{i\theta+X}^{i\theta+\infty} \exp(tu^2 - \beta e^{4u} + ibu) \ du.$$

One can similarly split

$$J_{t,\theta}(b,\beta) = J_{t,\theta, \leq X}(b,\beta) + J_{t,\theta, \geq X}(b,\beta)$$

Proposition 7.1. Let b=x-ia for some x,a>0, let $0 \le \theta < \frac{\pi}{8}$, and let $\beta > 0$ and $X,t \ge 0$.

(i) One has the upper bounds and

(69)
$$|I_{t,\theta,\leq X}(b,\beta)| \leq \exp(-t\theta^2 - \theta x) \int_0^X \exp(tv^2 - \beta e^{4v} \cos(4\theta) + av) du$$
 and

$$(70) |J_{t,\theta,\leq X}(b,\beta)| \leq \exp(-t\theta^2 - \theta x) \int_0^X \exp(tv^2 - \beta e^{4v} \cos(4\theta) + av)(\theta^2 + u^2)^{1/2} du.$$

(ii) If one has the hypothesis

(71)
$$\beta e^{4X} \cos(4\theta) > \max(\frac{t}{2}, \frac{a + 2tX}{4})$$

then one has

$$|I_{t,\theta,\geq X}(b,\beta)| \leq \frac{\exp(-t\theta^2 + tX^2 - \beta e^{4X}\cos(4\theta) - \theta x + aX)}{4\beta e^{4X}\cos(4\theta) - a - 2tX}$$

and similarly

(73)

$$|J_{t,\theta,\geq X}(b,\beta)| \leq \exp(-t\theta^2 + tX^2 - \beta e^{4X}\cos(4\theta) - \theta x + aX) \left(\frac{|X+i\theta|}{4\beta e^{4X}\cos(4\theta) - a - 2tX} + \frac{1}{(4\beta e^{4X}\cos(4\theta) - a - 2tX)^2}\right).$$

In particular, setting X = 0, we see that if

(74)
$$\beta \cos(4\theta) > \max(\frac{t}{2}, \frac{a}{4})$$

then

(75)
$$|I_{t,\theta}(b,\beta)| \le \frac{\exp(-t\theta^2 - \beta\cos(4\theta) - \theta x)}{4\beta\cos(4\theta) - a}$$

and similarly

$$(76) \qquad |J_{t,\theta}(b,\beta)| \le \exp(-t\theta^2 - \beta\cos(4\theta) - \theta x) \left(\frac{\theta}{4\beta\cos(4\theta) - a} + \frac{1}{(4\beta\cos(4\theta) - a)^2}\right).$$

In practice, the tail estimates (72), (73) become useful when θ is close to $\pi/8$ (to get the most gain out of the $\exp(-\theta x)$ factor), and X is large. Similarly, (75), (76) become useful when θ is close to $\pi/8$ and β is large.

Proof. We first prove (i). Writing $u = i\theta + v$ and b = x - ia we have

$$I_{t,\theta,\leq X}(b,\beta) = \int_0^X \exp(t(-\theta^2 + v^2 + 2i\theta v) - \beta e^{4v}\cos(4\theta) - i\beta e^{4v}\sin(4\theta) - \theta x + ivx + av + ia\theta) dv$$

and the claim (69) then follows from the triangle inequality. The claim (70) is proven similarly, with an additional factor of $i\theta + v = O_{\leq}((\theta^2 + v^2)^{1/2})$ in the integrand.

Now we prove (ii). Writing $u = i\theta + X + v$ and b = x - ia, we have

$$I_{t,\theta, \geq X}(b,\beta) = \int_0^\infty \exp(t(-\theta^2 + X^2 + 2Xv + v^2 + 2i\theta(X+v)) - \beta e^{4X}e^{4v}\cos(4\theta) - i\beta e^{4X}e^{4v}\sin(4\theta) - \theta x + ix(X+v) + aX + av + ia\theta) dv$$

and hence by the triangle inequality

$$|I_{t,\theta,\geq X}(b,\beta)| \leq \exp(-t\theta^2 + tX^2 - \beta e^{4X}\cos(4\theta) - \theta x + aX) \int_0^\infty \exp(tv^2 + 2tXv - \beta e^{4X}(e^{4v} - 1)\cos(4\theta) + av) dv.$$

