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

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ABSTRACT. For each $t \in \mathbb{R}$, define the entire function

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

where Φ is the super-exponentially decaying function

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

Newman showed that there exists a finite constant Λ (the *de Bruijn-Newman constant*) such that the zeroes of H_t are all real precisely when $t \geq \Lambda$. The Riemann hypothesis is the equivalent to the assertion $\Lambda \leq 0$, and Newman conjectured the complementary bound $\Lambda \geq 0$.

1. INTRODUCTION

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

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

where ξ denotes the Riemann xi function

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

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

It is a classical fact (see [18, p. 255]) that H_0 has the Fourier representation

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

where Φ is the super-exponentially decaying function

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

The sum defining $\Phi(u)$ converges absolutely for negative u also. From Poisson summation one can verify that Φ satisfies the functional equation $\Phi(u) = \Phi(-u)$ (i.e., Φ is even).

De Bruijn [1] introduced the more general family of functions $H_t \colon \mathbb{C} \to \mathbb{C}$ for $t \in \mathbb{R}$ by the formula

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

As noted in [5, p.114], one can view H_t as the evolution of H_0 under the backwards heat equation $\partial_t H_t(z) = -\partial_{zz} H_t(z)$. As with H_0, each of the H_t are entire even functions with functional equation $H_t(\overline{z}) = \overline{H_t(z)}$. De Bruijn showed that the zeroes of H_t are purely real for $t \geq 1/2$, and if H_t has purely real zeroes for some t, then $H_{t'}$ has purely real zeroes for all $t' > t$. Newman [10] strengthened this result by showing that there is an absolute constant $-\infty < \Lambda \leq 1/2$, now known as the *De Bruijn-Newman constant*, with the property that H_t has purely real zeroes if and only if $t \geq \Lambda$. The Riemann hypothesis is then clearly equivalent to the upper bound $\Lambda \leq 0$. Recently in [13] the complementary bound $\Lambda \geq 0$ was established, answering a conjecture of Newman [10]. Furthermore, Ki, Kim, and Lee [6] sharpened the upper bound $\Lambda \leq 1/2$ of de Bruijn [1] slightly to $\Lambda < 1/2$.

2. Applying the fundamental solution for the heat equation

We can write H_t in terms of H_0 using the fundamental solution to the heat equation. Namely, for any $t > 0$, we have the gaussian integral identity

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

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

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

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

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

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

$$H_t(z) = \int_{\mathbb{R}} \frac{1}{8} \xi\left(\frac{1+iz}{2} + \sqrt{t}v\right) \frac{1}{\sqrt{\pi}} e^{-v^2}\, dv. \tag{5}$$

We now combine this formula with expansions of the Riemann ξ-function. From [18, (2.10.6)] we have the Riemann-Siegel formula

$$\frac{1}{8}\xi(s) = R_{0,0}(s) + R^*_{0,0}(1-s) \tag{6}$$

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

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

with $0 \swarrow 1$ any infinite line oriented in the direction $e^{5\pi i/4}$ that crosses the interval $[0,1]$, and we use the convention $F^*(s) := \overline{F(\overline{s})}$ for the reflection of a function F. From the residue theorem (and the gaussian decrease of $e^{i\pi w^2}$ along the $e^{\pi i/4}$ and $e^{5\pi i/4}$ directions) we may expand

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

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

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

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 (5), (6) we conclude that

$$H_t(z) = \sum_{n=1}^{N} r_{t,n}(\frac{1+iz}{2}) + \sum_{n=1}^{N} r^*_{t,n}(\frac{1-iz}{2}) + R_{t,N}(\frac{1+iz}{2}) + R^*_{t,N}(\frac{1-iz}{2}) \tag{7}$$

for any $t > 0$, any z that is not purely imaginary, and any non-negative integer N, where $r_{t,n}(s), R_{t,N}(s)$ are defined for non-real s by the formulae

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

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

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

$$r_{t,n}(s) := \exp(-\frac{t}{4}\alpha_n^2)\int_{\mathbb{R}} \exp(-\sqrt{t}v\alpha_n) r_{0,n}(s+\sqrt{t}v+\frac{t}{2}\alpha_n)\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv \tag{8}$$

