No. 5: Some results on the $\xi(\mathbf{s})$ and $\boldsymbol{\Xi}(\mathbf{t})$ functions associated with Riemann's $\zeta(\mathbf{s})$ function *

Towards a Proof of the Riemann Hypothesis

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2016/01/22

Abstract

We report on some properties of the $\xi(s)$ function and its value on the critical line, $\Xi(t) = \xi\left(\frac{1}{2} + it\right)$. First, we present some identities that hold for the log derivatives of a holomorphic function. We then re-examine Hadamard's product-form representation of the $\xi(s)$ function, and present a simple proof of the horizontal monotonicity of the modulus of $\xi(s)$. We then show that the $\Xi(t)$ function can be interpreted as the autocorrelation function of a weakly stationary random process, whose power spectral function $S(\omega)$ and $\Xi(t)$ form a Fourier transform pair. We then show that $\xi(s)$ can be formally written as the Fourier transform of $S(\omega)$ into the complex domain $\tau = t - i\lambda$, where $s = \sigma + it = \frac{1}{2} + \lambda + it$. We then show that the function $S_1(\omega)$ studied by Pólya has $g(s)$ as its Fourier transform, where $\xi(s) = g(s)\zeta(s)$. Finally we discuss the properties of the function $g(s)$, including its relationships to Riemann-Siegel's $\vartheta(t)$ function, Hardy's Z-function, Gram's law and the Riemann-Siegel asymptotic formula.

Key words: Riemann's $\zeta(s)$ function, $\xi(s)$ and $\Xi(t)$ functions, Riemann hypothesis, Monotonicity of the modulus $\xi(t)$, Hadamard's product formula, Pólya's Fourier transform representation, Fourier transform to the complex domain, Riemann-Siegel's asymptotic formula, Hardy's Z-function.

1 Definition of $\xi(\mathrm{s})$ and its properties

The Riemann zeta function is defined by

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s}, \quad \text{for} \quad \Re(s) > 1, \tag{1}$$

which is then defined for the entire s-domain by analytic continuation (See Riemann [15] and Edwards [3]). In this article we investigate some properties of the function $\xi(s)$ [1] defined by (see Appendix A)

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

The function $\xi(s)$ is an *entire* function with the following "reflective" property:

$$\xi(1-s) = \xi(s). \tag{3}$$

*This article is based on the results reported in No. 3 and No. 4, with the last section 4.3 added. This paper was submitted to arXiv, an online publication and is posted, dated January 22, 2016. Click on `https://arxiv.org/submit/1461454/view`.

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[1] In Riemann's 1859 seminal paper [15] he was primarily concerned with the properties of this function evaluated on the critical line $s = \frac{1}{2} + it$, which he denoted as $\xi(t)$. We write it as $\Xi(t)$ instead, as defined in (7). See, e.g., Titchmarsh [18] p. 16. Edwards [3] writes explicitly $\xi(\frac{1}{2} + it)$ for $\Xi(t)$.

If we write

$$s = \sigma + it = \tfrac{1}{2} + \lambda + it,$$

the property (3) is paraphrased as

$$\Re\left\{\xi\left(\tfrac{1}{2} + \lambda + it\right)\right\} = \Re\left\{\xi\left(\tfrac{1}{2} - \lambda + it\right)\right\}, \tag{4}$$

$$\Im\left\{\xi\left(\tfrac{1}{2} + \lambda + it\right)\right\} = -\Im\left\{\xi\left(\tfrac{1}{2} - \lambda + it\right)\right\}, \tag{5}$$

By setting $\lambda = 0$ in (5), we find

$$\Im\left\{\xi\left(\tfrac{1}{2} + it\right)\right\} = 0, \quad \text{for all} \quad t, \tag{6}$$

which implies that $\xi(s)$ is real on the "critical line." Thus, if we define a real-valued function

$$\Xi(t) = \xi\left(\tfrac{1}{2} + it\right) = \Re\left\{\xi\left(\tfrac{1}{2} + it\right)\right\}, \tag{7}$$

the Riemann hypothesis can be paraphrased as "The zeros of $\Xi(t)$ are all real," which is indeed the way Riemann stated his conjecture, now known as the *Riemann hypothesis* or RH for short.

