# 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  $\Phi$  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  $\Lambda$  (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  $\Lambda \le 0$ , and Newman conjectured the complementary bound  $\Lambda \ge 0$ .

#### ...

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

It is a classical fact (see [20, p. 255]) that  $H_0$  has the Fourier representation

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

where  $\Phi$  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  $\Phi$  satisfies the functional equation  $\Phi(u) = \Phi(-u)$  (i.e.,  $\Phi$  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 [15] 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  $\xi$ -function. From [20, (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

$$R_{0,0}(s) := \frac{1}{8} \frac{s(s-1)}{2} \pi^{-s/2} \Gamma\left(\frac{s}{2}\right) \int_{0, t_1} \frac{w^{-s} e^{i\pi w^2}}{e^{\pi i w} - e^{-\pi i w}} dw$$

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  $\alpha_n$  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  $\beta_N$  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  $\alpha_n$ ,  $\beta_N$  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

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

(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), (3.1), (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

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

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  $\Gamma$  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  $\sigma$  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  $\alpha_n$  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  $\alpha_n$  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

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

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  $\int_{N \swarrow N+1} \frac{w^{-s}e^{i\pi v^2}}{e^{\pi iw}-e^{-\pi iw}}$  appearing in (9):

**Proposition 5.2.** Let  $\sigma$  be real and T' > 0, and define the quantities

$$(24) s \coloneqq \sigma + iT'$$

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

$$(26) N \coloneqq \lfloor a \rfloor$$

$$(27) p := 1 - 2(a - N)$$

(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  $\sigma$  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

(30) 
$$|C_k(p,\sigma)| \le \frac{\sqrt{2}}{2\pi} \frac{9^{\sigma} \Gamma(k/2)}{2^k}$$

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<sub>K</sub>(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  $\sigma$  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

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

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  $\delta$ . 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

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

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

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

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  $\delta_1$ , we translate u by  $\sigma$  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  $\delta_3$ , which will end up being extremely small compared to  $\delta_1$  or  $\delta_2$ . 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  $9^{\sigma}$ , 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

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

where

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

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

In our application we will just need 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

$$H_t(x+iy) = A(x+iy) + B(x+iy) + O_{<}(E_A(x+iy) + E_B(x+iy) + E_{C,0}(x+iy))$$

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

(45) 
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{S_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{S_*}+\kappa}} + O_{\leq}(e_A + e_B + e_{C,0})$$

where

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

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

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

(49) 
$$e_A := e_A(x+iy) := |\gamma| \sum_{n=1}^N n^y \frac{b_n^t}{n^{\operatorname{Re}(s) + \operatorname{Re}(\kappa)}} \varepsilon_{t,n}(\frac{1-y+ix}{2})$$

(50) 
$$e_B := e_B(x+iy) := \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s)}} \varepsilon_{t,n} (\frac{1+y+ix}{2})$$

(51) 
$$e_{C,0} := e_{C,0}(x+iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} (1 + \tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2})).$$

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

$$(52) x_N \le x < x_{N+1}$$

where

$$(53) x_N \coloneqq 4\pi N^2 - \frac{\pi t}{4}$$

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  $\gamma$ ,  $\kappa$ ,  $e_A$ ,  $e_B$ ,  $e_{C,0}$  be defined by (46)-(51).

(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

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

(vi) One has

$$e_{C,0} \le \left(\frac{T'}{2\pi}\right)^{-\frac{1+y}{4}} \exp\left(-\frac{t}{16}\log^2\frac{x}{4\pi}\right) (1.46 + \frac{1.33 \times (3^y + 3^{-y})}{a - 0.125}).$$

*Proof.* From the mean value theorem we have

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

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

(54) 
$$\alpha'\left(\sigma + \frac{ix}{2}\right) = O_{\leq}\left(\frac{1}{x - 6}\right)$$

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

(55) 
$$\alpha(\sigma + \frac{ix}{2}) = \frac{1}{2}\log\frac{x}{4\pi} + i\frac{\pi}{4} + O_{\leq}\left(\frac{2+\sigma}{x-6}\right).$$