Similarly one has

$$|J_{t,\theta,\geq X}(b,\beta)| \leq \exp(-t\theta^2 + tX^2 - \beta e^{4X}\cos(4\theta) - \theta x + aX) \int_0^\infty \exp(tv^2 + 2tXv - \beta e^{4X}(e^{4v} - 1)\cos(4\theta) + av)(|X + i\theta| + v) dv.$$

The exponent $tv^2 + 2tXv - \beta e^{4X}(e^{4v} - 1)\cos(4\theta) + av$ equals 0 when v = 0 and has derivative

$$2tv + 2tX - 4\beta e^{4X}\cos(4\theta)e^{4v} + a.$$

Note that $e^{4v} \ge 1 + 4v$. Hence by (74), this derivative will be bounded from below by the negative quantity $-(4\beta e^{4X}\cos(4\theta) - a - 2tX)$. This implies that

$$\exp(tv^2 - \beta e^{4X}(e^{4v} - 1)\cos(4\theta) + av) \le \exp(-v(4\beta e^{4X}\cos(4\theta) - a - 2tX))$$

and the bounds (72), (73) follow from the standard integral identities

$$\int_0^\infty \exp(a - bv) \, dv = \frac{\exp(a)}{b}$$
$$\int_0^\infty \exp(a - bv)v \, dv = \frac{\exp(a)}{b^2},$$

valid for any b > 0. Setting X = 0 we then obtain (75), (76).

Corollary 7.2. Let x, a, t > 0 and $0 \le \theta < \frac{\pi}{4}$, and let n_0 be a natural number such that

$$\pi n_0^2 \cos(4\theta) > \max(\frac{t}{2}, \frac{a}{4}).$$

Then we have

$$\left| \sum_{n \ge n_0} 2\pi^2 n^4 I_{t,\theta}(x - ia, \pi n^2) \right| \le \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2 \cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \times \left(n_0^4 G_0(\alpha) + 4n_0^3 G_1(\alpha) + 6n_0^2 G_2(\alpha) + 4n_0 G_3(\alpha) + G_4(\alpha) \right)$$

and

(78)
$$\left| \sum_{n \ge n_0} 3\pi n^2 I_{t,\theta}(x - ia, \pi n^2) \right| \le \frac{3\pi \exp(-t\theta^2 - \theta x - \pi n_0^2 \cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \times (n_0^2 G_0(\alpha) + 2n_0 G_1(\alpha) + G_2(\alpha))$$

where $\alpha := e^{-\pi n_0 \cos(4\theta)}$, and $G_k(\alpha)$ are the generalised geometric series

$$G_k(\alpha) := \sum_{m=0}^{\infty} m^k \alpha^m.$$

Similarly one has

$$\left| \sum_{n \ge n_0} 2\pi^2 n^4 J_{t,\theta}(x - ia, \pi n^2) \right| \le 2\pi^2 \exp(-t\theta^2 - \pi n_0^2 \cos(4\theta) - \theta x) \left(\frac{\theta}{4\pi n_0^2 \cos(4\theta) - a} + \frac{1}{(4\pi n_0^2 \cos(4\theta) - a)^2} \right) \times \left(n_0^4 G_0(\alpha) + 4n_0^3 \alpha G_1(\alpha) + 6n_0^2 G_2(\alpha) + 4n_0 G_3(\alpha) + G_4(\alpha) \right)$$

and

(80)

$$\left| \sum_{n \ge n_0} 3\pi n^2 J_{t,\theta}(x - ia, \pi n^2) \right| \le 3\pi \exp(-t\theta^2 - \pi n_0^2 \cos(4\theta) - \theta x) \left(\frac{\theta}{4\pi n_0^2 \cos(4\theta) - a} + \frac{1}{(4\pi n_0^2 \cos(4\theta) - a)^2} \right) \times \left(n_0^2 G_0(\alpha) + 2n_0 G_1(\alpha) + G_2(\alpha) \right).$$

We remark that $G_k(\alpha)$ can be computed explicitly for small k and $|\alpha| < 1$ as

$$G_0(\alpha) = \frac{1}{1-\alpha}$$

$$G_1(\alpha) = \frac{\alpha}{(1-\alpha)^2}$$

$$G_2(\alpha) = \frac{\alpha^2 + \alpha}{(1-\alpha)^3}$$

$$G_3(\alpha) = \frac{\alpha^3 + 4\alpha^2 + \alpha}{(1-\alpha)^4}$$

$$G_4(\alpha) = \frac{\alpha^4 + 11\alpha^3 + 11\alpha^2 + \alpha}{(1-\alpha)^5}$$

In general one has

$$G_k(\alpha) = \frac{\sum_{j=0}^{k-1} A(k, j) \alpha^{j+1}}{(1 - \alpha)^{k+1}}$$

for any $k \ge 1$ and $|\alpha| < 1$; where A(k, j) are the Eulerian numbers [15].