By applying Laplace's equation to $\Im\{\xi(s)\}$ and using (6), we readily find

$$\left.\frac{\partial^2 \Im\{\xi(s)\}}{\partial \lambda^2}\right|_{\lambda=0} = 0. \tag{8}$$

Thus, it follows that $\Im\{\xi(s)\}$ must be a polynomial in λ of degree 1 in the vicinity of $\lambda = 0$, viz.,

$$\Im\{\xi(s)\} \approx b(t)\lambda, \quad \text{for } \lambda \approx 0, \tag{9}$$

where $b(t)$ is a function of t only, independent of λ.

Similarly, by applying Laplace's equation to $\Re\{\xi(s)\}$ and using the Cauchy-Riemann equation:

$$\frac{\partial \Re\{\xi(s)\}}{\partial t} = -\frac{\partial \Im\{\xi(s)\}}{\partial \lambda}. \tag{10}$$

and using (9), we find that the real part of $\xi(s)$ is a polynomial in λ of degree 2:

$$\Re\{\xi(s)\} \approx \frac{b'(t)}{2}\lambda^2, \quad \text{for } \lambda \approx 0, \tag{11}$$

where $b'(t) = \dfrac{db(t)}{dt}$.

2 Preliminaries

2.1 Logarithmic Differentials of Holomorphic Functions

We begin with the following lemma that is applicable to any holomorphic function.

Lemma 2.1. *For a holomorphic function $f(s)$ we have*

$$\frac{1}{|f(s)|} \cdot \frac{\partial |f(s)|}{\partial \sigma} = \Re\left\{\frac{f'(s)}{f(s)}\right\}, \tag{12}$$

$$\frac{1}{|f(s)|} \cdot \frac{\partial |f(s)|}{\partial t} = -\Im\left\{\frac{f'(s)}{f(s)}\right\}, \tag{13}$$

wherever $f(s) \neq 0$, where $f'(s) = \dfrac{df(s)}{ds}$.

Proof. See Kobayashi [8]. □

By differentiating the logarithm of $f(s)$ further, we obtain

Corollary 2.1. *For the holomorphic function $f(s)$ of Lemma 2.1 the following identities also hold:*

$$\frac{1}{|f(s)|}\frac{\partial^2|f(s)|}{\partial\sigma^2} - \left(\frac{1}{|f(s)|}\frac{\partial|f(s)|}{\partial\sigma}\right)^2 = \Re\left\{\frac{f''(s)}{f(s)} - \left(\frac{f'(s)}{f(s)}\right)^2\right\}, \tag{14}$$

$$\frac{1}{|f(s)|}\frac{\partial^2|f(s)|}{\partial t^2} - \left(\frac{1}{|f(s)|}\frac{\partial|f(s)|}{\partial t}\right)^2 = -\Re\left\{\frac{f''(s)}{f(s)} - \left(\frac{f'(s)}{f(s)}\right)^2\right\}. \tag{15}$$

wherever $f(s) \neq 0$, where $f''(s) = \dfrac{d^2 f(s)}{ds^2}$.

Proof. See Kobayashi [8]. □

2.2 The Product Formula for ξ(s)

Hadamard [5] obtained in 1893 the following product-form representation

$$\xi(s) = \tfrac{1}{2}e^{Bs}\prod_n\left[\left(1 - \frac{s}{\rho_n}\right)e^{s/\rho_n}\right], \tag{16}$$

using Weirstrass's factorization theorem, which asserts that any entire function can be represented by a product involving its zeroes. In (16), the product is taken over all (infinitely many) zeros ρ_n's of the function $\xi(s)$, and B is a real constant. Detailed accounts of this formula are found in many books (see e.g., Edwards [3], Iwaniec [7] Patterson [13] and Titchmarsh [18]). Sondow and Dumitrescu [16] and Matiyasevich et al. [11] explored the use of the above product form, hoping to find a possible proof of the Riemann hypothesis.