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  $\alpha$  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 (54) and the fundamental theorem of calculus. Now we turn to (iv), (v). From (55) 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

$$(56) \qquad |\alpha(\frac{1\pm y+ix}{2}) - \log n|^2 = \frac{1}{4}\log^2\frac{x}{4\pi n^2} + \frac{\pi^2}{16} + O_{\leq}\left(\frac{3|\log\frac{x}{4\pi n^2} + i\frac{\pi}{2}|}{x-6} + \frac{9}{(x-6)^2}\right).$$

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 (49), (50) 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

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

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 (56) 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

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

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  $T' \ge \frac{x}{2} \ge 100$  in (13), one has

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

and

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

and hence by (35)

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

and hence

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

giving the claim.

#### 6. Bounding Dirichlet series

In view of the approximation (45), it is of interest to obtain lower bounds for the quantity

(57) 
$$X := \left| \sum_{n=1}^{N} \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^{N} n^y \frac{b_n^t}{n^{\overline{s_*} + \kappa}} \right|$$

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

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

It is thus of interest to obtain lower bounds for differences

(58) 
$$\Delta := \left( \left| \sum_{n=1}^{N} \frac{\beta_n}{n^s} \right| - \left| \sum_{n=1}^{N} \frac{\alpha_n}{n^s} \right| \right)_{+}$$

of magnitudes of Dirichlet series for various coefficients  $\beta_n$ ,  $\alpha_n$ . 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  $\sigma, T$ , and let  $\alpha_n, \beta_n$  be complex numbers for n = 1, ..., N with  $\beta_1 = 1$ . Let  $\Delta$  denote the quantity (58).

(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  $\alpha_n, \beta_n$  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  $\alpha_n$ ,  $\beta_n$  with the  $\lambda_d$ :

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

*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  $\beta_n$ ,  $\alpha_n$  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  $\Delta$  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  $\theta$ . By the triangle inequality, we then have

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

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

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

By the cosine rule, we have

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

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

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

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  $\tilde{\Delta}$ ,  $\Delta$  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 (57), we conclude from Lemma 6.1(i) with s replaced by  $s_*$ ,  $\beta_n$  replaced by  $b_n^t$ , and  $\alpha_n$  replaced by  $|\gamma|n^{\gamma-\overline{k}}b_n^t$  that

(59) 
$$X \ge 1 - |\gamma| - \sum_{n=2}^{N} \frac{b_n^t}{n^{\sigma}} (1 + |\gamma| n^{y - \operatorname{Re}(\kappa)}),$$

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  $|\lambda| n^{y-\bar{k}} b_n^t$  quantity need not be real, so that Lemma 6.1(ii) is not directly available. However, by writing

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

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

(60) 
$$X \ge \frac{1 - \tilde{\alpha}_1 - \sum_{n=2}^{N} \frac{\max(|\tilde{\beta}_n - \tilde{\alpha}_n|, \frac{1 - \tilde{\alpha}_1}{1 + \tilde{\alpha}_1}|\tilde{\beta}_n + \tilde{\alpha}_n|)}{n^{\sigma}} - |\gamma| \sum_{n=1}^{N} \frac{b_n^t(n^{|\kappa|} - 1)}{n^{\sigma - y}}$$

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

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

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

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

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  $\lambda_d$  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 (60) 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

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

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  $\Phi$  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

(62) 
$$H'_t(z) = \frac{i}{2} \int_{i\theta}^{i\theta + \infty} e^{tu^2} \Phi(u) u e^{izu} du - \frac{i}{2} \overline{\int_{i\theta}^{i\theta + \infty} e^{tu^2} \Phi(u) u e^{i\overline{z}u} du}.$$

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

(63)

$$\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)} \\ &= \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)} \\ &= \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)} \\ &= \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)} \\ &= \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)} \\ &= \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)} \\ &= \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-(9-y)i,\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-(9-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-(9-y)i,\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-(9-y)i,\pi n^2) + 2\pi^2 n^4 I_{t,$$

and

(64)