Proof. From (75) one has

$$\begin{split} |\sum_{n\geq n_0} 2\pi^2 n^4 I_{t,\theta}(x-ia,\pi n^2)| &\leq \sum_{n\geq n_0} 2\pi^2 n^4 \frac{\exp(-t\theta^2 - \pi n^2\cos(4\theta) - \theta x)}{4\pi n^2\cos(4\theta) - a} \\ &\leq \frac{2\pi^2 \exp(-t\theta^2 - \theta x)}{4\pi n_0^2 \cos(4\theta) - a - 2tX} \sum_{n\geq n_0} n^4 \exp(-\pi n n_0\cos(4\theta)) \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \sum_{m=0}^{\infty} (n_0^4 + 4n_0^3 m + 6n_0^2 m^2 + 4n_0 m^3 + m^4) \alpha^m \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \\ &\times \left(n_0^4 G_0(\alpha) + 4n_0^3 \alpha G_1(\alpha) + 6n_0^2 G_2(\alpha) + 4n_0 G_3(\alpha) + G_4(\alpha)\right) \end{split}$$

giving (77) as desired. The estimates (78), (79), (80) are proven similarly.

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

In this section we prove

Theorem 8.1. We have $\Lambda \leq 0.48$.

We first recall from [3, Theorem 13] that if $t \in \mathbb{R}$ and $\Delta > 0$ are such that all the zeroes of H_t lie in the strip $\{z : |\mathrm{Im}(z)| \leq \Delta\}$, then for any t' > t, the zeroes of $H_{t'}$ lie in the strip $\{z : |\mathrm{Im}(z)| \leq (\Delta^2 - 2(t-t'))_+^{1/2}\}$. In particular this implies that $\Lambda \leq t + \frac{\Delta^2}{2}$. Thus, to prove the theorem, it suffices to show that the zeroes of $H_{0.4}$ lie in the strip $\{|\mathrm{Im}(z)| \leq 0.4\}$. On the other hand, since the zeroes of $H_{0}(z) = \frac{1}{8}\xi\left(\frac{1+iz}{2}\right)$ lie in the strip $\{|\mathrm{Im}(z)| \leq 1\}$, the zeroes of $H_{0.4}$ lie in the strip $\{z : |\mathrm{Im}(z)| \leq \frac{1}{\sqrt{5}}\}$. Since $H_{0.4}$ is even with $H_{0.4} = H_{0.4}^*$, it thus suffices to show that

$$H_{0.4}(x+iy) \neq 0$$

whenever $x \ge 0$ and $0.4 \le y \le \frac{1}{\sqrt{5}}$.

Henceforth t = 0.4. As in Section 5, we introduce the quantities

$$T := \frac{x}{2}$$

$$T' := T + \frac{\pi t}{8} = \frac{x}{2} + \frac{\pi}{20}$$

$$a := \sqrt{\frac{T'}{2\pi}} = \sqrt{\frac{x}{4\pi} + \frac{\pi}{40}}$$

$$N := \lfloor a \rfloor$$

and we split into cases depending on the value of N.

- 8.1. The case of very large N: $N \ge 2000$
- 8.2. The case of large N: $300 \le N < 2000$
- 8.3. The case of medium *N*: $11 \le N < 300$
- 8.4. The case of small N: $N \le 10$

9. Asymptotic results

In this section we use the effective estimates from Section 5 to obtain asymptotic information about the function H_t , which improves (and makes more effective) the results of Ki, Kim, and Lee [8]. We use the usual asymptotic notation X = O(Y) to denote the bound $X = O_{\leq}(CY)$ for an absolute constant C.

Proposition 9.1. *Let* $0 < t \le 1/2$, $x \ge 200$, and $-3 \le y \le 3$.

(i) If $x \ge \exp(\frac{C}{t})$ 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 (19).

