EFFECTIVE APPROXIMATION OF HEAT FLOW EVOLUTION OF THE RIEMANN XI FUNCTION, AND AN UPPER BOUND FOR THE DE BRUIJN-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 $t \geq \Lambda$. The Riemann hypothesis is the equivalent to the assertion $\Lambda \leq 0$, and Newman conjectured the complementary bound $\Lambda \geq 0$.

1. Introduction

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

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

where ξ denotes the Riemann xi function

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

(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 [20, 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

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

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 $H_t\colon \mathbb{C} \to \mathbb{C}$ for $t \in \mathbb{R}$ by the formula

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

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 $t \geq 1/2$, 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 $-\infty < \Lambda \leq 1/2$, 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 [15] the complementary bound $\Lambda \geq 0$ was established, answering a conjecture of Newman [12]. Furthermore, Ki, Kim, and Lee [8] sharpened the upper bound $\Lambda \leq 1/2$ 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

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

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

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

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

We now combine this formula with expansions of the Riemann ξ-function. From [20, (2.10.6)] we have the Riemann-Siegel formula

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

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

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

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

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

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

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

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

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

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

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

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

for any complex number β_N with $\mathrm{Im}(s), \mathrm{Im}(s + \frac{t}{2}\beta_N)$ 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 $b \geq 0$ 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*

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

(v) *If z is a complex number with $|\mathrm{Im}(z)| \geq 1$ or $\mathrm{Re} z \geq 1$, 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 $a, b > 0$ and $x \geq x_0 \geq \exp(b/a)$, then*

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

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 $0 \leq t < x$.

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 $\mathrm{Im}(z) \geq 0$. We use equations (1.13), (3.1), (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

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

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

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

for $\mathrm{Re}(z) \leq 0$, 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 $\mathrm{Im}(z) \geq 1$ by hypothesis, and hence $|1 - e^{2\pi i z}| \geq 1 - e^{-2\pi}$. 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 $x \mapsto \frac{\log^a x}{x^b}$ is nonincreasing for $x \geq \exp(b/a)$. Taking logarithms and writing $y = \log x$, it suffices to show that $a \log y - by$ is non-increasing for $y \geq b/a$, but this is clear from taking a derivative. □

5. Initial approximations

In this section we give some initial estimates on the functions $r_{t,n}, R_{t,N}$ appearing in Section 3, and use this to approximate H_t.

We begin with the estimation of $r_{t,n}$. We will need the function

$$M_0(s) := \frac{1}{8}\frac{s(s-1)}{2}\pi^{-s/2}\sqrt{2\pi}\exp\left(\left(\frac{s}{2}-\frac{1}{2}\right)\log\frac{s}{2}-\frac{s}{2}\right) \tag{13}$$

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

$$\alpha := \frac{M_0'}{M_0} \tag{14}$$

of this function as

$$\begin{aligned} \alpha(s) &= \frac{1}{s} + \frac{1}{s-1} - \frac{1}{2}\log\pi + \frac{1}{2}\log\frac{s}{2} - \frac{1}{2s} \\ &= \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2}\log\frac{s}{2\pi}. \end{aligned} \tag{15}$$

We can also compute one further derivative:

$$\alpha'(s) = -\frac{1}{2s^2} - \frac{1}{(s-1)^2} + \frac{1}{2s}. \tag{16}$$

If $\mathrm{Im}(s) > 3$, we conclude in particular that

$$\begin{aligned} \alpha'(s) &= O_{\leq}\left(\frac{1}{2\mathrm{Im}\,(s)^2}\right) + O_{\leq}\left(\frac{1}{\mathrm{Im}\,(s)^2}\right) + O_{\leq}\left(\frac{1}{2\mathrm{Im}\,(s)}\right) \\ &= O_{\leq}\left(\frac{1}{2(\mathrm{Im}\,(s)-3)}\right) \end{aligned} \tag{17}$$

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

$$M_t(s) := \exp(\frac{t}{4}\alpha(s)^2)M_0(s) \tag{18}$$

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

$$b_n^t := \exp(\frac{t}{4}\log^2 n). \tag{19}$$

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

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

where

$$\varepsilon_{t,n}(\sigma+iT) := \exp\left(\frac{\frac{t^2}{8}|\alpha(\sigma+iT)-\log n|^2 + \frac{t}{4} + \frac{1}{6}}{T-3.33}\right) - 1, \tag{20}$$