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

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

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

(65) 
$$I_{t,\theta}(b,\beta) := \int_{i\theta}^{i\theta+\infty} \exp(tu^2 - \beta e^{4u} + ibu) du$$

(66) 
$$J_{t,\theta}(b,\beta) := \int_{i\theta}^{i\theta+\infty} \exp(tu^2 - \beta e^{4u} + ibu)u \ du.$$

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

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

for any cutoff  $X \ge 0$ , where

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

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

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

**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

(67) 
$$|I_{t,\theta,\leq X}(b,\beta)| \leq \exp(-t\theta^2 - \theta x) \int_0^X \exp(tv^2 - \beta e^{4v} \cos(4\theta) + av) du$$

and

(68) 
$$|J_{t,\theta,\leq X}(b,\beta)| \leq \exp(-t\theta^2 - \theta x) \int_0^X \exp(tv^2 - \beta e^{4v} \cos(4\theta) + av)(\theta^2 + u^2)^{1/2} du.$$

(ii) If one has the hypothesis

(69) 
$$\beta e^{4X} \cos(4\theta) > \max(\frac{t}{2}, \frac{a + 2tX}{4})$$

then one has

(70) 
$$|I_{t,\theta,\geq X}(b,\beta)| \leq \frac{\exp(-t\theta^2 + tX^2 - \beta e^{4X}\cos(4\theta) - \theta x + aX)}{4\beta e^{4X}\cos(4\theta) - a - 2tX}$$

and similarly

(71)

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

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

(72) 
$$\beta \cos(4\theta) > \max(\frac{t}{2}, \frac{a}{4})$$

then

(73) 
$$|I_{t,\theta}(b,\beta)| \le \frac{\exp(-t\theta^2 - \beta\cos(4\theta) - \theta x)}{4\beta\cos(4\theta) - a}$$

and similarly

$$(74) \qquad |J_{t,\theta}(b,\beta)| \le \exp(-t\theta^2 - \beta\cos(4\theta) - \theta x) \left(\frac{\theta}{4\beta\cos(4\theta) - a} + \frac{1}{(4\beta\cos(4\theta) - a)^2}\right).$$

In practice, the tail estimates (70), (71) become useful when  $\theta$  is close to  $\pi/8$  (to get the most gain out of the  $\exp(-\theta x)$  factor), and X is large. Similarly, (73), (74) become useful when  $\theta$  is close to  $\pi/8$  and  $\beta$  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 (67) then follows from the triangle inequality. The claim (68) is proven similarly, with an additional factor of  $i\theta + v = O_{<}((\theta^2 + v^2)^{1/2})$  in the integrand.

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

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

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 (72), 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 (70), (71) 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 (73), (74).

**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

(75)

$$\begin{split} \left| \sum_{n \geq n_0} 2\pi^2 n^4 I_{t,\theta}(x - ia, \pi n^2) \right| &\leq \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2 \cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \\ &\times \left( \frac{n_0^4}{1 - \alpha} + \frac{4n_0^3 \alpha}{(1 - \alpha)^2} + \frac{6n_0^2 (\alpha^2 + \alpha)}{(1 - \alpha)^3} + \frac{4n_0 (\alpha^3 + 4\alpha^2 + \alpha)}{(1 - \alpha)^4} + \frac{\alpha^4 + 11\alpha^3 + 11\alpha^2 + \alpha}{(1 - \alpha)^5} \right) \end{split}$$

and

(76) 
$$\left| \sum_{n \ge n_0} 3\pi n^2 I_{t,\theta}(x - ia, \pi n^2) \right| \le \frac{3\pi \exp(-t\theta^2 - \theta x - \pi n_0^2 \cos(4\theta))}{4\pi n_0^2 \cos(4\theta) - a} \times \left( \frac{n_0^2}{1 - \alpha} + \frac{2n_0\alpha}{(1 - \alpha)^2} + \frac{\alpha^2 + \alpha}{(1 - \alpha)^3} \right)$$

where  $\alpha := e^{-\pi n_0 \cos(4\theta)}$ . Similarly one has

(77)

