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

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

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: $F = F^*$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

One can differentiate the expansion (10) term-by-term to conclude that

$$H_t'(z) = \frac{i}{2}\sum_{n=1}^N r_{t,n}'(\frac{1+iz}{2}) - \frac{i}{2}\sum_{n=1}^N (r_{t,n}')^*(\frac{1-iz}{2}) + \frac{i}{2}R_{t,N}'(\frac{1+iz}{2}) - \frac{i}{2}(R_{t,N}')^*(\frac{1-iz}{2}).$$

Differentiating (11), (12) under the integral sign (which can be justified using the Cauchy integral formula and the subgaussian nature of $r_{0,n}, R_{0,N}$) we also obtain the formulae

$$r_{t,n}'(s) = \exp(-\frac{t}{4}\alpha_n^2) \int_{\mathbb{R}} (\alpha_n + \frac{2v}{\sqrt{t}}) \exp(-\sqrt{t}v\alpha_n) r_{0,n}(s + \sqrt{t}v + \frac{t}{2}\alpha_n) \frac{1}{\sqrt{\pi}} e^{-v^2}\, dv \tag{13}$$

and

$$R_{t,N}'(s) = \exp(-\frac{t}{4}\beta_N^2) \int_{\mathbb{R}} (\beta_N + \frac{2v}{\sqrt{t}}) \exp(-\sqrt{t}v\beta_N) R_{0,N}(s + \sqrt{t}v + \frac{t}{2}\beta_N) \frac{1}{\sqrt{\pi}} e^{-v^2}\, dv. \tag{14}$$

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*

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

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

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

(ii) *If $x > 1$, then*

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

or equivalently

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

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

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

(iv) *We have*

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

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

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

(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

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

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

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

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 $\Gamma(\overline{z}) = \overline{\Gamma(z)}$ 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

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

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

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

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

$$|R_2(z)| \leq \frac{0.0205}{|z|^2}$$

and hence by Claim (i)

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

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 estimation of $r_{t,n}, R_{t,N}$

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

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

$$M_0(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \sqrt{2\pi} \exp((\frac{s}{2} - \frac{1}{2}) \log \frac{s}{2} - \frac{s}{2}) \tag{15}$$

defined for all s away from the negative axis. Clearly this function is non-vanishing. We may compute the logarithmic derivative $\alpha := \frac{M_0'}{M_0}$ of this function as

$$\begin{aligned} \alpha(s) &= \frac{1}{s} + \frac{1}{s-1} - \frac{1}{2} \log \pi + \frac{1}{2} \log \frac{s}{2} - \frac{1}{2s} \\ &= \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2} \log \frac{s}{2\pi}. \end{aligned} \tag{16}$$

We can also compute one further derivative:

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

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

$$\begin{aligned} \alpha'(s) &= O_{\leq}(\frac{1}{2\mathrm{Im}\,(s)^2}) + O_{\leq}(\frac{1}{\mathrm{Im}\,(s)^2}) + O_{\leq}(\frac{1}{2\mathrm{Im}\,(s)}) \\ &= O_{\leq}(\frac{1}{2(\mathrm{Im}\,(s) - 3)}) \end{aligned} \tag{18}$$

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

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

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

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

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

$$r_{t,n}(\sigma+iT) = M_t(\sigma+iT)\frac{b_n}{n^{\sigma+iT+\frac{t}{2}\alpha(\sigma+iT)}}(1+O_{\leq}(\exp(\frac{1}{T-3.33}(\frac{t^2}{8}|\alpha(\sigma+iT)-\log n|^2+\frac{t}{4}+\frac{1}{6}))-1))$$

Proof. From (8), (15) and Lemma 4.1(v) one has

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

whenever $\mathrm{Im}(s) > 1$. Set $\alpha_n :=:= \alpha(\sigma+iT) - \log n$ (this is the logarithmic derivative of $M(s)n^{-s}$ at $s = \sigma+iT$). From (11) we have

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

By (16) 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

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

From (18) we have

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

for all s 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

$$M_0(\sigma+iT+\sqrt{t}v+\frac{t}{2}\alpha_n) = M_0(\sigma+iT)\exp(\alpha(\sigma+iT)(\sqrt{t}v+\frac{t}{2}\alpha_n)+O_{\leq}(\frac{1}{4(T-3.08)}|\sqrt{t}v+\frac{t}{2}\alpha_n|^2)).$$

