# 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

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

From the work of de Bruijn and Newman, 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 equivalent to the assertion  $\Lambda \le 0$ ; recently, Rodgers and Tao established the matching lower bound  $\Lambda \ge 0$ . Ki, Kim and Lee established the upper bound  $\Lambda < \frac{1}{2}$ .

In this paper we establish several effective estimates on  $H_t(x + iy)$ , including some that are accurate for small or medium values of x. By combining these estimates with numerical computations, we are able to obtain a new upper bound  $\Lambda \le 0.22$ ; we also obtain some new estimates controlling the asymptotic behavior of zeroes of  $H_t(x + iy)$  as  $x \to \infty$ .

## 1. Introduction

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

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

where  $\xi$  denotes the Riemann xi function

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

(after removing all singularities) and  $\zeta$  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 [24, 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 [4] 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 [8, p.114], one can view  $H_t$  as the evolution of  $H_0$  under the backwards heat equation  $\partial_t H_t(z) = -\partial_{zz} H_t(z)$ . As with  $H_0$ , each of the  $H_t$  are entire even functions with functional equation  $H_t(\overline{z}) = \overline{H_t(z)}$ ; from the super-exponential decay of  $e^{tu^2}\Phi(u)$  we see that the  $H_t$  are in fact entire of order 1. It follows from the work of Pólya [18] that if  $H_t$  has purely real zeroes for some t, then  $H_{t'}$  has purely real zeroes for all t' > t; de Bruijn showed that the zeroes of  $H_t$  are purely real for  $t \ge 1/2$ . Newman [13] 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 [19] the complementary bound  $\Lambda \ge 0$  was established, answering a conjecture of Newman [13], and improving upon several previous lower bounds for  $\Lambda$  [5, 14, 7, 6, 15, 20]. Furthermore, Ki, Kim, and Lee [9] sharpened the upper bound  $\Lambda \le 1/2$  of de Bruijn [4] slightly to  $\Lambda < 1/2$ .

In this paper we improve the upper bound:

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

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

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

- (i) (Numerical verification of RH at initial time 0) There are no zeroes ζ(σ + iT) = 0 with <sup>1+y<sub>0</sub></sup>/<sub>2</sub> ≤ σ ≤ 1 and 0 ≤ T ≤ <sup>X</sup>/<sub>2</sub>.
   (ii) (Asymptotic zero-free region at final time t<sub>0</sub>) There are no zeroes H<sub>t<sub>0</sub></sub>(x + iy) = 0 with
- (ii) (Asymptotic zero-free region at final time t<sub>0</sub>) There are no zeroes H<sub>t0</sub>(x + iy) = 0 with x ≥ X + √1 y<sub>0</sub><sup>2</sup> and y<sub>0</sub> ≤ y ≤ √1 2t<sub>0</sub>.
   (iii) (Barrier at intermediate times) There are no zeroes H<sub>t</sub>(x + iy) = 0 with X ≤ x ≤
- (iii) (Barrier at intermediate times) There are no zeroes  $H_t(x + iy) = 0$  with  $X \le x \le X + \sqrt{1 y_0^2}$ ,  $\sqrt{y_0^2 + 2(t_0 t)} \le y \le \sqrt{1 2t}$ , and  $0 \le t \le t_0$ .

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

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

We will obtain Theorem 1.1 by applying Theorem 1.2 with the specific numerical choices  $t_0 = 0.2$ ,  $X = 6 \times 10^{10} + 83952 - 0.5$ , and  $y_0 = 0.2$ . The reason we choose X close to  $6 \times 10^{10}$ 

is that this is near the limit of known numerical verifications of the Riemann hypothesis such as [17], which we need for the hypothesis (i) of the above theorem; the shift 83952 - 0.5 is in place to make the partial Euler product  $\prod_{p \le 11} (1 - \frac{1}{n^{\frac{1-iX}{2}}})^{-1}$  large, which helps in keeping the functions

 $H_t(x+iy)$ ,  $H_{t_0}(x+iy)$  large in magnitude, which in turn is helpful for numerical verifications of (ii) and (iii). The choices  $t_0 = 0.2$ ,  $y_0 = 0.2$  are then close to the limit of our ability to numerically verify hypothesis (ii) for this choice of X. (The hypothesis (iii) is also verified numerically, but can be done relatively quickly compared to (ii), and so does not present the main bottleneck to further improvements to Theorem 1.1.)

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

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

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

We will need some notation to describe the approximations of  $H_t(x + iy)$  we will use in this paper. We will need the function  $M_0 : \mathbb{C} \setminus (-\infty, 1] \to \mathbb{C} \setminus \{0\}$  defined by the formula

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

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

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

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

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

is given explicitly by the formula

(9) 
$$\alpha(s) = \frac{1}{s} + \frac{1}{s-1} - \frac{1}{2}\log\pi + \frac{1}{2}\log\frac{s}{2} - \frac{1}{2s}$$
$$= \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2}\log\frac{s}{2\pi}.$$

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

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

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

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

As it turns out,  $B_t(x + iy)$  is an asymptotic approximation to  $H_t(x + iy)$  in the region (5), in the sense that

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

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

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

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

where

(14) 
$$f_t(x+iy) := \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{s_*}+\kappa}}$$

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

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

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

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

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

and  $e_A$ ,  $e_B$ ,  $e_{C,0}$  are certain explicitly computable positive quantities<sup>1</sup> depending on t and x + iy. Furthermore, we have the following bounds:

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

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

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

$$(23) e_A + e_B \le \sum_{n=1}^{N} (1 + |\gamma| N^{|\kappa|} n^{\gamma}) \frac{b_n^t}{n^{\text{Re}(s_*)}} \left( \exp\left(\frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi n^2} + 0.626}{x - 6.66}\right) - 1 \right)$$

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

<sup>&</sup>lt;sup>1</sup>See (71)-(74) for the precise definition of these quantities.