$$\begin{split} |\sum_{n\geq n_0} 2\pi^2 n^4 J_{t,\theta}(x-ia,\pi n^2)| &\leq 2\pi^2 \exp(-t\theta^2 - \pi n_0^2 \cos(4\theta) - \theta x) (\frac{\theta}{4\pi n_0^2 \cos(4\theta) - a} + \frac{1}{(4\pi n_0^2 \cos(4\theta) - a)^2}) \\ &\qquad \times (\frac{n_0^4}{1-\alpha} + \frac{4n_0^3\alpha}{(1-\alpha)^2} + \frac{6n_0^2(\alpha^2 + \alpha)}{(1-\alpha)^3} + \frac{4n_0(\alpha^3 + 4\alpha^2 + \alpha)}{(1-\alpha)^4} + \frac{\alpha^4 + 11\alpha^3 + 11\alpha^2 + \alpha}{(1-\alpha)^5}) \end{split}$$

and

(78)

$$\begin{split} |\sum_{n\geq n_0} 3\pi n^2 J_{t,\theta}(x-ia,\pi n^2)| &\leq 3\pi \exp(-t\theta^2 - \pi n_0^2 \cos(4\theta) - \theta x) (\frac{\theta}{4\pi n_0^2 \cos(4\theta) - a} + \frac{1}{(4\pi n_0^2 \cos(4\theta) - a)^2}) \\ &\qquad \times (\frac{n_0^2}{1-\alpha} + \frac{2n_0\alpha}{(1-\alpha)^2} + \frac{\alpha^2 + \alpha}{(1-\alpha)^3}). \end{split}$$

Proof. From (73) one has

$$\begin{split} |\sum_{n\geq n_0} 2\pi^2 n^4 I_{t,\theta}(x-ia,\pi n^2)| &\leq \sum_{n\geq n_0} 2\pi^2 n^4 \frac{\exp(-t\theta^2 - \pi n^2\cos(4\theta) - \theta x)}{4\pi n^2\cos(4\theta) - a} \\ &\leq \frac{2\pi^2 \exp(-t\theta^2 - \theta x)}{4\pi n_0^2\cos(4\theta) - a - 2tX} \sum_{n\geq n_0} n^4 \exp(-\pi n n_0\cos(4\theta)) \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2\cos(4\theta) - a} \sum_{m=0}^{\infty} (n_0^4 + 4n_0^3 m + 6n_0^2 m^2 + 4n_0 m^3 + m^4) \alpha^m \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2\cos(4\theta) - a} \\ &= \frac{2\pi^2 \exp(-t\theta^2 - \theta x - \pi n_0^2\cos(4\theta))}{4\pi n_0^2\cos(4\theta) - a} \\ &\times (\frac{n_0^4}{1 - \alpha} + \frac{4n_0^3 \alpha}{(1 - \alpha)^2} + \frac{6n_0^2(\alpha^2 + \alpha)}{(1 - \alpha)^3} + \frac{4n_0(\alpha^3 + 4\alpha^2 + \alpha)}{(1 - \alpha)^4} + \frac{\alpha^4 + 11\alpha^3 + 11\alpha^2 + \alpha}{(1 - \alpha)^5}) \end{split}$$

giving (75) as desired, where we use the Euler number identities

$$\sum_{m=0}^{\infty} \alpha^m = \frac{1}{1-\alpha}$$

$$\sum_{m=0}^{\infty} m\alpha^m = \frac{\alpha}{(1-\alpha)^2}$$

$$\sum_{m=0}^{\infty} m^2 \alpha^m = \frac{\alpha^2 + \alpha}{(1-\alpha)^3}$$

$$\sum_{m=0}^{\infty} m^3 \alpha^m = \frac{\alpha^3 + 4\alpha^2 + \alpha}{(1-\alpha)^4}$$

$$\sum_{m=0}^{\infty} m^4 \alpha^m = \frac{\alpha^4 + 11\alpha^3 + 11\alpha^2 + \alpha}{(1-\alpha)^5}.$$

The estimates (76), (77), (78) 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  $H_{0.2} = \frac{1}{8}\xi\left(\frac{1+iz}{2}\right)$  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

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

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

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

$$N := |a|$$

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  $0 \le y \le 10$ .

