ZEROES OF THE HEAT FLOW EVOLUTION OF THE RIEMANN ξ FUNCTION AT NEGATIVE TIMES: NUMERICAL EXPERIMENTS AND HEURISTIC JUSTIFICATIONS

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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

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

This is essentially the heat flow evolution of the Riemann ξ function, introduced by de Bruijn. The Riemann hypothesis asserts that the zeroes of H_0 are all real; recently, it was shown by Rodgers and Tao that the zeroes are no longer all real for $t < 0$.

In this paper we investigate, through a combination of numerical experiments and heuristic asymptotics, the behavior of the zeroes of H_t for negative times t. The numerical experiments uncovered several striking patterns in the zeroes, for which we now also have heuristic justifications. Firstly, there are complex zeroes $H_t(x + iy)$ clustered around the curves

$$y = |t| \log \frac{N}{\sqrt{n(n+1)}} - 1$$

for natural numbers n, where $N := \sqrt{\frac{x}{4\pi} + \frac{t}{16}}$. Secondly, for large values of the quantity

$$v := \frac{t^2}{64\pi^2 N^3},$$

the only surviving real zeroes $H_t(x+iy)$ occur when N is close to a half-integer, while for medium-sized values of v, the zeroes take on a "sharkfin pattern" that can be described asymptotically in terms of the zeroes of the Airy function.

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 ξ function

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

(after removing all singularities) and ζ is the Riemann ζ 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 [16, 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 (with somewhat different notation) the more general family of functions $H_t\colon \mathbb{C} \to \mathbb{C}$ for $t \in \mathbb{R}$, defined 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 $H_t(\overline{z}) = \overline{H_t(z)}$; 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 [10] 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 $t \geq 1/2$. Newman [7] 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 [7], and improving upon several previous lower bounds for Λ [2, 8, 4, 3, 9, 14]. Furthermore, Ki, Kim, and Lee [6] sharpened the upper bound $\Lambda \leq 1/2$ of de Bruijn [1] slightly to $\Lambda < 1/2$; recently [11], we improved this bound further to $\Lambda \leq 0.22$.

In this paper we investigate, through a combination of numerics and heuristic approximations, the behaviour of the zeroes $H_t(x+iy) = 0$ when t is negative. For both the numerics and the heuristics, it is convenient to work with the heat kernel exact formula

$$H_t(x+iy) = \int_{\mathbb{R}} \frac{1}{8}\xi\Big(\frac{1+ix-y}{2} + i|t|^{1/2}v\Big)\frac{1}{\sqrt{\pi}}e^{-v^2}\,dv, \tag{5}$$

valid whenever $t < 0$; see [13, (15)] (as well as [11, (35)] for the analogous formula for $t > 0$).

describe numerical experiments of H_t

It is convenient to introduce the following coordinates: the shifted real argument

$$\tilde{x} := x + \frac{\pi t}{4}, \tag{6}$$

a normalised version

$$N := \sqrt{\frac{\tilde{x}}{4\pi}} = \sqrt{\frac{x}{4\pi} + \frac{t}{16}} \tag{7}$$

of that coordinate, and a further coordinate

$$w := \frac{t^2}{64\pi^2 N^3}.$$

For future reference we observe that

$$\tilde{x} = 4\pi N^2 \tag{8}$$

and (for negative values of t)

$$t = -8\pi N^{3/2} w^{1/2}. \tag{9}$$

Claim 1.1 (Numerically observed phenomena). (i) *For each natural number n, some of the complex zeroes of $H_t(x+iy)$ concentrate on the curve*

$$y = |t| \log \frac{N}{\sqrt{n(n+1)}} - 1. \tag{10}$$

(ii) *For large values of w, the real zeroes of $H_t(x+iy)$ occur when N is close to a half-integer.*

(iii) *For medium values of w, the real zeroes of $H_t(x+iy)$ are confined to the region*

$$(\frac{9w}{4})^{1/3} - w < \{2N + \frac{1}{2}\} < 1 - w$$

and occur when

$$\frac{4\sqrt{N}}{3}(1 - \{2N + \frac{1}{2}\} - w)^{3/2} + \frac{1}{4}$$

is close to an integer.