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

$$R_{t,N}(s) := \exp(-\frac{t}{4}\beta_N^2)\int_{\mathbb{R}} \exp(-\sqrt{t}v\beta_N) R_{0,N}(s+\sqrt{t}v+\frac{t}{2}\beta_N)\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv \tag{9}$$

for any complex number β_N with $\mathrm{Im}(s), \mathrm{Im}(s+\frac{t}{2}\beta_N)$ having the same sign. In the spirit of the saddle point method, we will select the parameters α_n, β_N later in the paper in order to make the phases in $r_{0,n}, R_{0,N}$ close to stationary, in order to obtain good estimates and approximations for these terms.

One can differentiate the expansion (7) term-by-term to conclude that

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

Differentiating (8), (9) under the integral sign (which can be justified using the Cauchy integral formula and the subgaussian nature of $r_{0,n}, R_{0,N}$) we also obtain the formulae

$$r_{t,n}'(s) = \exp(-\frac{t}{4}\alpha_n^2)\int_{\mathbb{R}}(\alpha_n + \frac{2v}{\sqrt{t}})\exp(-\sqrt{t}v\alpha_n)r_{0,n}(s+\sqrt{t}v+\frac{t}{2}\alpha_n)\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv \tag{10}$$

and

$$R_{t,N}'(s) = \exp(-\frac{t}{4}\beta_N^2)\int_{\mathbb{R}}(\beta_N + \frac{2v}{\sqrt{t}})\exp(-\sqrt{t}v\beta_N)R_{0,N}(s+\sqrt{t}v+\frac{t}{2}\beta_N)\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv. \tag{11}$$

3. Elementary estimates

To obtain effective estimates, it is convenient to use the notation $O_\leq(X)$ to denote any quantity that is bounded in magnitude by X. Any expression of the form $A = B$ using this notation should be interpreted as the assertion that any quantity of the form A is also of the form B, thus for instance $O_\leq(1) + O_\leq(1) = O_\leq(3)$. (In particular, the equality relation is no longer symmetric with this notation.)

We have the following elementary estimates:

Lemma 3.1 (Elementary estimates)**.** *Let $x > 0$.*

(i) *If $a > 0$ and $b \geq 0$ are such that $x > b/a$, then*

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

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

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

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

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

or equivalently

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

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

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

(iv) *We have*

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

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

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

(vi) *If* $a, b > 0$ *and* $x \geq x_0 \geq \exp(b/a)$*, then*

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

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

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

whenever $0 \leq t < x$.

For Claim (ii), we use the Taylor expansion of the logarithm to note that

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

which on comparison with the geometric series formula

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

gives the claim. Similarly for Claim (iii), we may compare the Taylor expansion

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

with the geometric series formula

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

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

Claim (iv) follows from the trivial identity $e^x = 1 + (e^x - 1)$ and the elementary inequality $e^{-x} \geq 1 - (e^x - 1)$. For Claim (v), we may use the functional equation $\Gamma(\overline{z}) = \overline{\Gamma(z)}$ to assume that $\mathrm{Im}(z) \geq 0$. We use equations (1.13), (3.1), (3.14) and (3.15) of [**?**] to obtain the Stirling approximation

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

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

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

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

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

for $\mathrm{Re}(z) \leq 0$, where C_2 is the constant

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

In the latter case, we have $\mathrm{Im}(z) \geq 1$ by hypothesis, and hence $|1 - e^{2\pi i z}| \geq 1 - e^{-2\pi}$. We conclude that in all ranges of z of interest, we have

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

and hence by Claim (i)

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

and the claim then follows by Claim (ii).

For Claim (vi), it suffices to show that the function $x \mapsto \frac{\log^a x}{x^b}$ is nonincreasing for $x \geq \exp(b/a)$. Taking logarithms and writing $y = \log x$, it suffices to show that $a \log y - by$ is nonincreasing for $y \geq b/a$, but this is clear from taking a derivative. □

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