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

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

for an absolute constant c > 0, where  $\gamma$  is defined in (46).

(ii) If instead we have  $5 \le y \le 10$  and  $x \ge C$  for a sufficiently large absolute constant C, then

$$\frac{H_t(x+iy)}{B_0(x+iy)} = 1 + O_{\le}(0.7).$$

*Proof.* We begin with (i). We apply the decomposition (45) followed by Proposition 5.6. (Strictly speaking, the estimates there required  $y \le 1$  rather than  $y \le 10$ ; 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

(79) 
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{s_*}+\kappa}} + O_{\leq}(e_A + e_B + e_{C,0})$$

where

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

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

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

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

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

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

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

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

so it will suffice 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

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

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 (79). We have

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

$$= O(x^{-y/2} \sum_{n=1}^{N} \frac{1}{n^{\frac{1-y}{2}}})$$

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

since  $y \ge 5$ ; similar arguments give  $e_A$ ,  $e_B = O(\frac{\log^2 x}{x})$ . We conclude that

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

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

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

**Corollary 9.2.** 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  $4\pi$  such that

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

(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  $x + iy = x_n + O_{\le}(\frac{c}{\log x_n})$ . By Proposition 9.1(i), (46), (44) one has

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

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

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

Using (18) and Taylor expansion, and also bounding

(81) 
$$\alpha(s) = \frac{1}{2} \log \frac{x_n}{4\pi} + \frac{\pi i}{4} + O(\frac{1}{x_n}) = \frac{1}{2} \log x_n + O(1)$$

when  $s = \frac{ix_n}{2} + O(1)$ , we conclude that

$$M_t(\frac{1+y+ix}{2}) = M_t(\frac{1+ix_n}{2}) \exp(\frac{i(x-x_n)+y}{4} \log x_n + O(\frac{1}{\log x_n}))$$

and similarly

$$M_t(\frac{1-y+ix}{2}) = M_t(\frac{1+ix_n}{2}) \exp(\frac{i(x-x_n)-y}{4} \log x_n + O(\frac{1}{\log x_n}))$$

and hence

$$H_t(x+iy) = \overline{M_t(\frac{1+ix_n}{2})} \exp(\frac{-i(x-x_n)+y}{4}\log x_n) + M_t(\frac{1-y+ix}{2}) \exp(\frac{i(x-x_n)-y}{4}\log x_n) + O(\frac{1}{\log x_n}|M_t(\frac{1+ix_n}{2})|).$$

Now we investigate the argument of  $M_t(\frac{1+ix_n}{2})$  modulo  $\pi$ . From (19), (16), (14), (81) we have

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

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

$$= \frac{t\pi}{16}\log\frac{x_{n}}{4\pi} - \frac{x_{n}}{4}\log\pi + \frac{x_{n}}{4}\log\frac{x_{n}}{4} - \frac{\pi}{8} + O(\frac{\log x_{n}}{x_{n}}) \bmod\pi$$

$$= \frac{t\pi}{16}\log\frac{x_{n}}{4\pi} - \frac{\pi}{8} + \frac{x_{n}}{4}\log\frac{x_{n}}{4\pi} - \frac{x_{n}}{4} + O(\frac{\log x_{n}}{x_{n}}) \bmod\pi$$

$$= \pi n + \frac{5\pi}{8} - \frac{\pi}{8} + O(\frac{\log x_{n}}{x_{n}}) \bmod\pi$$

$$= \frac{\pi}{2} + O(\frac{\log x_{n}}{x_{n}}) \bmod\pi$$

and thus

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

We conclude that

$$H_t(x+iy) = M_t(\frac{1+ix_n}{2})(\exp(\frac{i(x-x_n)-y}{4}\log x_n) - \exp(\frac{-i(x-x_n)+y}{4}\log x_n) + O(\frac{1}{\log x_n}))$$

$$= 2iM_t(\frac{1+ix_n}{2})(\sin(\frac{(x+iy-x_n)\log x_n}{4}) + O(\frac{1}{\log x_n})).$$

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, 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  $x \ge \exp(\frac{C}{t})$ . By symmetry we may assume  $y \ge 0$ . We can assume  $y \le 1$  since it is known (e.g., from [3, Theorem 13]) that there are no zeroes with y > 1.