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

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

Writing $\alpha_n = \alpha(\sigma+iT) - \log n$ and using (19) we see that

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

and so it suffices to show that

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

Since $\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv$ integrates to one, it suffices by Lemma 4.1(iv) to show that

$$\int_{\mathbb{R}}\exp(\frac{1}{T-3.08}(\frac{t}{2}v^2+\frac{t^2}{8}|\alpha_n|^2+\frac{1}{6}))\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv \leq \exp(\frac{1}{T-3.33}(\frac{t^2}{8}|\alpha_n|^2+\frac{t}{4}+\frac{1}{6})). \tag{20}$$

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

$$\exp(\frac{1}{T-3.08}(\frac{t^2}{8}|\alpha_n|^2+\frac{1}{6}))(1-\frac{t}{2(T-3.08)})^{-1/2}.$$

Applying Lemma 4.1(ii) and using the hypotheses $t \leq 1/2$, $T \geq 10$, one has

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

and hence (bounding $\frac{1}{T-3.08}$ by $\frac{1}{T-3.33}$), we obtain the claim. □

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*

$$s := \sigma + iT' \tag{21}$$

$$a := \sqrt{\frac{T'}{2\pi}} \tag{22}$$

$$N := \lfloor a \rfloor \tag{23}$$

$$p := 1 - 2(a-N) \tag{24}$$

$$U := \exp(-i(\frac{T'}{2}\log\frac{T'}{2\pi} - \frac{T'}{2} - \frac{\pi}{8})). \tag{25}$$

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

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

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

$$C_0(p) = \frac{e^{\pi i(\frac{p^2}{2}+\frac{3}{8})} - i\sqrt{2}\cos\frac{\pi p}{2}}{2\cos(\pi p)} \tag{26}$$

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

$$|C_k(p,\sigma)| \leq \frac{\sqrt{2}}{2\pi}\frac{9^\sigma\Gamma(k/2)}{2^k} \tag{27}$$

for $\sigma > 0$ and

$$|C_k(p,\sigma)| \leq \frac{2^{\frac{1}{2}-\sigma}}{2\pi}\frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2}} \tag{28}$$

for $\sigma \leq 0$, while the error term $RS_K(s)$ obeys the bounds

$$|RS_K(s)| \leq \frac{1}{7}2^{3\sigma/2}\frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}} \tag{29}$$

for $\sigma \geq 0$, and

$$|RS_K(s)| \leq \frac{1}{2}(\frac{9}{10})^{\lceil -\sigma \rceil}\frac{\Gamma((K+1)/2)}{(a/1.1)^{K+1}} \tag{30}$$

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

$$|C_0(p)| \leq \frac{1}{2} \tag{31}$$

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* (22)*,* (23)*,* (25)*,* (26) *Then*

$$R_{t,N}(\sigma+iT) = (-1)^{N-1} U e^{\pi i\sigma/4} \exp(\frac{t\pi^2}{64}) M_0(iT')(C_0(p)+O_{\leq}((\frac{0.366\times 9^\sigma + 0.887}{a-0.125}+\frac{5}{3(T'-3.33)})\exp(\frac{4.89}{T'-3.33}))).$$

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

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

From (9) we have

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

for any positive integer K_v that we permit to depend on v, where $s_v := \sigma+iT'+\sqrt{t}v$. From (15) and Lemma 4.1(v) we thus have

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

From (18) and Taylor expansion of a logarithm of M, we have

$$M_0(s_v) = M_0(iT')\exp(\alpha(iT')(\sigma+\sqrt{t}v)+O_{\leq}(\frac{1}{4(T'-0.33)}(\sigma+\sqrt{t}v)^2));$$

from (16), (22) one has

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

Bounding $\frac{3}{2T'}$ by $\frac{6}{4(T'-0.33)}$, we conclude that

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

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

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

putting all this together, we obtain

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

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

$$R_{t,N}(\sigma+iT) = (-1)^{N-1} U e^{\pi i\sigma/4} \exp(\frac{t\pi^2}{64}) M_0(iT')(C_0(p)(1+O_{\leq}(\epsilon)) + O_{\leq}(\delta)) \tag{32}$$

where

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

and

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

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

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

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

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

and hence

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

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

$$\epsilon \leq \frac{10}{3(T'-3.33)} \exp(\frac{10}{3(T'-3.33)}). \tag{33}$$

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

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

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 $\lfloor -\sigma \rfloor + 3$ 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

$$\frac{\sqrt{2}}{2\pi}\frac{9^u\Gamma(1/2)}{2a} + \frac{1}{7}2^{3u/2}\frac{\Gamma(1)}{(a/1.1)^2} \leq \frac{0.200\times 9^u}{a} + \frac{0.173\times 2^{3u/2}}{a^2} \tag{34}$$