2. Heuristic approximations

We now make some heuristic approximations to (5) in the regime $t < 0$, $y \geq 0$, and $x \gg 1$, with y not too large compared with x (later on we will refine the approximation in certain subregimes).

From the functional equation for $H_t(x+iy) = H_t(-x-iy)$, we have

$$H_t(x+iy) = \int_{\mathbb{R}} \frac{1}{8}\xi(\frac{1-ix+y}{2} - i|t|^{1/2}v)\frac{1}{\sqrt{\pi}}e^{-v^2}\, dv.$$

To cancel off an exponential decay factor in the ξ function, it is convenient to shift the v variable by $\pi|t|^{1/2}/8$, thus

$$\begin{aligned} H_t(x+iy) &= \frac{1}{8\sqrt{\pi}}\int_{\mathbb{R}} \xi(\frac{1-ix+y}{2} - i|t|^{1/2}v + \pi i|t|/8)e^{-(v-\pi|t|^{1/2}/8)^2}\, dv \\ &= \frac{\exp(\pi^2 t/64)}{8\sqrt{\pi}}\int_{\mathbb{R}} \xi(\frac{1+y}{2} - \frac{i\tilde{x}}{2} - i|t|^{1/2}v)e^{-v^2+\pi|t|^{1/2}v/4}\, dv \end{aligned}$$

where $\tilde{x}$ was defined by (6). Next, from the definition of ξ and the Stirling approximation we have

$$\frac{1}{8}\xi(s) \approx M_0(s)\zeta(s)$$

where

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

where Log denotes the standard branch of the complex logarithm. Thus

$$H_t(x+iy) \approx \frac{\exp(\pi^2 t/64)}{\sqrt{\pi}}\int_{\mathbb{R}} M_0(\frac{1+y}{2} - \frac{i\tilde{x}}{2} - i|t|^{1/2}v)\zeta(\frac{1+y}{2} - \frac{i\tilde{x}}{2} - i|t|^{1/2}v)e^{-v^2+\pi|t|^{1/2}v/4}\, dv.$$

By Taylor expansion we have

$$M_0(\frac{1+y}{2} - \frac{i\tilde{x}}{2} - i|t|^{1/2}v) \approx M_0(\frac{1+y}{2} - \frac{i\tilde{x}}{2}) \exp(-\alpha(\frac{1+y}{2} - \frac{i\tilde{x}}{2})i|t|^{1/2}v + \alpha'(\frac{1+y}{2} - \frac{i\tilde{x}}{2})\frac{-|t|v^2}{2})$$

where

$$\alpha(s) := \frac{M_0'(s)}{M_0(s)} = \frac{1}{2s} + \frac{1}{s-1} + \frac{1}{2}\mathrm{Log}\frac{s}{2\pi}$$

is the logarithmic derivative of M_0. Assuming that y is small compared to $\tilde{x}$, we have the approximations

$$\alpha(\frac{1+y}{2} - \frac{i\tilde{x}}{2}) \approx \frac{1}{2}\log\frac{\tilde{x}}{4\pi} - \frac{i\pi}{4}$$

and

$$\alpha'(\frac{1+y}{2} - \frac{i\tilde{x}}{2}) \approx \frac{i}{\tilde{x}}.$$

Using (6), we thus have

$$H_t(x+iy) \approx \frac{\exp(\pi^2 t/64)}{\sqrt{\pi}} M_0(\frac{1+y}{2} - 2\pi i N^2) \int_{\mathbb{R}} \exp(-i|t|^{1/2}v\log N - \frac{\pi|t|^{1/2}v}{4} - \frac{i|t|v^2}{8\pi N^2})\zeta(\frac{1+y}{2} - 2\pi i N^2 - i|t|^{1/2}v) e^{-v^2 + \frac{\pi|t|^{1/2}v}{4}}\ dv.$$