(ii) If instead we have $x \ge C$ for a sufficiently large absolute constant C, then

$$H_t(x+3i) = (1+O_{\leq}(0.7))M_t\left(2-\frac{ix}{2}\right).$$

Proof. We begin with (i). Since $H_t = H_t^*$ and $M_t = M_t^*$, we may assume without loss of generality that $y \ge 0$. Using (47), (44) we may write the desired estimate as

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

We apply the decomposition (46) followed by Proposition 5.6. (Strictly speaking, the estimates there required $y \le 1$ rather than $y \le 3$; however, as remarked at the beginning of Section 5, all the estimates in that section would continue to hold under this weaker hypothesis if one adjusted all the numerical constants appropriately.) This gives

(81)
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{S_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{S_*}+\kappa}} + O_{\leq}(e_A + e_B + e_{C,0})$$

where

$$\gamma = O(x^{-y/2})$$

$$\kappa = O(x^{-1})$$

$$Re(s_*) \ge \frac{1+y}{2} + \frac{t}{2} \log \frac{x}{4\pi} - O(x^{-2})$$

$$e_A = O\left(x^{-y/2} \sum_{n=1}^{N} b_n^t n^{-\frac{1-y}{2} - \frac{t}{2} \log \frac{x}{4\pi} - O(x^{-1})} \frac{\log^2 x}{x}\right)$$

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

$$e_{C,0} = O\left(x^{-\frac{1+y}{4}}\right)$$

Since $N = O(x^{1/2})$, we have $x^{-y/2}n^y = O(1)$ and $n^{O(x^{-1})} = O(1)$ for all $1 \le n \le N$. 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 (20) 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 $2 \le n \le N$, we have

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

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 $x \ge \exp(C/t)$ 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 (81), now with y = 3. We have

$$\gamma \sum_{n=1}^{N} n^{3} \frac{b_{n}^{t}}{n^{\overline{s_{*}} + \kappa}} = O\left(x^{-3/2} \sum_{n=1}^{N} \frac{b_{n}^{t}}{n^{-1 + \frac{t}{2} \log \frac{x}{4\pi}}}\right)$$
$$= O\left(x^{-3/2} \sum_{n=1}^{N} n\right)$$
$$= O(x^{-1/2})$$

since $y \ge 5$; similar arguments give $e_A = O(\frac{\log^2 x}{x^{3/2}})$, while

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

We conclude that

$$\frac{H_t(x+3i)}{B_0(x+3i)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_n}} + O(x^{-1/2})$$

$$= 1 + O_{\leq} \left(\sum_{n=2}^N n^{-2-\frac{t}{2} \log \frac{x}{4\pi} - O(x^{-1})} \right) + O(x^{-1/2})$$

$$= 1 + O_{\leq} \left(\sum_{n=2}^N n^{-2} \right) + O(x^{-1/2})$$

$$= 1 + O_{\leq} \left(\frac{\pi^2}{6} - 1 \right) + O(x^{-1/2})$$

$$= 1 + O_{\leq}(0.7)$$

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

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

Lemma 9.2. Let $0 < t \le 1/2$, 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 $\arg M_t\left(\frac{1+ix_*}{2}\right)$ for all large real x_* such that

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

Proof. By (19), (15), the log-derivative of M_t is given by

$$\frac{M_t'}{M_t} = \alpha + \frac{t}{2}\alpha\alpha'.$$

For $s = \frac{ix_*}{2} + O(1)$, we have from (16) that

(83)
$$\alpha(s) = \frac{1}{2} \log \frac{x_*}{4\pi} + \frac{\pi i}{4} + O\left(\frac{1}{x_*}\right)$$

and from this and (18) 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

$$\arg M_{t} \left(\frac{1+ix_{*}}{2}\right) = \frac{t}{4} \operatorname{Im}\alpha \left(\frac{1+ix_{*}}{2}\right)^{2} + \pi - \frac{x_{*}}{4} \log \pi + \operatorname{Im} \left(\frac{-1+ix_{*}}{4} \log \frac{1+ix_{*}}{4} - \frac{1+ix_{*}}{4}\right)$$

$$= \frac{t}{4} \left(\frac{\pi}{4} \log \frac{x_{*}}{4\pi} + O(\frac{\log x_{*}}{x_{*}})\right) + \pi - \frac{x_{*}}{4} \log \pi + \operatorname{Im} \left(\frac{-1+ix_{*}}{4} \left(\log \frac{x_{*}}{4} + \frac{i\pi}{2} - \frac{i}{x_{*}} + O\left(\frac{1}{x_{*}^{2}}\right)\right)\right) - \frac{x_{*}}{4}$$

$$= \frac{t\pi}{16} \log \frac{x_{*}}{4\pi} + \pi + \frac{x_{*}}{4} \log \pi + \frac{x_{*}}{4} \log \frac{x_{*}}{4} - \frac{\pi}{8} + O\left(\frac{\log x_{*}}{x_{*}}\right)$$

$$= \frac{t\pi}{16} \log \frac{x_{*}}{4\pi} + \frac{7\pi}{8} + \frac{x_{*}}{4} \log \frac{x_{*}}{4\pi} - \frac{x_{*}}{4} + O\left(\frac{\log x_{*}}{x_{*}}\right)$$

as desired.