for $u \geq 0$ and

$$\sum_{1 \leq k \leq \lfloor -u \rfloor + 3} \frac{2^{\frac{1}{2}-\sigma}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2} a^k} + \frac{1}{2}(9/10)^{\lceil -u \rceil} \frac{\Gamma((\lfloor -u \rfloor + 4)/2)}{(a/1.1)^{\lfloor -u \rfloor + 4}} \tag{35}$$

for $u < 0$. One easily verifies that

$$\frac{2^{\frac{1}{2}-\sigma}}{2\pi} \frac{\Gamma(k/2)}{2\pi((3-2\log 2)\pi)^{k/2} a^k} \leq \frac{1}{2}(9/10)^{\lceil -\sigma \rceil} \frac{\Gamma(k/2)}{(a/1.1)^k}$$

and so we can bound (35) by

$$\frac{1}{2}(9/10)^{\lceil -u \rceil} \sum_{1 \leq k \leq -u+4} \frac{\Gamma(k/2)}{(a/1.1)^k}.$$

For $u \geq 0$, we can estimate (34) 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 $k \leq \frac{a^2}{1.21} = \frac{T'}{2.42\pi}$ then

$$\frac{\Gamma(k+2/2)}{(a/1.1)^{k+2}} = \frac{1.21k}{2a^2} \frac{\Gamma(k/2)}{(a/1.1)^k} \leq \frac{1}{2} \frac{\Gamma(k/2)}{(a/1.1)^k}$$

and hence by the geometric series formula

$$\sum_{2 \leq k \leq \frac{T'}{2.42\pi}, k \text{ even}} \frac{\Gamma(k/2)}{(a/1.1)^k} \leq 2 \frac{\Gamma(2/2)}{(a/1.1)^2} = \frac{2.42}{a^2}$$

and similarly

$$\sum_{3 \leq k \leq \frac{T'}{2.42\pi}, k \text{ odd}} \frac{\Gamma(k/2)}{(a/1.1)^k} \leq 2 \frac{\Gamma(3/2)}{(a/1.1)^3} = \frac{1.331\sqrt{\pi}}{a^3}$$

and hence we can bound (35) by

$$\frac{1}{2}(9/10)^{\lceil -u \rceil} (\frac{1.1\sqrt{\pi}}{a} + \frac{2.42}{a^2} + \frac{1.331\sqrt{\pi}}{a^3} + \sum_{\frac{T'}{2.42\pi} \leq k \leq -u+4} \frac{\Gamma(k/2)}{(a/1.1)^k}).$$

By Lemma 4.1(i) we have

$$\frac{1.1\sqrt{\pi}}{a} + \frac{2.42}{a^2} + \frac{1.331\sqrt{\pi}}{a^3} \leq \frac{1.1\sqrt{\pi}}{a - 1.25}$$

and thus (bounding $(9/10)^{\lceil -u \rceil}$ by $1/(1.1)$) we can bound (35) by

$$\frac{1}{2}(\frac{\sqrt{\pi}}{a - 1.25} + \sum_{\frac{T'}{2.2\pi} \leq k \leq -u+4} (1.1)^{k-1} \frac{\Gamma(k/2)}{a^k}).$$

Putting this together, we conclude that

$$\sum_{k=1}^{\tilde{K}_u} \frac{|C_k(p,u)|}{a^k} + |RS_{\tilde{K}_u}(u+iT')| \leq \frac{0.2 \times 9^u}{a - 0.865} + \frac{\sqrt{\pi}}{2(a-1.25)} + \frac{1}{2} \sum_{\frac{T'}{2.2\pi} \leq k \leq -u+4} (1.1)^{k-1} \frac{\Gamma(k/2)}{a^k}$$

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

$$\begin{aligned}
\delta_1 &:= \int_{\mathbb{R}} \exp(\frac{1}{T'-0.33}(u^2+\frac{5}{6}))\frac{\sqrt{\pi}}{2(a-1.25)}\frac{1}{\sqrt{\pi t}}e^{-(u-\sigma)^2/t}\,du\\
\delta_2 &:= \int_{\mathbb{R}} \exp(\frac{1}{T'-0.33}(u^2+\frac{5}{6}))\frac{0.2\times 9^u}{a-0.865}\frac{1}{\sqrt{\pi t}}e^{-(u-\sigma)^2/t}\,du\\
\delta_3 &:= \int_{\mathbb{R}} \exp(\frac{1}{T'-0.33}(u^2+\frac{5}{6}))\frac{1}{2}\sum_{\frac{T'}{2.2\pi}\leq k\leq -u+4}(1.1)^{k-1}\frac{\Gamma(k/2)}{a^k}\frac{1}{\sqrt{\pi t}}e^{-(u-\sigma)^2/t}\,du.
\end{aligned}$$