The two factors of $\exp(\frac{\pi|t|^{1/2}v}{4})$ cancel. In practice, the $\exp(-\frac{i|t|v^2}{8\pi N^2})$ term has proven to be fairly negligible, so we drop it to conclude that

$$H_t(x+iy) \approx \frac{\exp(\pi^2 t/64)}{\sqrt{\pi}} M_0(\frac{1+y}{2} - 2\pi i N^2) \int_{\mathbb{R}} \exp(-i|t|^{1/2}v\log N)\zeta(\frac{1+y}{2} - 2\pi i N^2 - i|t|^{1/2}v) e^{-v^2}\ dv.$$

If we formally write $\zeta(s) = \sum_{n=1}^\infty \frac{1}{n^s}$ (ignoring convergence issues), we obtain

$$H_t(x+iy) \approx \frac{\exp(\pi^2 t/64)}{\sqrt{\pi}} M_0(\frac{1+y}{2} - 2\pi i N^2) \sum_{n=1}^\infty \int_{\mathbb{R}} \exp(-i|t|^{1/2}v\log N) n^{-\frac{1+y}{2} + 2\pi i N^2 + i|t|^{1/2}v} e^{-v^2}\ dv.$$

We therefore expect zeroes $H_t(x+iy)$ to obey the approximate equation

$$\sum_{n=1}^\infty \int_{\mathbb{R}} \exp(-i|t|^{1/2}v\log\frac{N}{n}) n^{-\frac{1+y}{2} + 2\pi i N^2} e^{-v^2}\ dv. \approx 0.$$

Evaluating the gaussian integral, we arrive at

$$\sum_{n=1}^\infty f_n(N,y,t) \approx 0 \tag{11}$$

where

$$f_n(N,y,t) := \exp(-\frac{|t|}{4}\log^2\frac{N}{n}) n^{-\frac{1+y}{2} + 2\pi i N^2}. \tag{12}$$

We now focus on two subregimes: one in which $|t|$ is small compared with $\tilde{x}$, and the other where $y = 0$.

2.1. **Small $|t|$.** The magnitude of $f_n(N,y,t)$ can be computed as

$$|f_n(N,y,t)| = \exp(\frac{1+y}{2}\log n - \frac{|t|}{4}\log^2\frac{N}{n}). \tag{13}$$

The function $x \mapsto \frac{1+y}{2}\log x - \frac{|t|}{4}\log^2\frac{N}{x}$ has first derivative

$$\frac{1+y}{2x} - \frac{|t|}{2x}\log\frac{N}{x}$$

and is thus increasing in the region $y > |t|\log\frac{N}{x} - 1$ and decreasing outside of this region. In particular, in the region

$$|t|\log\frac{N}{n+1} - 1 < y < |t|\log\frac{N}{n}$$

for some fixed natural number n, we expect the terms f_n, f_{n+1} to dominate the sum (11), so the zeroes of $H_t(x+iy) = 0$ should be close to the zeroes of

$$f_n(N,y,t) + f_{n+1}(N,y,t) = 0.$$

The latter of course lies on the curve $|f_n(N,y,t)| = |f_{n+1}(N,y,t)|$, which by (13) and some algebra may be simplified to

$$y = |t|\log\frac{N}{\sqrt{n(n+1)}} - 1.$$

This supports Claim 1.1(i).

add remark about how one can see finer oscillations in the zeroes by retaining a few more terms in (11)**.**

2.2. **Real zeroes.** Now we take $y = 0$. We substitute (9) into (12) and use the Taylor approximation $\log\frac{N}{n} \approx \frac{n-N}{N}$ to then obtain

$$f_n(N,0,t) \approx \exp(-2\pi N^{-1/2}w^{1/2}(n-N)^2 - \frac{1}{2}\log n + 2\pi i N^2\log n).$$

The gaussian factor $\exp(-2\pi N^{-1/2}w^{1/2}(n-N)^2)$ localises n to N, and we then use the approximations

$$\frac{1}{2}\log n \approx \frac{1}{2}\log N$$

and

$$2\pi i N^2\log n \approx 2\pi i N^2(\log N + \frac{n-N}{N} - \frac{(n-N)^2}{2N^2} + \frac{(n-N)^3}{3N^3})$$

so (11) then becomes (after canceling some terms independent of n)

$$\sum_{n=1}^{\infty}\exp(-2\pi N^{-1/2}w^{1/2}(n-N)^2 + 2\pi i N(n-N) - \pi i(n-N)^2 + \frac{2\pi i}{3N}(n-N)^3) \approx 0.$$