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

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

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

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

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

In the asymptotic limit  $x \to \infty$ , one easily sees that  $e_A + e_B = O(\frac{\log^2 x}{x})$ ,  $e_{C,0} = O(x^{-\frac{3+y}{4}} \exp(-\frac{t}{16}\log^2 x))$ , and  $f_t(x+iy) = 1 + O(x^{-\frac{t}{4}\log 2})$ , thus giving the cruder asymptotic (12) in the region (5) at least. In practice, the  $e_{C,0}$  term numerically dominates the  $e_A + e_B$  term, although both errors will be quite small in the ranges of x under consideration; in particular, for the ranges needed to verify conditions (ii) and (iii) of Theorem 1.2, we can make  $e_A + e_B$  and  $e_{C,0}$  both significantly smaller than  $|f_t(x+iy)|$ . In the spirit of expanding the Riemann-Siegel approximation to higher order, we also obtain an even more accurate explicit approximation in which a correction term is added to  $f_t$ , and the error term  $e_{C,0}$  is replaced by a smaller quantity  $e_C$ .

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

**Theorem 1.5** (Distribution of zeroes of  $H_t$ ). Let  $0 < t \le 1/2$ , let C > 0 be a sufficiently large absolute constant, and let c > 0 be a sufficiently small absolute constant. For all  $n \ge C$ , let  $x_n$  be the unique real number greater than  $4\pi$  such that

(26) 
$$\frac{x_n}{4\pi} \log \frac{x_n}{4\pi} - \frac{x_n}{4\pi} + \frac{11}{8} + \frac{t}{16} \log \frac{x_n}{4\pi} = n.$$

(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

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

for some n.

- (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 (counting multiplicity) is

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

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

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

and

$$N_t(X) = \frac{X}{4\pi} \log \frac{X}{4\pi} - \frac{X}{4\pi} + O(\log(2+X)).$$

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

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

$$N_t(X) = \lfloor \frac{X}{4\pi} \log \frac{X}{4\pi} - \frac{X}{4\pi} + \frac{11}{8} + \frac{t}{16} \log \frac{X}{4\pi} + O(X^{-ct}) \rfloor$$

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

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

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

The results in Theorem 1.5 refine previous results of Ki, Kim, and Lee [9, Theorems 1.3, 1.4], which gave similar results but with constants that depended on t in a non-uniform (and ineffective) fashion, and error terms that were of shape o(1) rather than  $O(x^{-ct})$  in the limit  $x \to \infty$  (holding t fixed). The results may also be compared with those in [2], who (in our notation) show that assuming RH, the zeroes of  $H_0$  are precisely the solutions  $x_n$  to the equation

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

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

## 2. Notation

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

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

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

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

If F is a meromorphic function, we use F' to denote its derivative. We also use  $F^*$  to denote the reflection  $F^*(s) := \overline{F(s)}$  of F. Observe from analytic continuation that if  $F: \Omega \to \mathbb{C}$  is

holomorphic on a connected open domain  $\Omega \subset \mathbb{C}$  containing an interval in  $\mathbb{R}$ , and is real-valued on  $\Omega \cap \mathbb{R}$ , then it is equal to its own reflection:  $F = F^*$  (since the holomorphic function  $F - F^*$  has an uncountable number of zeroes).

## 3. Dynamics of zeroes

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

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

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

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

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

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

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

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

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

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

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

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

The differential equation (28) was previously derived in [8, Lemma 2.4] in the case  $t > \Lambda$  (in which all zeroes are real and simple). The  $x_1, \ldots, x_m$  can be given explicitly for small values of m as

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

when m = 2,

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

when m = 3, and

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

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

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

$$H_t(z_i(t)) = 0$$

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

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

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

$$\frac{\partial H_t}{\partial t} = -H_t^{"}$$

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

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

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

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

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

$$H_t(z) = H_t(0) \prod_{t=1}^{r} \left(1 - \frac{z}{z_k}\right),\,$$

where the prime indicates that the k and -k factors are multiplied together. Note that the product converges absolutely since the number of zeroes in D(0,R) grows like  $O(R^{1+o(1)})$ . Taking logarithmic derivatives, we conclude that

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

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

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

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

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

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

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

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

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

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

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

Next, we recall the following bound of de Bruijn:

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

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

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

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

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

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

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

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

for some 0 < x < X.

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

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

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

The right-hand side of (34) is

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

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

$$2\sum_{k\neq i}' \frac{Y(t_1) - y_k}{(x - x_k)^2 + (Y(t_1) - y_k)^2}$$

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

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

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

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

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

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

#### 4. Applying the fundamental solution for the heat equation

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

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

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

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

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

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

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

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

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

We now combine this formula with expansions of the Riemann  $\xi$ -function. From [24, (2.10.6)] we have the Riemann-Siegel formula

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

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

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

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

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

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

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

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

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 (35), (36) we conclude that

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

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

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

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

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

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 integrands in (40), (41) close to stationary in phase, in order to obtain good estimates and approximations for these terms.

# 5. Elementary estimates

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

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

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

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

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

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

whenever  $0 \le t < x$ .

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  $\text{Im}(z) \ge 0$ . From the work of Boyd [3, (1.13), (3.1), (3.14), (3.15)] we have the effective Stirling approximation

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

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

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

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

### 6. Estimates for large *x*

We can now begin the proof of Theorem 1.3. The strategy is to use the expansion (39), which turns out to be an effective approximation in the region (5), since we will be able to ensure that quantities such as  $s + \sqrt{t}v + \frac{t}{2}\alpha_n$  or  $s + \sqrt{t}v + \frac{t}{2}\beta_N$ , with  $s = \frac{1+i(x+iy)}{2}$ , stay away from the real axis where the poles of  $\Gamma$  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 4. We will treat these two functions separately.

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

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

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

(43) 
$$\alpha'(s) = O_{\leq}\left(\frac{1}{2\operatorname{Im}(s)^{2}}\right) + O_{\leq}\left(\frac{1}{\operatorname{Im}(s)^{2}}\right) + O_{\leq}\left(\frac{1}{2\operatorname{Im}(s)}\right)$$
$$= O_{\leq}\left(\frac{1}{2\operatorname{Im}(s) - 6}\right)$$

thanks to Lemma 5.1(i).