Using (5), we may evaluate δ_1 exactly as

$$\delta_1 = \frac{\sqrt{\pi}}{2(a-1.25)}\exp(\frac{5}{6(T'-0.33)})(1-\frac{t}{T'-0.33})^{-1/2}.$$

From Lemma 4.1(ii) and the hypothesis $t \leq 1/2$ we have

$$(1-\frac{t}{T'-0.33})^{-1/2} \leq \exp(\frac{t}{2(T'-0.83)}) \tag{36}$$

and hence

$$\delta_1 \leq \frac{\sqrt{\pi}}{2(a-1.25)}\exp(\frac{5+3t}{6(T'-0.83)}).$$

For δ_2, we translate u by σ to obtain

$$\delta_2 = \frac{0.2\times 9^\sigma}{a-0.865}\int_{\mathbb{R}}\exp(\frac{1}{T'-0.33}(u^2+2\sigma u+\sigma^2+\frac{5}{6})+2u\log 3)\frac{1}{\sqrt{\pi t}}e^{-u^2/t}\,du$$

and hence by (5)

$$\delta_2 = \frac{0.2\times 9^\sigma}{a-0.865}\exp(\frac{\sigma^2+\frac{5}{6}}{T'-0.33}+\frac{t(\log 3+\frac{\sigma}{T'-0.33})^2}{1-\frac{t}{T'-0.33}})(1-\frac{t}{T'-0.33})^{-1/2}.$$

One can write

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

and hence by (36)

$$\delta_2 \leq \frac{0.2\times 9^\sigma}{a-0.865}\exp(\frac{5+3t+6\sigma^2}{6(T'-0.83)}+t(\log 3+\frac{\sigma}{T'-0.33})^2(1+\frac{t}{T'-0.83})).$$

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

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

and then

$$(\log 3 + \frac{\sigma}{T' - 0.33})^2(1 + \frac{t}{T' - 0.83}) \leq \log^2 3(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - \frac{2\sigma t/\log 3}{2\sigma/\log 3 + t}})$$
$$\leq \log^2 3(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 0.83 - t})$$
$$\leq \log^2 3(1 + \frac{\frac{2\sigma}{\log 3} + t}{T' - 1.33})$$

and thus

$$\delta_2 \leq \frac{0.2 \times 9^\sigma \exp(t \log^2 3)}{a - 0.865} \exp(\frac{5 + 3t + 6\sigma^2 + 12\sigma \log 3 + 6t \log^2 3}{6(T' - 1.33)}).$$

Now we turn to δ_3. By the Fubini-Tonelli theorem, we have

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

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 $\frac{1}{T'-0.33}(u^2 + \frac{5}{6}) - \frac{u^2}{t}$ by $-\frac{u^2}{2t}$, thus

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

We can bound $e^{-u^2} \leq e^{(k-4)u/2t}$, and thus

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

and thus

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

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

$$\frac{0.2}{a - 0.865} + \frac{2 \times 10^{-30}}{a^{14}} \leq \frac{0.2}{a - 1.25}$$

we have

$$\delta_2 + \delta_3 \leq \frac{0.2 \times 9^\sigma \exp(t \log^2 3)}{a - 0.125} \exp(\frac{5 + 3t + 6\sigma^2 + 12\sigma \log 3 + 6t \log^2 3}{6(T' - 1.33)})$$

and therefore

$$\delta \leq \frac{0.2 \times 9^{\sigma} \exp(t \log^2 3) + \frac{\sqrt{\pi}}{2}}{a - 0.125} \exp(\frac{5 + 3t + 6\sigma^2 + 12\sigma \log 3 + 6t \log^2 3}{6(T' - 1.33)}).$$

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

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

$$\frac{\sqrt{\pi}}{2} \leq 0.887$$

$$\frac{5 + 3t + 6\sigma^2 + 12\sigma \log 3 + 6t \log^2 3}{6} \leq 4.89$$

and hence

$$\delta \leq \frac{0.366 \times 9^{\sigma} + 0.887}{a - 0.125} \exp(\frac{4.89}{T' - 1.33}).$$

Inserting this and (33), (31) into (32) we obtain the claim. □

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