This lets us control the zeroes of $H_t(x + iy)$ for x large enough:

Corollary 9.3 (Distribution of zeroes of H_t). Let $0 < t \le 1/2$, let C > 0 be a sufficiently large absolute constant, and let c > 0 be a sufficiently small absolute constant. For all $n \ge C$, let x_n be the unique real number greater than 4π such that

(84)
$$\frac{x_n}{4\pi} \log \frac{x_n}{4\pi} - \frac{x_n}{4\pi} + \frac{5}{8} + \frac{t}{16} \log \frac{x_n}{4\pi} = n.$$

(This is well-defined since the left-hand side is an increasing function of x_n for $x_n \ge 4\pi$.)

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

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

- (ii) Conversely, for each $n \ge \exp(\frac{C}{t})$ there is exactly one zero H_t in the disk $\{x + iy : |x + iy x_n| \le \frac{c}{\log x_n}\}$ (and by part (i), this zero will be real and lie within $O(x^{-ct})$ of x_n).
- (iii) If $X \ge \exp(\frac{C}{t})$, the number $N_t(X)$ of zeroes with real part between 0 and X is

$$N_t(X) = \frac{X}{4\pi} \log \frac{X}{4\pi} - \frac{X}{4\pi} + \frac{t}{16} \log \frac{X}{4\pi} + O(1).$$

These results refine Theorems 1.3 and 1.4 of [8], 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 $x \to \infty$ (holding t fixed).

Proof. We begin with (ii). Let $n \ge \exp(\frac{C}{t})$, and suppose that $x + iy = x_n + O(1)$. By Proposition 9.1(i) and Lemma 9.2 we have

(85)
$$H_{t}(x+iy) = \overline{M_{t}\left(\frac{1+ix_{n}}{2}\right)} \exp\left((-i(x-x_{n})+y)\left(\frac{1}{4}\log\frac{x_{n}}{4\pi} - \frac{\pi i}{8}\right) + O(x_{n}^{-ct})\right) + M_{t}\left(\frac{1+ix_{n}}{2}\right) \exp\left((i(x-x_{n})-y)\left(\frac{1}{4}\log\frac{x_{n}}{4\pi} + \frac{\pi i}{8}\right) + O(x_{n}^{-ct})\right).$$

From Lemma 9.2 and (84) one has

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

and hence

(86)
$$\overline{M_t\left(\frac{1+ix_n}{2}\right)} = -\exp\left(O(\frac{\log x_n}{x_n})\right)M_t\left(\frac{1+ix_n}{2}\right).$$

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

(87)

$$H_{t}(x+iy) = -M_{t} \left(\frac{1+ix_{n}}{2}\right) e^{-\pi(x-x_{n})/8} \exp\left((-i(x-x_{n})+y)\frac{1}{4}\log\frac{x_{n}}{4\pi} + O(|y|\log x_{n} + x_{n}^{-ct})\right) + M_{t} \left(\frac{1+ix_{n}}{2}\right) e^{-\pi(x-x_{n})/8} \exp\left((i(x-x_{n})-y)\frac{1}{4}\log\frac{x_{n}}{4\pi} + O(|y|\log x_{n} + x_{n}^{-ct})\right) = 2iM_{t} \left(\frac{1+ix_{n}}{2}\right) e^{-\pi(x-x_{n})/8} \left(\sin\left(\frac{x+iy-x_{n}}{4}\log\frac{x_{n}}{4\pi}\right) + O(|y|\log x_{n} + x_{n}^{-ct})\right).$$

In particular, if x + iy traverses the circle $\{x_n + \frac{c}{\log n}e^{i\theta} : 0 \le \theta \le 2\pi\}$ 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 $x \ge \exp(\frac{C}{t})$. We can assume $|y| \le 1$ since it is known (e.g., from [3, 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 (84) in x_n is comparable to $\log x_n$. From (85) we have

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

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 (87) 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.