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

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

More precisely, we have

**Proposition 6.1** (Estimate for  $r_{t,n}$ ). Let  $\sigma$  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

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

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

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

whenever Im(s) > 2. Let  $\alpha_n$  denote the quantity

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

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

(46) 
$$\operatorname{Im}(\alpha_n) \ge -\frac{1}{2T} - \frac{1}{T} \ge -0.15;$$

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

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

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

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

From (43) we have

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

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

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

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

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

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

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

and so it suffices to show that

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

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

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

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

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

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

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

Applying Lemma 5.1(ii) and using the hypotheses  $t \le 1/2$ ,  $T \ge 10$ , 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.

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

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

$$(48) s \coloneqq \sigma + iT'$$

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

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

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

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

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

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

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

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

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

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

for  $\sigma > 0$  and

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

for  $\sigma \leq 0$ , while the error term RS<sub>K</sub>(s) is a complex number obeying the bounds

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

for  $\sigma \geq 0$ , and

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

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].

Maybe insert a plot of  $|C_0(p)|$  for  $-1 \le p \le 1$  here?

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

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

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

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

In fact we have the more general approximation

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

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

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

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

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

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

where

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

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

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

From (38) 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 (6) and Lemma 5.1(v) we thus have

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

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

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

From (9), (49) one has

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

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

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

We conclude that

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

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

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

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

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

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 (27) 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 5.1(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

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

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 6.2 applies. The expression

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

is then bounded by

(62) 
$$\frac{\sqrt{2}}{2\pi} \frac{9^{u} \Gamma(1/2)}{2a} + \frac{1}{7} 2^{3u/2} \frac{\Gamma(1)}{(a/11)^{2}} \le \frac{0.200 \times 9^{u}}{a} + \frac{0.173 \times 2^{3u/2}}{a^{2}}$$

for  $u \ge 0$  and

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

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 (63) 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 (62) by

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

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

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

and hence by the geometric series formula

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

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 (63) by

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

By Lemma 5.1(i) we have

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

and thus we can bound (63) by

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

Putting this together, we conclude that

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

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

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

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

$$\delta_{3} := \int_{\mathbb{R}} \exp\left(\frac{u^{2} + \frac{5}{6}}{T' - 0.33}\right) \frac{2^{-u}}{2} \sum_{\frac{T'}{2} \leq k \leq -u + 4} (1.1)^{k} \frac{\Gamma(k/2)}{a^{k}} \frac{1}{\sqrt{\pi t}} e^{-(u - \sigma)^{2}/t} du.$$
(64)

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 (27)

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

One can write

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

while by Lemma 5.1(ii) we have

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

We conclude that

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

From Lemma 5.1(i) and the hypothesis  $0 \le \sigma \le 1$ , 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 5.1(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 (65), we have

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

We can bound  $(-\log \sqrt{2} + \frac{\sigma}{T'-0.33})^2$  by  $\log^2 \sqrt{2}$ . Using (66), (67) 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 (64) and the Fubini-Tonelli theorem, we have

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

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

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

We can bound  $e^{-\frac{u^2}{2t}} \le e^{\frac{(k-4)u}{2t}}$ , 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

$$\delta_3 \le \frac{\sqrt{t}}{\sqrt{\pi}} \sum_{k \ge \frac{T'}{23-k}} (1.1)^k \frac{\Gamma(k/2)}{(k-6)a^k} e^{-(k-4)^2 + (k-4)\log 2}.$$

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

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

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

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

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

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

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

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

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

$$\begin{split} E_{A}(x+iy) &:= \left| M_{t} \left( \frac{1-y+ix}{2} \right) \right| \sum_{n=1}^{N} \frac{b_{n}^{t}}{n^{\frac{1-y}{2} + \frac{t}{2} \operatorname{Re}\alpha(\frac{1-y+ix}{2})}} \varepsilon_{t,n}(\frac{1-y+ix}{2}) \\ E_{B}(x+iy) &:= \left| M_{t} \left( \frac{1+y+ix}{2} \right) \right| \sum_{n=1}^{N} \frac{b_{n}^{t}}{n^{\frac{1+y}{2} + \frac{t}{2} \operatorname{Re}\alpha(\frac{1+y+ix}{2})}} \varepsilon_{t,n}(\frac{1+y+ix}{2}) \\ E_{C}(x+iy) &:= \exp\left( \frac{t\pi^{2}}{64} \right) |M_{0}(iT')| \left( \tilde{\varepsilon}(\frac{1-y+ix}{2}) + \tilde{\varepsilon}(\frac{1+y+ix}{2}) \right) \end{split}$$

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

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

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

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

where

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

We can now prove Theorem 1.3. Dividing by the expression  $B_0$  from (11), and using (14), we conclude that

(69) 
$$\frac{H_t(x+iy)}{B_0(x+iy)} = f_t(x+iy) + \frac{C(x+iy)}{B_0(x+iy)} + O_{\leq}(e_A + e_B + e_C)$$

and

(70) 
$$\frac{H_t(x+iy)}{B_0(x+iy)} = f_t(x+iy) + O_{\leq}(e_A + e_B + e_{C,0})$$

where

(71) 
$$e_A := e_A(x + iy) := |\gamma| \sum_{n=1}^N n^y \frac{b_n^t}{n^{\operatorname{Re}(s) + \operatorname{Re}(\kappa)}} \varepsilon_{t,n} \left( \frac{1 - y + ix}{2} \right)$$

(72) 
$$e_B := e_B(x+iy) := \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s)}} \varepsilon_{t,n} \left( \frac{1+y+ix}{2} \right)$$

(73) 
$$e_C := e_C(x+iy) := \frac{\exp\left(\frac{t\pi^2}{64}\right)|M_0(iT')|}{|M_t(\frac{1+y+ix}{2})|} \left(\tilde{\varepsilon}\left(\frac{1-y+ix}{2}\right) + \tilde{\varepsilon}\left(\frac{1+y+ix}{2}\right)\right).$$

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

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

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

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

(i) One has

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

(ii) One has

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

(iii) One has

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

(iv) One has

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

(v) One has

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

(vi) One has

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

and

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

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

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

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

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

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

From (43) one has

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

and from Taylor expansion we also have

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

from (9) one has

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

and hence

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

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 (5), 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  $x \ge 200$  thanks to Lemma 5.1(vi), hence

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

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 (48) to show that

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

By (9) one has

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

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

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

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

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

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

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

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

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 (5), 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

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

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

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

Similarly, in (5) we also have

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

We conclude from (44) 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 (71), (72), we obtain claims (iv), (v).