Proof. From (8), (13) 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 $\mathrm{Im}(s) > 2$. Let α_n denote the quantity

$$\alpha_n := \alpha(\sigma + iT) - \log n; \tag{21}$$

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

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

By (15) and the hypothesis $T \geq 10$, the imaginary part of α_n may be lower bounded by

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

since $t \leq 1/2$, 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 (17) 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 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 (21), (18), (19) 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 $\frac{1}{T-3.08} \leq \frac{1}{T-3.33}$, it suffices by Lemma 4.1(iv) to show that

$$\int_{\mathbb{R}} \exp\left(\frac{tv^2}{2(T-3.08)}\right) \frac{1}{\sqrt{\pi}} e^{-v^2}\, dv \leq \exp\left(\frac{t}{4(T-3.33)}\right). \tag{22}$$

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 $t \leq 1/2$, $T \geq 10$, 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. □

Now we begin the 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*

$$s := \sigma + iT' \tag{23}$$

$$a := \sqrt{\frac{T'}{2\pi}} \tag{24}$$

$$N := \lfloor a \rfloor \tag{25}$$

$$p := 1 - 2(a - N) \tag{26}$$

$$U := \exp\left(-i\left(\frac{T'}{2}\log\frac{T'}{2\pi} - \frac{T'}{2} - \frac{\pi}{8}\right)\right). \tag{27}$$

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

$$C_0(p) := \frac{e^{\pi i(\frac{p^2}{2}+\frac{3}{8})} - i\sqrt{2}\cos\frac{\pi p}{2}}{2\cos(\pi p)} \tag{28}$$

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

$$|C_k(p,\sigma)| \leq \frac{\sqrt{2}}{2\pi} \frac{9^{\sigma}\Gamma(k/2)}{2^k} \tag{29}$$

for $\sigma > 0$ and

$$|C_k(p,\sigma)| \leq \frac{2^{\frac{1}{2}-\sigma}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2}} \tag{30}$$

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

$$|RS_K(s)| \leq \frac{1}{7} 2^{3\sigma/2} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}} \tag{31}$$

for $\sigma \geq 0$*, and*

$$|RS_K(s)| \leq \frac{1}{2}\left(\frac{9}{10}\right)^{\lceil -\sigma \rceil} \frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}} \tag{32}$$

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)]. □

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

$$|C_0(p)| \leq \frac{1}{2} \tag{33}$$

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* $0 \leq \sigma \leq 1$*, 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* (24)*,* (25)*,* (27)*,* (28)*. 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

$$\tilde{\varepsilon}(\sigma + iT) := \left(\frac{0.397 \times 9^{\sigma}}{a - 0.125} + \frac{5}{3(T' - 3.33)}\right) \exp\left(\frac{3.49}{T' - 3.33}\right). \tag{34}$$

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

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

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 (13) 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 (17) 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 (15), (24) 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

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

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

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

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

$$R_{t,N}(\sigma+iT) = (-1)^{N-1}Ue^{\pi i\sigma/4}\exp\left(\frac{t\pi^2}{64}\right)M_0(iT')\left(C_0(p)(1+O_{\leq}(\epsilon))+O_{\leq}(\delta)\right) \tag{35}$$

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 (5) 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 4.1(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

$$\epsilon \leq \frac{10}{3(T' - 3.33)} \exp\left(\frac{10}{3(T' - 3.33)}\right). \tag{36}$$

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 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

$$\frac{\sqrt{2}}{2\pi} \frac{9^u \Gamma(1/2)}{2a} + \frac{1}{7} 2^{3u/2} \frac{\Gamma(1)}{(a/1.1)^2} \leq \frac{0.200 \times 9^u}{a} + \frac{0.173 \times 2^{3u/2}}{a^2} \tag{37}$$

for $u \geq 0$ and

$$\sum_{1 \leq k \leq \tilde{K}_u} \frac{2^{\frac{1}{2}-u}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3 - 2\log 2)\pi)^{k/2} a^k} + \frac{1}{2}(9/10)^{\lceil -u \rceil} \frac{\Gamma((\tilde{K}_u + 1)/2)}{(a/1.1)^{\tilde{K}_u + 1}} \tag{38}$$

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 (38) 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 (37) by

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

thanks to Lemma 4.1(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 (38) 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 4.1(i) we have