Finally, 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 $n \ge \exp(\frac{C}{t})$. 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 $\{x + iy : 0 \le x \le X; -3 \le y \le 3\}$ traversed clockwise, since there are no zeroes with imaginary part of magnitude greater than one. By compactness, the variation on the left edge $\{iy : -3 \le y \le 3\}$ is O(1), and similarly for any fixed portion $\{x + 3i : 0 \le y \le C\}$ of the upper edge. From Proposition 9.1 (and (85)), we see that the variation of $H_t(x + iy)/M_t(\frac{1+y-ix}{2})$ on the remaining upper edge $\{x + 3i : C \le x \le X\}$ and on the top half $\{X + iy : 0 \le y \le 3\}$ 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 9.2.

Remark 9.4. The above proposition gives good control on $H_t(x + iy)$ whenever $x \ge \exp(C/t)$. As a consequence (and assuming for sake of argument that the Riemann hypothesis holds), then for any $\Lambda_0 > 0$, the bound $\Lambda \le \Lambda_0$ 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 9.5. Our discussion here will be informal. In view of the results of [7], it is expected that the zeroes $z_j(t)$ of $H_t(x+iy)$ should evolve according to the system of ordinary differential equations

$$\partial_t z_k(t) = 2 \sum_{j \neq k}^{\prime} \frac{1}{z_k(t) - z_j(t)}$$

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 [7, 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 9.3, 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 $|x| \le c \log \frac{1}{\Lambda}$ for some small absolute constant c > 0. This suggests that the time complexity bound in Remark 9.4 is likely to be best possible (unless one is able to prove the Riemann hypothesis, of course).

In [7, 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 9.1 and Corollary 9.3 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. maybe supply some numerically computed graphics here?

REFERENCES

- [1] J. Arias de Reyna, *High-precision computation of Riemann's zeta function by the Riemann-Siegel asymptotic formula, I*, Mathematics of Computation, Volume 80, Number 274, April 2011, Pages 9951009.
- [2] 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), pp. 609–630.
- [3] N. C. de Bruijn, The roots of trigonometric integrals, Duke J. Math. 17 (1950), 197-226.
- [4] G. Csordas, T. S. Norfolk, R. S. Varga, A lower bound for the de Bruijn-Newman constant Λ, Numer. Math. 52 (1988), 483–497.
- [5] 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 Lambda, Electronic Transactions on Numerical Analysis. 1 (1993), 104–111.
- [6] 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.
- [7] 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.
- [8] H. Ki, Y. O. Kim, and J. Lee, *On the de Bruijn-Newman constant*, Advances in Mathematics, **22** (2009), 281–306.
- [9] D. H. Lehmer, On the roots of the Riemann zeta-function, Acta Math. 95 (1956) 291–298.
- [10] H. L. Montgomer y, *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), pp. 181–193. Amer. Math. Soc., Providence, R.I., 1973.
- [11] H. L. Montgomery, R. C. Vaughan, Multiplicative number theory. I. Classical theory. Cambridge Studies in Advanced Mathematics, 97. Cambridge University Press, Cambridge, 2007.
- [12] C. M. Newman, Fourier transforms with only real zeroes, Proc. Amer. Math. Soc. 61 (1976), 246–251.
- [13] T. S. Norfolk, A. Ruttan, R. S. Varga, A lower bound for the de Bruijn-Newman constant Λ II., in A. A. Gonchar and E. B. Saff, editors, Progress in Approximation Theory, 403–418. Springer-Verlag, 1992.
- [14] A. M. Odlyzko, An improved bound for the de Bruijn-Newman constant, Numerical Algorithms 25 (2000), 293–303
- [15] T. K. Petersen, Eulerian numbers. With a foreword by Richard Stanley. Birkhäuser Advanced Texts: Basler Lehrbücher. Birkhäuser/Springer, New York, 2015.
- [16] B. Rodgers, T. Tao, The De Bruijn-Newman constant is nonnegative, preprint.
- [17] Y. Saouter, X. Gourdon, P. Demichel, An improved lower bound for the de Bruijn-Newman constant, Mathematics of Computation. 80 (2011), 2281–2287.
- [18] J. Stopple, *Notes on Low discriminants and the generalized Newman conjecture*, Funct. Approx. Comment. Math., vol. 51, no. 1 (2014), pp. 23–41.
- [19] J. Stopple, Lehmer pairs revisited, Exp. Math. 26 (2017), no. 1, 45–53.

- [20] H. J. J. te Riele, A new lower bound for the de Bruijn-Newman constant, Numer. Math., 58 (1991), 661–667.
- [21] 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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