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

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

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

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

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

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

and from (9) one has

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

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 (77) we have

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

As before, in the region (5) we have

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

and thus

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

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

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

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

and hence by (59)

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

Hence

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

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

# give table illustrating accuracy of approximation

# 7. Bounding Dirichlet series

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

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

It is thus of interest to obtain lower bounds for differences

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

of magnitudes of Dirichlet series for various coefficients  $\beta_n$ ,  $\alpha_n$ . Our tools for this will be as follows.

**Lemma 7.1.** 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 (78).

(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

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

for some phase  $\theta$ . By the triangle inequality, we then have

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

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

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

By the cosine rule, we have

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

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

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

and the claim follows.

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

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

between Dirichlet convolution and Dirichlet series, which implies that

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

Since  $\tilde{\Delta}$ ,  $\Delta$  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  $f_t(x+iy)$ , we conclude from Lemma 7.1(i) with s replaced by  $s_*$ ,  $\beta_n$  replaced by  $b_n^t$ , and  $\alpha_n$  replaced by  $|\gamma|n^{y-\overline{k}}b_n^t$  that

(79) 
$$|f_t(x+iy)| \ge 1 - |\gamma| - \sum_{n=2}^{N} \frac{b_n^t}{n^{\sigma}} (1 + |\gamma| n^{y - \text{Re}(\kappa)}),$$

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

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

we see from the triangle inequality that

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

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

$$|f_{t}(x+iy)| \ge \frac{1 - \tilde{\alpha}_{1} - \sum_{n=2}^{N} \frac{\max(|\tilde{\beta}_{n} - \tilde{\alpha}_{n}|, \frac{1 - \tilde{\alpha}_{1}}{1 + \tilde{\alpha}_{1}}|\tilde{\beta}_{n} + \tilde{\alpha}_{n}|)}{\sum_{d=1}^{D} \frac{|\lambda_{d}|}{d^{\sigma}}} - |\gamma| \sum_{n=1}^{N} \frac{b_{n}^{t}(n^{|\kappa|} - 1)}{n^{\sigma - y}}$$

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

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

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

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

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

for some small prime P, where the product is over primes p up to P. For instance, if P=3, then we would take D=6,  $\lambda_1=1$ ,  $\lambda_2=-b_2^t$ ,  $\lambda_3=-b_3^t$ ,  $\lambda_6=b_2^tb_3^t$ , and all other  $\lambda_d$  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 (80) favorable. (For instance, it makes  $\tilde{\beta}_p$  vanish for all primes  $p \leq P$ .) In the literature one also sees other choices of mollifier than this Euler product used, for instance to control the extreme values of Dirichlet polynomials; however our numerical experimentations with alternative mollifiers to (81) turned out to give inferior results for our application.

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

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

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

# perhaps say more about how exactly we found the shift 83952?

To search for a good shift, in practice we can evaluate  $eulerprod = |\prod_{p=1}^{P} \frac{1}{1 - \frac{1}{p^{1-ix/2}}}|$ , the exponent corresponding to y=1 (where min |(A + B)/B0| for a rectangle contour is expected), and  $x = \frac{1}{p^{1-ix/2}}$ 

X + (q - 0.5, q, q + 0.5), q an integer from 1 to N (say 100,000). We can then choose candidates q where  $min(eulerprod_{(q-0.5,q,q+0.5)})$  is above a treshold (say 4).

For each of the chosen candidates, we can then evaluate  $\min(|(A+B)/B0|_{(q-0.5,q,q+0.5)})$  at t=0, and finally select a candidate where this is highest.

Hence for X near  $6 \times 10^{10}$ , using the above scheme with the first 10 primes, we get 7 candidates, q=(1046, 22402, 24198, 52806, 77752, 83952, 99108).

Among these, q=83952 gives the highest min  $|(A + B)/B0|_{(q=0.5, q, q+0.5)} \approx 4.32$ .

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

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

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

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

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

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

**Proposition 8.1.** Let (x, y, t) lie in one of the following regions:

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

Define

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

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

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

so in particular

(82) 
$$\log \frac{x}{4\pi} \ge 2\log N - \log(1 + \frac{\pi t}{4x}),$$

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

(83) 
$$|f_t(x+iy)| > e_A + e_B + e_{C.0}$$

Note that if  $x \ge X_0 - 0.5$  then  $N \ge N_0 := 69098$ , with  $N = N_0$  when  $X_0 - 0.5 \le x \le X_0 + 0.5$ . We calculate a somewhat crude upper bound for the right-hand side of (83):

the estimate below needs to be redone for the new range of parameters

**Lemma 8.2.** For (x, y, t) in either of the regions (ii), (iii) in Proposition 8.1, one has

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

*Proof.* From Theorem 1.3 we have

(84) 
$$e_A + e_B \le (e^{\delta_1} - 1)(F_{N,t}(\text{Re}(s_*)) + |\gamma|F_{N,t}(\text{Re}(s_*) - y - |\kappa|))$$

where

(85) 
$$F_{N,t}(\sigma) := \sum_{n=1}^{N} \frac{b_n^t}{n^{\sigma}}.$$

and

(86) 
$$\delta_1 := \frac{\frac{t^2}{16} \log^2 \frac{x}{4\pi} + 0.626}{x - 6.66}.$$