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

and thus we can bound (38) 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

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

$$\delta_2 := \int_{\mathbb{R}} \exp\left(\frac{u^2+\frac{5}{6}}{T'-0.33}\right)\frac{0.029\times 2^{-u}}{a-1.25}\frac{1}{\sqrt{\pi t}}e^{-(u-\sigma)^2/t}\,du$$

$$\delta_3 := \int_{\mathbb{R}} \exp\left(\frac{u^2+\frac{5}{6}}{T'-0.33}\right)\frac{2^{-u}}{2}\sum_{\frac{T'}{\pi}\leq k\leq -u+4}(1.1)^k\frac{\Gamma(k/2)}{a^k}\frac{1}{\sqrt{\pi t}}e^{-(u-\sigma)^2/t}\,du. \tag{39}$$

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)

$$\delta_1 = \frac{0.2\times 9^\sigma}{a-0.865}\exp\left(\frac{\sigma^2+\frac{5}{6}}{T'-0.33} + \frac{t(\log 3+\frac{\sigma}{T'-0.33})^2}{1-\frac{t}{T'-0.33}}\right)\left(1-\frac{t}{T'-0.33}\right)^{-1/2}. \tag{40}$$

One can write

$$\frac{1}{1-\frac{t}{T'-0.33}} = 1 + \frac{t}{T'-0.33-t} \leq 1 + \frac{t}{T'-0.83} \tag{41}$$

while by Lemma 4.1(ii) we have

$$1-\frac{t}{T'-0.33} = \exp\left(O_{\leq}\left(\frac{t}{T'-0.33-t}\right)\right) = \exp\left(O_{\leq}\left(\frac{t}{T'-0.83}\right)\right). \tag{42}$$

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 4.1(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 4.1(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 (40), 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 (41), (42) 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 (39) 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 (36), (33) into (35), and crudely bounding $2^{-\sigma}$ by 9^{σ}, we obtain the claim. □

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* $0 \leq y \leq 1$, $x \geq 200$, *and* $0 < t \leq 1/2$. *Set*

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

and then define $a, N, p, U, C_0(p)$ *using* (24), (25), (27), (28). *Define the quantities*

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

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

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

where M_0, b_n^t *were defined in* (18), (19). *Then*

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

where

$$E_A(x+iy) := |M_t(\frac{1-y+ix}{2})|\sum_{n=1}^{N}\frac{b_n^t}{n^{\frac{1-y}{2}+\frac{t}{2}\mathrm{Re}\alpha(\frac{1-y+ix}{2})}}\varepsilon_{t,n}(\frac{1-y+ix}{2})$$

$$E_B(x+iy) := |M_t(\frac{1+y+ix}{2})|\sum_{n=1}^{N}\frac{b_n^t}{n^{\frac{1+y}{2}+\frac{t}{2}\mathrm{Re}\alpha(\frac{1+y+ix}{2})}}\varepsilon_{t,n}(\frac{1+y+ix}{2})$$

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

and $\varepsilon_{t,n}, \tilde{\varepsilon}$ *were defined in* (20), (34).

In our application we will just need the cruder "$A + B$" approximation that is immediate from the above corollary and (33):

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

$$B_0(x+iy) := M_t(\frac{1+y-ix}{2}) \tag{43}$$

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

$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^{N}\frac{b_n^t}{n^{s_*}} + \lambda\sum_{n=1}^{N} n^y \frac{b_n^t}{n^{\overline{s_*}+\kappa}} + O_{\leq}\left(e_A + e_B + e_{C,0}\right) \tag{44}$$

where

$$\lambda := \lambda(x+iy) := \frac{M_t(\frac{1-y+ix}{2})}{M_t(\frac{1+y-ix}{2})} \tag{45}$$

$$s_* = s_*(x+iy) := \frac{1+y-ix}{2} + \frac{t}{2}\alpha(\frac{1+y-ix}{2}) \tag{46}$$

$$\kappa := \kappa(x+iy) := \frac{t}{2}(\alpha(\frac{1-y+ix}{2}) - \alpha(\frac{1+y+ix}{2})) \tag{47}$$

$$e_A := e_A(x+iy) := |\lambda| \sum_{n=1}^N n^y \frac{b_n^t}{n^{\mathrm{Re}(s)+\mathrm{Re}(\kappa)}} \varepsilon_{t,n}(\frac{1-y+ix}{2}) \tag{48}$$

$$e_B := e_B(x+iy) := \sum_{n=1}^N \frac{b_n^t}{n^{\mathrm{Re}(s)}} \varepsilon_{t,n}(\frac{1+y+ix}{2}) \tag{49}$$

$$e_{C,0} := e_{C,0}(x+iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|}(1+\tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2})). \tag{50}$$

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

$$x_N \leq x < x_{N+1} \tag{51}$$

where

$$x_N := 4\pi N^2 - \frac{\pi t}{4}. \tag{52}$$

Similarly one has

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

Proposition 5.6. *Let the notation and hypotheses be as in Corollary 5.4, and let* $\lambda, \kappa, e_A, e_B, e_{C,0}$ *be defined by* (45)-(50).