We compute

$$\begin{aligned}\exp(2\pi i N(n-N) - \pi i(n-N)^2) &= \exp(-\pi i n^2 + 4\pi i N n - 3\pi i N^2)\\ &= \exp(\pi i n + 4\pi i N n - 3\pi i N^2)\\ &= \exp(2\pi i\{2N + \frac{1}{2}\}n - 3\pi i N^2)\end{aligned}$$

where $\{x\}$ denotes the fractional part of x. The above equation thus becomes

$$\sum_{n=1}^{\infty} \exp(-2\pi N^{-1/2} w^{1/2} (n-N)^2 + 2\pi i n \{2N + \frac{1}{2}\} + \frac{2\pi i}{3N}(n-N)^3) \approx 0.$$

In view of the gaussian factor, we now allow n to range over the integers rather than the natural numbers. Using Poisson summation, we arrive at

$$\sum_m g_m(N,w) \approx 0$$

where

$$g_m(N,w) := \int_{\mathbb{R}} \exp(-2\pi N^{-1/2} w^{1/2} (X-N)^2 - 2\pi i X (m - \{2N + \frac{1}{2}\}) + \frac{2\pi i}{3N}(X-N)^3)\, dX.$$

We can shift X by N to obtain

$$g_m(N,w) = e^{-2\pi i N(m - \{2N+\frac{1}{2}\})} \int_{\mathbb{R}} \exp(-2\pi N^{-1/2} w^{1/2} X^2 - 2\pi i X (m - \{2N + \frac{1}{2}\}) + \frac{2\pi i}{3N} X^3)\, dX.$$

Suppose we neglect the third order term $\frac{2\pi i}{3N} X^3$. Then

$$g_m(N,w) \approx e^{2\pi i N(m - \{2N+\frac{1}{2}\})} \int_{\mathbf{R}} \exp(-2\pi N^{-1/2} w^{1/2} X^2 - 2\pi i X (m - \{2N + \frac{1}{2}\})\, dX$$

$$\approx \sqrt{\frac{N^{1/2}}{2w^{1/2}}} e^{-2\pi i N(m - \{2N+\frac{1}{2}\})} \exp(-\frac{(m - \{2N+\frac{1}{2}\})^2 N^{1/2}}{4w^{1/2}}). \tag{14}$$

This decays quickly for m far from $\{2N + \frac{1}{2}\}$, so we expect the $m = 0$ and $m = 1$ terms to dominate, thus we arrive at

$$g_0(N,w) + g_1(N,w) \approx 0. \tag{15}$$

Inserting the approximation (14), and cancelling common terms, we arrive at

$$1 + e^{-2\pi i N} \exp(-\frac{(1 - 2\{2N + \frac{1}{2}\}) N^{1/2}}{4w^{1/2}}) \approx 0.$$

This has solutions when N is a half-integer. This supports Claim 1.1(ii).

Now we look at smaller values of w. Here we do not omit the $\frac{2\pi i}{3N} X^3$ term, but continue to use the simplified equation (15). We may write

$$g_m(N,w) = \exp(-iNc_m) \int_{\mathbb{R}} \exp(\frac{ia}{3} X^3 - ibX^2 - ic_m X)\, dX$$

where

$$a := \frac{2\pi}{N}$$
$$b := -2\pi i N^{-1/2} w^{1/2}$$
$$c_m := 2\pi(m - \{2N + \frac{1}{2}\}).$$

If we make the change of variables $X = a^{-1/3}(t + ba^{-2/3})$ and formally shift the contour of integration, we obtain

$$g_m(N, w) = a^{-1/3} \exp(-iNc_m - 2ib^3a^{-2}/3 - ibc_m a^{-1}) \int_{\mathbb{R}} \exp(\frac{it^3}{3} - i(c_m a^{-1/3} + b^2a^{-4/3})t)\, dt.$$