By taking the logarithm of (16) and differentiating it, we obtain

$$\frac{\xi'(s)}{\xi(s)} = B + \sum_n\left(\frac{1}{s-\rho_n} + \frac{1}{\rho_n}\right). \tag{17}$$

From the definition of $\xi(s)$ in (2), we have

$$\frac{\xi'(s)}{\xi(s)} = \frac{1}{s} + \frac{1}{s-1} - \frac{\log\pi}{2} + \Psi(\tfrac{s}{2}) + \frac{\zeta'(s)}{\zeta(s)}, \tag{18}$$

where

$$\Psi(s) = \frac{\Gamma'(s)}{\Gamma(s)}$$

is the digamma function.

We equate (17) to (18), use the identity $\Psi(\frac{s}{2}+1) = \frac{1}{s} + \frac{1}{2}\Psi(\frac{s}{2})$, and set $s = 0$, obtaining

$$B + \sum_n\left(-\frac{1}{\rho_n} + \frac{1}{\rho_n}\right) = -1 - \tfrac{1}{2} + \tfrac{1}{2}\Psi(1) + \frac{\zeta'(0)}{\zeta(0)}. \tag{19}$$

By using $\zeta'(0)/\zeta(0) = \log(2\pi)$, and $\Psi(1) = \Gamma'(1) = -\gamma$ (where $\gamma = 0.5772218\ldots$ is the Euler constant), we determine the constant B as

$$B = \log(2\pi) - 1 - \tfrac{1}{2}\log\pi - \gamma/2 = \tfrac{1}{2}\log(4\pi) - 1 - \gamma/2 = -0.0230957\ldots. \tag{20}$$

Davenport ([1] pp. 81-82) derives an alternative expression for B. The reflective property of $\xi(s)$ gives the identity

$$\frac{\xi'(s)}{\xi(s)} = -\frac{\xi'(1-s)}{\xi(1-s)}, \tag{21}$$

which, together with (17), yields

$$B + \sum_n \left(\frac{1}{s-\rho_n} + \frac{1}{\rho_n} \right) = -B - \sum_n \left(\frac{1}{1-s-\rho_n} + \frac{1}{\rho_n} \right). \tag{22}$$

Thus,

$$\begin{aligned} B &= -\sum_n \frac{1}{\rho_n} - \frac{1}{2} \left(\sum_n \frac{1}{s-\rho_n} - \sum_n \frac{1}{s-(1-\rho_n)} \right) \\ &= -\sum_n \frac{1}{\rho_n} = -2 \sum_{n=1}^{\infty} \frac{\sigma_n}{\sigma_n^2 + t_n^2}, \end{aligned} \tag{23}$$

Note that the two summed terms in the parenthesis in the first line of the above cancel to each other, because if ρ_n is a zero, so is $1-\rho_n$. To obtain the final expression in the above, we use the property that when $\rho_n = \sigma_n + it_n$ is a zero, so is its complex conjugate $\rho_n^* = \sigma_n - it_n$, thus we enumerate zeros in such a way that $\rho_n^* = \rho_{-n}$.

By substituting (23) back into (16), we obtain

$$\begin{aligned} \xi(s) &= \tfrac{1}{2} \exp\left(-s \sum_n \frac{1}{\rho_n} \right) \prod_n \left(1 - \frac{s}{\rho_n} \right) e^{s/\rho_n} = \tfrac{1}{2} \prod_n e^{-s/\rho_n} \left(1 - \frac{s}{\rho_n} \right) e^{s/\rho_n} \\ &= \tfrac{1}{2} \prod_n \left(1 - \frac{s}{\rho_n} \right). \end{aligned} \tag{24}$$

This is nothing but the product form

$$\xi(s) = \xi(0) \prod_n \left(1 - \frac{s}{\rho_n} \right),$$

which Edwards (see [3] p. 18 and pp. 46-47) attributes to Riemann.