(i) *One has*

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

(ii) *One has*

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

(iii) *One has*

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

(iv) *One has*

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

(v) *One has*

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

(vi) *One has*

$$e_C \leq \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2 \frac{x}{4\pi}\right)(1.46 + \frac{1.33 \times (3^y + 3^{-y})}{a - 0.125}).$$

Proof. From the mean value theorem we have

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

for some $\frac{1-y}{2} \leq \sigma \leq \frac{1+y}{2}$. From (14), (18) we have

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

From (17) one has

$$\alpha'\left(\sigma + \frac{ix}{2}\right) = O_{\leq}\left(\frac{1}{x-6}\right) \tag{53}$$

and from Taylor expansion we also have

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

from (15) 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

$$\alpha(\sigma + \frac{ix}{2}) = \frac{1}{2}\log\frac{x}{4\pi} + i\frac{\pi}{4} + O_{\leq}\left(\frac{2+\sigma}{x-6}\right). \tag{54}$$

Inserting these bounds, we conclude that

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

Expanding this out, we have

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

With $\sigma \leq 1$, $0 < t \leq 1/2$, and $x \geq 200$ one has

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

and thus

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

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

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

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 (23) to show that

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

By (15) one has

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

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

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

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

Claim (iii) is immediate from (53) and the fundamental theorem of calculus. Now we turn to (iv), (v). From (54) 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

$$|\alpha(\frac{1\pm y+ix}{2}) - \log n|^2 = \frac{1}{4}\log^2\frac{x}{4\pi n^2} + \frac{\pi^2}{16} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2}\right). \tag{55}$$

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

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

since $x \geq 200$ and $0 < t \leq 1/2$, 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

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

and for $x \geq 200$ one can check that $\frac{|\log\frac{x}{4\pi}+i\frac{\pi}{2}|}{x-6}$ is decreasing in x. Thus

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

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

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

We conclude from (20) 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 (48), (49) and using claims (i), (ii), we obtain claims (iv), (v).

Now we establish (vi). From (18) 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 (17) 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 $\log M_0$, we conclude that

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

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

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

and hence

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

By repeating the proof of (55) we have

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

As before we have

$$\frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2} \leq \frac{3|\log\frac{200}{4\pi n^2} + i\frac{\pi}{2}|}{200-6} + \frac{9}{(200-6)^2}$$
$$\leq 0.05$$

and thus

$$\frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} = \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + O_{\leq}\left(0.05 + \frac{3.58}{x-6}\right)\right)$$
$$\leq \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi} + 0.069\right).$$

Finally, since $T' \geq \frac{x}{2} \geq 100$, one has

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

and

$$\frac{5}{3(T' - 3.33)} \leq 0.173$$

and hence by (34)

$$\tilde{\varepsilon}(\frac{1 \pm y + ix}{2}) \leq \frac{1.24 \times 3^{\pm y}}{a - 0.125} + 0.18$$

and hence

$$\exp(0.069)(1 + \tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2})) \leq 1.46 + \frac{1.33 \times (3^y + 3^{-y})}{a - 0.125}$$

giving the claim.

... □

6. Bounding Dirichlet series

...

7. Estimation for small x

...

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 $x \geq 0$ and $0.4 \leq y \leq \frac{1}{\sqrt{5}}$.

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

$$T := \frac{x}{2}$$
$$T' := T + \frac{\pi t}{8} = \frac{x}{2} + \frac{\pi}{20}$$
$$N := \sqrt{\frac{T'}{2\pi}} = \sqrt{\frac{x}{4\pi} + \frac{\pi}{40}}$$

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

8.1. The case of large N: $N \geq 2000$. ...

8.2. The case of medium N: $11 \leq N < 2000$. ...

8.3. The case of small N: $N \leq 10$. ...

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