Since the Airy function Ai is given by the formula

$$\begin{aligned}\mathrm{Ai}(x) &= \frac{1}{\pi} \int_0^\infty \cos(\frac{t^3}{3} + xt)\, dt \\ &= \frac{1}{2\pi} \int_{\mathbf{R}} \exp(i\frac{t^3}{3} + ixt)\, dt\end{aligned}$$

we conclude that

$$g_m(N, w) = 2\pi a^{-1/3} \exp(-iNc_m - 2ib^3a^{-2}/3 - ibc_m a^{-1})\mathrm{Ai}(-(c_m a^{-1/3} + b^2a^{-4/3})).$$

Inserting this into (15), we arrive at

$$\mathrm{Ai}(-(c_0a^{-1/3} + b^2a^{-4/3})) + \exp(-2\pi iN - 2\pi iba^{-1})\mathrm{Ai}(-(c_0a^{-1/3} + b^2a^{-4/3} + 2\pi a^{-1/3}))) \approx 0.$$

Substituting the definitions of a, b, c_0,we obtain

(16)

$$\mathrm{Ai}((2\pi)^{2/3}N^{1/3}(\{2N+\frac{1}{2}\}+w))+\exp(-2\pi iN-2\pi N^{1/2}w^{1/2})\mathrm{Ai}((2\pi)^{2/3}N^{1/3}(\{2N+\frac{1}{2}\}+w-1)) \approx 0.$$

The Airy function oscillates for negative reals and is positive for positive reals. We then expect the zeroes of the above equation to be located in the region where

$$\{2N + \frac{1}{2}\} + w - 1 < 0$$

and in which the amplitude of the second term dominates that of the first term. Up to polynomial factors, $\mathrm{Ai}(x)$ behaves like $e^{-\frac{2}{3x^{3/2}}}$ for positive x and oscillates with bounded amplitude for negative x, thus we expect

$$\exp(-\frac{2}{3}[(2\pi)^{2/3}N^{1/3}(\{2N + \frac{1}{2}\} + w)]^{3/2}) \leq \exp(-2\pi N^{1/2}w^{1/2})$$

which after some algebra simplifies to

$$\{2N + \frac{1}{2}\} + w - (\frac{9w}{4})^{1/3} > 0.$$

In this region, the second term in (16) dominates, leading us to

$$\mathrm{Ai}((2\pi)^{2/3}N^{1/3}(\{2N + \frac{1}{2}\} + w - 1)) \approx 0.$$

The zeroes of $\mathrm{Ai}(x) = 0$ occur when $\frac{2}{3}(-x)^{3/2} + \frac{\pi}{4}$ is close to a multiple of π, so we arrive at

$$\frac{2}{3}2\pi N^{1/2}(1 - \{2N + \frac{1}{2}\} - w)^{3/2} + \frac{\pi}{4} \approx 0 \bmod \pi$$

or equivalently

$$\frac{4\sqrt{N}}{3}(1 - \{2N + \frac{1}{2}\} - w)^{3/2} + \frac{1}{4} \approx 0 \bmod 1.$$

This supports Claim 1.1(iii).

Remark 2.1. *The above analysis also allows one to predict how many zeroes one would expect to participate in the patterns observed in Claim 1.1. In the region* $0 \leq x \leq x_*$*, the Riemann-von Mangoldt formula for* H_t *(see* [13, Theorem 4.2]*) shows that the number of zeroes of* $H_t(x+iy) = 0$ *is approximately*

$$\frac{x_*}{4\pi} \log \frac{x_*}{4\pi} - \frac{x_*}{4\pi} \approx N_*^2 \log N_*^2$$

where $N_* := \frac{x_*}{4\pi}$*. On the other hand, by inspecting the variation in phase of* $f_{n+1}(N, y, t)/f_n(N, y, t)$*, we expect the number of such zeroes lying near the curve* (10) *with* $0 \leq x \leq x_*$ *to be roughly* $N_*^2 \log \frac{n+1}{n}$ *for a fixed choice of t. The number of zeroes obeying Claim 1.1(ii) should be approximately* N_**, while the number obeying Claim 1.1(ii) is* $O(N_*^{3/2})$*. In particular only a small minority of the zeroes should remain real as t becomes negative.*

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