From Lemma 5.1(vi), the quantity  $\delta_1$  is monotone decreasing in x in the region (5). Thus we have

(87) 
$$\delta_1 \le \frac{\frac{(0.2)^2}{16} \log^2 \frac{X_0 - 0.5}{4\pi} + 0.626}{X_0 - 0.5 - 6.66}$$

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

$$\delta_1 < 2.07 \times 10^{-11}$$

and hence by Taylor expansion

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

(say). Also, from Theorem 1.3 and (85) we can bound

$$|\gamma|F_{N,t}(\operatorname{Re}(s_*) - y - |\kappa|) \le |\gamma|N^y N^{|\kappa|}F_{N,t}(\operatorname{Re}(s_*))$$

$$\leq \exp(0.02y + y(\log N - \frac{1}{2}\log \frac{x}{4\pi}) + \frac{ty}{2(x-6)}\log N)F_{N,t}(\operatorname{Re}(s_*))$$

$$\leq \exp(0.02y + (y + \frac{ty}{2(x-6)})\frac{1}{2}\log(1 + \frac{\pi t}{4x}) + \frac{ty}{4(x-6)}\log \frac{x}{4\pi})F_{N,t}(\operatorname{Re}(s_*)).$$

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

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

and

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

and thus

(88) 
$$|\gamma|F_{N_t}(\text{Re}(s_*) - y - |\kappa|) \le 1.021F_{N_t}(\text{Re}(s_*)).$$

Thus

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

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

$$\frac{t}{2x^2}(1-3y+\frac{4y(1+y)}{x^2})_+ \leq \frac{0.2}{2(X_0-0.5)^2}(1-3\times0.2+\frac{8}{(X_0-0.5)^2})_+ \leq 1.2\times10^{-23}$$

to obtain

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

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

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

Since

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

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

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

and hence by (15)

$$\frac{b_n^t}{n^{\frac{t}{4}\log\frac{x}{\pi}}} \le 1$$

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

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

and hence by the integral test

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

so that (by (86))

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

We have

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

(say), and hence

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

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

$$e_A + e_B \le 0.7220 \frac{0.0025 \log^2 \frac{X_0 - 0.5}{4\pi} + 0.626}{(X_0 - 0.5 - 6.66)^{0.79995}}$$
  
\$\le 3.221 \times 10^{-9}.\$

Meanwhile, from Proposition 6.6(vi) one has

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

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

that

(89)

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

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

It now suffices to establish the bound

$$(90) |f_t(x+iy)| > 1.25 \times 10^{-3}$$

in the following regions:

- (i) (90) holds when  $6 \times 10^{10} + 83952 0.5 \le x \le 6 \times 10^{10} + 83952 + 0.5$ ,  $0 \le t \le 0.2$ , and  $y \ge 0.2$ .
- (ii) (90) holds when  $x \ge 6 \times 10^{10} + 83952 0.5$ ,  $69098 \le N \le 80000$ , t = 0.2, and  $y \ge 0.2$ .
- (iii) (90) holds when  $80000 \le N \le 1.5 \times 10^6$ , t = 0.2, and  $y \ge 0.2$ .
- (iv) (90) holds when  $N \ge 1.5 \times 10^6$ , t = 0.2, and  $y \ge 0.2$ .

We begin with claim (i). We need some derivative estimates on the quantity  $f_t(x+iy)$ .

**Lemma 8.3.** In the region (5), and away from the jump discontinuities of N, we have

$$|\frac{\partial f_t}{\partial x}| = |\frac{\partial f_t}{\partial y}| \le \sum_{n=1}^N \frac{b_n^t}{n^{\text{Re}(s_*)}} (\frac{\log n}{2} + \frac{t \log n}{4(x-6)}) + |\gamma| N^{|\kappa|} \sum_{n=1}^N \frac{b_n^t n^y}{n^{\text{Re}(s_*)}} (\frac{t \log n}{4(x-6)} + (\log \frac{|1+y+ix|}{4\pi} + \pi + \frac{3}{x}) (\frac{1}{2} + \frac{t}{4(x-6)}))$$

and

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

*Proof.* We begin with the first estimate. Write

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

then

(91) 
$$f_t = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N \frac{b_n^t}{n^{s_{**}}}.$$

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

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

By the product and chain rules, we may calculate

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

From (17), (43) we have

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

Similarly we have

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

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

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

and hence by (8)

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

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

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

We have from (9) that

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

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

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

and thus

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

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

Now we estimate the time derivative. Since

$$\frac{\partial}{\partial t} \log b_n^t = \frac{1}{4} \log^2 n$$

$$\frac{\partial}{\partial t} s_* = \frac{1}{2} \alpha (\frac{1+y-ix}{2})$$

$$\frac{\partial}{\partial t} s_{**} = \frac{1}{2} \alpha (\frac{1-y+ix}{2})$$

$$\frac{\partial}{\partial t} \log \gamma = \frac{1}{4} (\alpha (\frac{1-y+ix}{2})^2 - \alpha^2 (\frac{1+y-ix}{2}))$$

we see from differentiating (91) that, we obtain

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

From (43), (9) we have

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

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

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

so in particular

$$\alpha(\frac{1-y+ix}{2})-\alpha(\frac{1+y-ix}{2})=\frac{\pi i}{2}+O_{\leq}(\frac{8}{x-6})$$

and

$$\alpha(\frac{1 - y + ix}{2}) + \alpha(\frac{1 + y - ix}{2}) = \log \frac{x}{4\pi} + O_{\leq}(\frac{8}{x - 6})$$

so that

$$|\alpha(\frac{1-y+ix}{2})^2 - \alpha^2(\frac{1+y-ix}{2}))| \le (\frac{\pi}{2} + \frac{8}{x-6})(\log\frac{x}{4\pi} + \frac{8}{x-6}).$$

We conclude from the triangle inequality that

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

П

giving the second claim.

...

Now we prove claim (ii).

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

Now we prove claim (iii).