Then, Eqn.(17) is simplified to

$$\frac{\xi'(s)}{\xi(s)} = \sum_n \frac{1}{s-\rho_n}. \tag{25}$$

From this and Lemma 2.1, we have

$$\frac{1}{|\xi(s)|} \frac{\partial |\xi(s)|}{\partial \sigma} = \Re \left(\sum_n \frac{1}{s-\rho_n} \right) = \sum_n \frac{\sigma - \sigma_n}{(\sigma-\sigma_n)^2 + (t-t_n)^2}. \tag{26}$$

Thus, we arrive at the following theorem concerning the monotonicity of the $|\xi(s)|$ function, which Sondow and Dumitrescu [16] proved in a little more complicated way based on (16) instead of (24). Matiyaesevich et al. [11] also discuss the monotonicity of the $\xi(s)$ and other functions.

Theorem 2.1 (Monotonicity of Modulus Function $|\xi(s)|$)**.** *Let $\sigma_{\sup}$ be the supremum of the real parts of all zeros:*

$$\sigma_{\sup} = \sup_n \{\sigma_n\}.$$

Then the modulus $|\xi(\sigma + it)|$ is a monotone increasing function of σ in the region $\sigma > \sigma_{\sup}$ for all real t. Likewise, the modulus is a monotone decreasing function of σ in the region $\sigma < \sigma_{\inf}$, where

$$\sigma_{\inf} = \inf_n \{\sigma_n\} = 1 - \sigma_{\sup}.$$

Proof. It is apparent from (26) that $|\xi(s)|$ is a monotone increasing function of σ in the range $\sigma > \sigma_{\sup} \geq \frac{1}{2}$ for all t. Because of the reflective property (3) it then readily follows that $|\xi(s)|$ is a monotone decreasing function of σ in the range $\sigma < 1 - \sigma_{\sup} \leq \frac{1}{2}$. □

Thus, if all zeta zeros are located on the critical line, i.e., if $\sigma_{\sup} = \sigma_{\inf} = \frac{1}{2}$, the derivative of the modulus $|\xi(s)|$ is positive for $\sigma > \frac{1}{2}$, and negative for $\sigma < \frac{1}{2}$. Thus, we have shown the necessity of monotonicity of the modulus function $|\xi(s)|$, which has been one of major concerns towards a proof of the Riemann hypothesis.

Corollary 2.2 (Monotonicity of Modulus Function $|\xi(s)|$, if the Riemann hypothesis is true)**.** *If all zeta zeros are on the critical line, the modulus $|\xi(\sigma + it)|$ is a monotone increasing function of σ in the right half plane, $\sigma > \frac{1}{2}$. Likewise, the modulus is a monotone decreasing function of σ in the left half plane, $\sigma < \frac{1}{2}$.*

Proof. The above discussion that has led to this corollary should suffice as a proof. □

2.3 Functions $\mathbf{a}(\lambda, \mathbf{t}), \mathbf{b}(\lambda, \mathbf{t}), \alpha(\lambda, \mathbf{t}), \beta(\lambda, \mathbf{t})$ and Their Properties

Take the imaginary part of both sides of (25) and set $s = \frac{1}{2} + it$. By noting that $\xi(s)$ is real for $\sigma = \frac{1}{2}$, we obtain

$$\frac{1}{\xi(s)} \frac{\partial \Im(\xi(s))}{\partial \sigma}\bigg|_{\sigma=\frac{1}{2}} = \sum_n \frac{t - t_n}{(t - t_n)^2 + (\frac{1}{2} - \sigma_n)^2}. \tag{27}$$

Recall the function $b(t)$ defined in (9). Then, the LHS of the above is $\dfrac{b(t)}{\Xi(t)}$, where

$$\Xi(t) = \xi\left(\tfrac{1}{2} + it\right) = \frac{1}{2} \prod_n \left(1 - \frac{\frac{1}{2} + it}{\sigma_n + it_n}\right) \tag{28}$$

$$b(t) = \frac{\partial \Im\{\xi(s)\}}{\partial \sigma}\bigg|_{\sigma=\frac{1}{2}} = \Xi(t) \cdot \sum_n \frac{t - t_n}{(t - t_n)^2 + (\frac{1}{2} - \sigma_n)^2}. \tag{29}$$