By Proposition 9.1(i) we then have

$$1 + \gamma + O(x^{-ct}) = 0$$

for some small absolute constant c > 0. On the other hand, from Proposition 5.6 we have  $\gamma = O(x^{-y/2})$ . This forces  $y = O(\frac{1}{\log x})$  (if C is large enough). Next, we apply (46) to conclude that

$$\overline{M_t(\frac{1+y+ix}{2})} + M_t(\frac{1-y+ix}{2}) = O(x^{-ct}|M_t(\frac{1+y+ix}{2})|).$$

By (80), (18), (81) as before, we have

$$M_t(\frac{1+y+ix}{2}) = M_t(\frac{1+ix}{2}) \exp(\frac{y}{4} \log \frac{x}{4\pi} + \frac{\pi i y}{8} + O(\frac{1}{x}))$$

and similarly

$$M_t(\frac{1-y+ix}{2}) = M_t(\frac{1+ix}{2}) \exp(-\frac{y}{4} \log \frac{x}{4\pi} - \frac{\pi i y}{8} + O(\frac{1}{x}))$$

and hence

$$\frac{\overline{M_t(\frac{1+ix}{2})}}{M_t(\frac{1+ix}{2})} + \exp(-\frac{y}{2}\log\frac{x}{4\pi}) = O(x^{-ct}).$$

This implies in particular that

$$\arg M_t(\frac{1+ix}{2}) = \frac{\pi}{2} + O(x^{-ct}) \bmod \pi$$

and that  $\frac{y}{2} \log \frac{x}{4\pi} = O(x^{-ct})$ , and hence  $y = O(\frac{x^{-ct}}{\log x})$ . Repeating the calculations used to prove (ii), we also have

$$\arg M_t(\frac{1+ix}{2}) = \frac{t\pi}{16} \log \frac{x}{4\pi} - \frac{\pi}{8} + \frac{x}{4} \log \frac{x}{4\pi} - \frac{x}{4} + O(\frac{\log x}{x}) \bmod \pi$$

and hence

$$\frac{x}{4\pi} \log \frac{x}{4\pi} - \frac{x}{4\pi} + \frac{3}{8} + \frac{t}{16} \log \frac{x}{4\pi} = n + O(x^{-ct})$$

for some natural number n. As the left-hand side has derivative positive comparable to  $\log x$ , we conclude in particular that

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

Applying part (ii) we now know that the zero is real, so y = 0 as claimed.

Finally, we prove (iii). In view of parts (i) and (ii), and adjusting C if necessary, we may assume that X takes the form  $X = x_n + \varepsilon$  for some  $n \ge \exp(\frac{C}{t})$  and some arbitrarily small  $\varepsilon$ . 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  $\{x + iy : 0 \le x \le X; -5 \le y \le 5\}$ , since there are no zeroes with imaginary part of magnitude greater than one. By compactness, the variation on the left edge  $\{iy : -5 \le y \le 5\}$  is O(1). From Proposition 9.1 (and the previously obtained asymptotics for  $H_t$  near  $x_n$ ), we see that the variation of  $H_t/B_0$  on the upper edge  $\{x + 5i : 0 \le x \le X\}$  and on the top half  $\{X + iy : 0 \le y \le 5\}$  of the right edge are both equal to O(1). We thus conclude that

$$N_t(X) = \frac{1}{\pi} \arg B_0(X) + O(1)$$

where we use a continuous branch of the argument of  $B_0$  that is bounded at 5i. By (44), (19), (14), we thus have

$$N_t(X) = \frac{1}{\pi} \text{Im}(\frac{t}{4}\alpha(\frac{1+iX}{2})^2 - \frac{X}{4}\log\pi + \frac{-1+iX}{4}\log\frac{1+iX}{4} - \frac{1+iX}{4}) + O(1)$$

and by repeating the calculations used in (i) we obtain the claim.

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