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

$$|f_{N+1}| >= |f_N| - \sum_{N=1}^{\infty} \text{ (additional terms corresponding to N+1)}$$

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

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

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

$$\begin{split} \beta_{n,N} &= \sum_{1 \leq d \leq D: d \mid n: n \leq dN} \lambda_d b^t_{n/d}, \\ \alpha_{n,N} &= \sum_{1 \leq d \leq D: d \mid n: n \leq dN} \lambda_d a^t_{n/d}, \\ g(n,N,N_{max}) &= \max(\frac{1 - |\gamma|_{N_{max}}}{1 + |\gamma|_{N_{max}}} |\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} - \alpha_{n,N}|, |\beta_{n,N} - |\frac{\gamma_{N_{max}}}{\gamma_N} |\alpha_{n,N}|), \end{split}$$

For the Triangle inequality bound,

$$|f_{N_{min}}| \geq \frac{1}{\sum_{d=1}^{D} \frac{|\lambda_{d}|}{d^{\sigma_{N_{min}}}}} (1 - |\gamma_{N_{min}}| - \sum_{n=2}^{DN_{min}} \frac{|\beta_{n,N_{min}}| + |\alpha_{n,N_{min}}|}{n^{\sigma_{N_{min}}}}) - |\gamma_{N_{min}}| \sum_{n=1}^{N_{min}} \frac{b_{n}^{t}(n^{|\kappa|} - 1)}{n^{\sigma_{N_{min}} - y}}$$

$$|f_{N+1}| \geq |f_{N}| - \frac{1}{\sum_{d=1}^{D} \frac{|\lambda_{d}|}{d^{\sigma_{N+1}}}} \sum_{1 \leq d \leq D: d|D} (\sum_{n=dN+1}^{dN+d} \frac{|\beta_{n,N+1}| + |\alpha_{n,N+1}|}{n^{\sigma_{N+1}}}) - |\gamma_{N+1}| \frac{b_{N+1}^{t}((N+1)^{|\kappa|} - 1)}{(N+1)^{\sigma_{N+1} - y}}$$

For the Lemma inequality bound,

$$|f_{N_{min}}| \ge \frac{1}{\sum_{d=1}^{D} \frac{|\lambda_{d}|}{d^{\sigma_{N_{min}}}}} (1 - |\gamma_{N_{min}}| - \sum_{n=2}^{DN_{min}} \frac{g(n, N_{min}, N_{max})}{n^{\sigma_{N_{min}}}}) - |\gamma_{N_{min}}| \sum_{n=1}^{N_{min}} \frac{b_n^t(n^{|\kappa|} - 1)}{n^{\sigma_{N_{min}} - y}}$$

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

- 1)  $\beta_{n,N} = \beta_{n,N+1}$  and  $\frac{\alpha_{n,N}}{\gamma_N} = \frac{\alpha_{n,N+1}}{\gamma_{N+1}}$  when  $n \notin [dN, dN + d]$  for d : d|D2)  $g(n, N, N_{max})$  can be seen to have the following properties with n fixed and N varying, resulting in it being constant or decreasing with increasing N,
- $\begin{aligned} & \bullet g(n,N,N_{max}) = |\beta_{n,N} \alpha_{n,N}| \text{ when } \beta_{n,N}\alpha_{n,N} \leq 0 \\ & \bullet g(n,N,N_{max}) = \max(\frac{1-|\gamma|_{N_{max}}}{1+|\gamma|_{N_{max}}}|\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} |\frac{\gamma_{N_{max}}}{\gamma_{N}}|\alpha_{n,N}|)) \text{ when } \beta_{n,N}\alpha_{n,N} > 0 \text{ and } |\beta_{n,N}| \geq 0 \end{aligned}$
- $\bullet g(n, N, N_{max}) = \max(\frac{1 |\gamma|_{N_{max}}}{1 + |\gamma|_{N_{max}}} |\beta_{n,N} + \alpha_{n,N}|, |\beta_{n,N} \alpha_{n,N}|, |\beta_{n,N} |\frac{\gamma_{N_{max}}}{\gamma_N} |\alpha_{n,N}|)) \text{ when } \beta_{n,N} \alpha_{n,N} > 0$ 0 and  $|\alpha_{n,N}| > |\beta_{n,N}|$

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

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

## all numbers need to be recalculated here

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

$$x \ge 4\pi N_0^2 - \frac{\pi t}{4} \ge 1.13 \times 10^{12}.$$

We use the triangle inequality bound

$$|X| \ge (2 - F_{N,t}(\operatorname{Re}(s_*)) - |\gamma| F_{N,t}(\operatorname{Re}(s_*) - y))_+$$

$$\ge \left(2 - F_{N,0.2}(0.7 + \frac{1}{20} \log \frac{x}{4\pi}) - |\gamma| F_{N,0.2}(0.3 + \frac{1}{20} \log \frac{x}{4\pi})\right)_+$$

so to prove (83) here, it suffices by Lemma 8.2 to show that

(92) 
$$F_{N,0.2}(0.7 + \frac{1}{20}\log\frac{x}{4\pi}) + |\gamma|F_{N,0.2}(0.3 + \frac{1}{20}\log\frac{x}{4\pi}) \le 2 - 4.38 \times 10^{-4}.$$

From Proposition 6.6(i) we have

$$|\gamma| \le e^{0.0016} \left(\frac{x}{4\pi}\right)^{-0.2}$$
.

We can then bound the left-hand side of (92) by  $Q_1 + Q_2 + Q_3$ , where

$$Q_{1} := F_{N_{0},0.2}(0.7 + \frac{1}{20}\log\frac{x}{4\pi})$$

$$Q_{2} := e^{0.0016} \left(\frac{x}{4\pi}\right)^{-0.2} F_{N_{0},0.2}(0.3 + \frac{1}{20}\log\frac{x}{4\pi})$$

$$Q_{3} := \sum_{N_{0} < n < N} \frac{\exp(\frac{1}{20}\log^{2}n)}{n^{0.7 + \frac{1}{20}\log\frac{x}{4\pi}}} (1 + e^{0.0016}(\frac{x}{4\pi n^{2}})^{-0.2}).$$

We have

$$Q_1 \le F_{N_0,0,2}(0.7 + \frac{1}{20}\log\frac{1.13 \times 10^{12}}{4\pi})$$
  
< 1.898

and

$$Q_2 \le e^{0.0016} \left( \frac{1.13 \times 10^{12}}{4\pi} \right)^{-0.2} F_{N_0, 0.2}(0.3 + \frac{1}{20} \log \frac{1.13 \times 10^{12}}{4\pi})$$

$$\le 0.047.$$

To estimate  $Q_3$ , we first observe that

$$\frac{x}{4\pi n^2} \ge \frac{x}{4\pi N^2}$$
$$\ge \left(1 + \frac{\pi t}{4x}\right)^{-1}$$
$$\ge 1 - 1.4 \times 10^{-13}$$

and hence

$$1 + e^{0.0016} \left(\frac{x}{4\pi n^2}\right)^{-0.2} \le 2.0017.$$

Also from (82) we have

$$\frac{1}{n^{\frac{1}{20}\log\frac{x}{4\pi}}} \le \frac{1}{n^{\frac{1}{20}\log N^2}} \exp(\log(1 + \frac{\pi t}{4x})\log N).$$

Using Proposition 5.1(vi) we can easily bound

$$\log(1 + \frac{\pi t}{4r})\log N \le 10^{-6}$$

(say), and hence

$$Q_3 \le 2.0018 \sum_{N_0 < n \le N} \frac{\exp(\frac{1}{20} \log^2 n)}{n^{0.7 + \frac{1}{20} \log N^2}}.$$

The function  $n \mapsto \frac{\exp(\frac{1}{20}\log^2 n)}{n^{0.7 + \frac{1}{20}\log N^2}}$  is decreasing for  $1 \le n < N$ , so by the integral test we have

$$Q_3 \le 2.0018 \int_{N_0}^N \frac{\exp(\frac{1}{20}\log^2 a)}{a^{0.7 + \frac{1}{20}\log N^2}} da.$$

Making the change of variables  $a = e^u$ , this becomes

$$Q_3 \le 2.0018 \int_{\log N_0}^{\log N} \exp(0.3u + \frac{1}{20}(u^2 - 2u\log N)) du.$$

The quadratic expression  $-0.3u + \frac{1}{20}(u^2 - 2u \log N)$  is convex in u, and is thus bounded by its maximum at the endpoints; thus

$$Q_3 \le 2.0018(\log \frac{N}{N_0}) \exp(\max(0.3\log N_0 - \frac{1}{20}\log N_0 \log \frac{N^2}{N_0}, 0.3\log N - \frac{1}{20}\log^2 N)).$$

Writing  $N = e^b N_0$  for some b > 0, this bound can be rewritten as

$$Q_3 \le \frac{2.0018}{N_0^{\frac{1}{20}\log N_0 - 0.3}} \exp(\log b + \frac{1}{20}(-2b\log N_0 + (6b - b^2)_+)).$$

A routine numerical maximisation shows that

$$\log b + \frac{1}{20}(-2b\log N_0 + (6b - b^2)_+) \le -1.009$$

and hence

$$Q_3 \le 0.0113$$
.

Combining these bounds we obtain (92).

## 9. Asymptotic results

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

We begin with an asymptotic

**Proposition 9.1.** *Let*  $0 < t \le 1/2$ ,  $x \ge 200$ , and  $-10 \le y \le 10$ .

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

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

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

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

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

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

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

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

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

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

(93) 
$$\frac{H_t(x+iy)}{B_0(x+iy)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + \gamma \sum_{n=1}^N n^y \frac{b_n^t}{n^{\overline{s_*} + \kappa}} + O_{\leq} (e_A + e_B + e_{C,0})$$

where

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Now we prove (ii). As before we have the expansion (93). We have

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

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

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

We conclude that

$$\frac{H_t(x+yi)}{B_0(x+yi)} = \sum_{n=1}^N \frac{b_n^t}{n^{s_*}} + O(x^{-\frac{y-1}{4}})$$

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

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

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

$$= 1 + O_{<}(0.7)$$

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

Finally we prove (iii). Again our starting point is (93). The right-hand side can be bounded crudely by  $O(x^{O(1)}) = O(x_0^{O(1)})$ , hence

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

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

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

giving the claim.

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

**Lemma 9.2.** Let  $0 < t \le 1/2$ , let  $x_* > 0$  be sufficiently large, and let  $x + iy = x_* + O(1)$ . Then

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

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

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

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

(94) 
$$\frac{M_t'}{M_t} = \alpha + \frac{t}{2}\alpha\alpha'.$$

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

(95) 
$$\alpha(s) = \frac{1}{2} \log \frac{x_*}{4\pi} + \frac{\pi i}{4} + O\left(\frac{1}{x_*}\right)$$

and from this and (43) we conclude that

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

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

For the second claim, we calculate

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

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

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

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

as desired.

Now we can prove Theorem 1.5. We begin with (ii). Let  $n \ge \exp(\frac{C}{t})$ , and suppose that  $x + iy = x_n + O(1)$ . By Proposition 9.1(i) and Lemma 9.2 we have

(96) 
$$H_{t}(x+iy) = \overline{M_{t}\left(\frac{1+ix_{n}}{2}\right)} \exp\left((-i(x-x_{n})+y)\left(\frac{1}{4}\log\frac{x_{n}}{4\pi} - \frac{\pi i}{8}\right) + O(x_{n}^{-ct})\right) + M_{t}\left(\frac{1+ix_{n}}{2}\right) \exp\left((i(x-x_{n})-y)\left(\frac{1}{4}\log\frac{x_{n}}{4\pi} + \frac{\pi i}{8}\right) + O(x_{n}^{-ct})\right).$$

From Lemma 9.2 and (26) one has

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

and hence

(97) 
$$\overline{M_t\left(\frac{1+ix_n}{2}\right)} = -\exp\left(O(\frac{\log x_n}{x_n})\right)M_t\left(\frac{1+ix_n}{2}\right).$$

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

(98)

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

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

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

Let *n* be a natural number that minimises  $|x - x_n|$ , then  $x = x_n + O\left(\frac{1}{\log x_n}\right)$  since the derivative of the left-hand side of (26) in  $x_n$  is comparable to  $\log x_n$ . From (96) we have

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

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

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

and hence  $y = O\left(\frac{x_n^{-ct}}{\log x_n}\right)$ . We can now apply (98) to conclude that

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

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

Next, we prove (iii). In view of parts (i) and (ii), and adjusting C if necessary, we may assume that X takes the form  $X = x_n + \frac{c}{\log x_n}$  for some  $n \ge \exp(\frac{C}{t})$ . By the argument principle,  $N_t(X)$  is equal to  $\frac{-1}{2\pi}$  times the variation in the argument of  $H_t$  on the boundary of the rectangle  $\{x + iy : 0 \le x \le X; -3 \le y \le 3\}$  traversed clockwise, since there are no zeroes with imaginary part of magnitude greater than one. By compactness, the variation on the left edge  $\{iy : -3 \le y \le 3\}$  is O(1), and similarly for any fixed portion  $\{x+3i : 0 \le y \le C\}$  of the upper edge. From Proposition 9.1 (and (96)), we see that the variation of  $H_t(x+iy)/M_t(\frac{1+y-ix}{2})$  on the remaining upper edge  $\{x+3i : C \le x \le X\}$  and on the top half  $\{X+iy : 0 \le y \le 3\}$  of the right edge are both equal to O(1). Since  $H_t = H_t^*$ , the variation on the lower half of the rectangle is equal to that of the upper half. We thus conclude that

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

where we use a continuous branch of the argument of  $M_t\left(\frac{1-iX}{2}\right)$  that is bounded at 3*i*. The claim now follows from Lemma 9.2.

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

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

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

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

Taking logarithmic derivatives, we conclude that

(99) 
$$\frac{H'_t(z)}{H_t(z)} = \sum_{n>0} \left( \frac{1}{z - z_n} + \frac{1}{z + z_n} \right).$$

Setting z = X + 4i, we see from Proposition 9.1 and the generalized Cauchy integral formula that the logarithmic derivative of  $H_t(x+iy)/M_t\left(\frac{1+y-ix}{2}\right)$  is equal to O(1) at X+4i for all sufficiently large X, and hence for all X by symmetry and compactness. On the other hand, from Stirling's formula (or the logarithmic growth of the digamma function) one easily verifies that the logarithmic derivative of  $M_t\left(\frac{1+y-ix}{2}\right)$  is equal to  $O(\log(2+X))$  at X+4i. Hence  $\frac{H_t'(X+4i)}{H_t(X+4i)} = O(\log(2+X))$ . Taking imaginary parts, we conclude that

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

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

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

where the sum now ranges over all zeroes, including any at the origin. Since  $|y_n| \le 1$ , every zero in [X, X+1] makes a contribution of at least  $\frac{1}{100}$  (say). As the summands are all positive, the first part of claim (iv) follows. To prove the second part, we may assume by compactness that  $x \ge C$ . Repeating the proof of (iii), and reduce to showing that the variation of  $\arg H_t$  on the short vertical interval  $\{X+iy:0\le y\le 3\}$  is  $O(\log X)$ . If we let  $\theta$  be a phase such that  $e^{i\theta}H_t(X+3i)$  is real and positive, we see that this variation is at most  $\pi(m+1)$ , where m is the number of zeroes of  $\operatorname{Re} e^{i\theta}H_t(X+yi)$  for  $0\le y\le 3$ , since every increment of  $\pi$  in  $\operatorname{arg} e^{i\theta}H_t$  must be accompanied by at least one such zero. As  $H_t=H_t^*$ , this is also the number of zeroes of  $e^{i\theta}H_t(X+yi)+e^{-i\theta}H_t(2X-(X+yi))$ . On the other hand, from Proposition 9.1(ii), (iii) and Jensen's formula we see that the number of such zeroes is  $O(\log X)$ , and the claim follows.

**Remark 9.3.** Theorem 1.5 gives good control on  $H_t(x + iy)$  whenever  $x \ge \exp(C/t)$ . As a consequence (and assuming for sake of argument that the Riemann hypothesis holds), then for any  $\Lambda_0 > 0$ , the bound  $\Lambda \le \Lambda_0$  should be numerically verifiable in time  $O(\exp(O(1/\Lambda_0)))$ , by applying the arguments of previous sections with t and y set equal to small multiples of  $\Lambda_0$ . We leave the details to the interested reader.

**Remark 9.4.** Our discussion here will be informal. In view of the results of [8], it is expected that the zeroes  $z_j(t)$  of  $H_t(x + iy)$  should evolve according to the system of ordinary differential equations

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

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

spaced. As a consequence, if the Riemann hypothesis fails and there is a zero x+iy of  $H_0$  with y comparable to 1, it should take time comparable to  $\frac{1}{\log x}$  for this zero to move towards the real axis, leading to the heuristic lower bound  $\Lambda \gg \frac{1}{\log x}$ . Thus, in order to obtain an upper bound  $\Lambda \leq \Lambda_0$ , it will probably be necessary to verify that there are no zeroes x+iy of  $H_0$  with y comparable to 1 and  $|x| \leq c \log \frac{1}{\Lambda}$  for some small absolute constant c > 0. This suggests that the time complexity bound in Remark 9.3 is likely to be best possible (unless one is able to prove the Riemann hypothesis, of course).

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

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

assuming that the zero is simple. By using the asymptotics in Proposition 9.1 and Corollary 1.5 together with the generalized Cauchy integral formula to then obtain asymptotics for  $H'_t$  and  $H''_t$ , it is possible to show that for the zeroes x(t) that are real and larger than  $\exp(C/t)$ , and move leftwards with velocity

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

we leave the details to the interested reader. maybe supply some numerically computed graphics here?

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