Differentiate (25) once more, and we obtain

$$\frac{\xi''(s)\xi(s) - \xi'^2(s)}{\xi^2(s)} = -\sum_n \frac{1}{(s - \rho_n)^2},$$

which can be rearranged to yield

$$\frac{\xi''(s)}{\xi(s)} = \left(\frac{\xi'(s)}{\xi(s)}\right)^2 - \sum_n \frac{1}{(s - \rho_n)^2}. \tag{30}$$

Taking the real part of both sides, and evaluating them at $s = \frac{1}{2} + it$, we find

$$\begin{aligned} \frac{2a(t)}{\Xi(t)} &= -\left(\frac{b(t)}{\Xi(t)}\right)^2 + \sum_n \frac{(t - t_n)^2 - (\frac{1}{2} - \sigma_n)^2}{\left[(\frac{1}{2} - \sigma_n)^2 + (t - t_n)^2\right]^2} \\ &= \frac{-b^2(t)^2 + b'(t)\Xi(t) - b(t)\Xi'(t)}{\Xi^2(t)}. \end{aligned} \tag{31}$$

where

$$2a(t) = \frac{\partial^2 \xi(s)}{\partial \sigma^2}\bigg|_{\sigma=\frac{1}{2}}. \tag{32}$$

From the Cauchy-Riemann equation we find

$$\Xi'(t) = -\frac{\partial \Im\{\xi(s)\}}{\partial \sigma}\bigg|_{\sigma=\frac{1}{2}} = -b(t). \tag{33}$$

By substituting this into (31), we obtain a surprisingly simple result:

$$a(t) = \tfrac{1}{2} b'(t) = -\tfrac{1}{2}\Xi''(t), \tag{34}$$

which can be alternatively obtained by applying the Laplace equation to (32).

The above formulae carry over to any point $s = \frac{1}{2} + \lambda + it$:

Lemma 2.2. *Let us define*

$$2a(\lambda,t)=\frac{\partial^2\Re\{\xi(s)\}}{\partial\lambda^2}=-\Re\{\xi''(t)\}, \tag{35}$$

$$b(\lambda,t)=\frac{\partial\Im\{\xi(s)\}}{\partial\lambda}, \tag{36}$$

where $\xi''(s)$ is the second partial derivative of $\xi(s)$ with respect to t. Then, the following relations hold:

$$a(\lambda,t)=\tfrac{1}{2}b'(\lambda,t), \tag{37}$$

$$b(\lambda,t)=-\Re\{\xi'(t)\} \tag{38}$$

Proof. By applying the Cauchy-Riemann equations and Laplace's equation, the above relations can be easily derived. □

We now derive similar functions and their relations by interchanging $\Re\{\xi(s)\}$ and $\Im\{\xi(s)\}$.

Corollary 2.3. *Let us define*

$$2\alpha(\lambda,t)=\frac{\partial^2\Im\{\xi(s)\}}{\partial\lambda^2}=-\Im\{\xi''(s)\}, \tag{39}$$

$$\beta(\lambda,t)=\frac{\partial\Re\{\xi(s)\}}{\partial\lambda}. \tag{40}$$

Then the following relations hold:

$$\alpha(\lambda,t)=-\tfrac{1}{2}\beta'(\lambda,t), \tag{41}$$

$$\beta(\lambda,t)=\Im\{\xi'(s)\}. \tag{42}$$

$$\frac{\partial a(\lambda,t)}{\partial\lambda}=\alpha'(\lambda,t),\qquad \frac{\partial\alpha(\lambda,t)}{\partial\lambda}=-a'(\lambda,t) \tag{43}$$

$$\frac{\partial\beta(\lambda,t)}{\partial\lambda}=b'(\lambda,t),\qquad \frac{\partial b(\lambda,t)}{\partial\lambda}=-\beta'(\lambda,t). \tag{44}$$

Proof. By applying the Cauchy-Riemann equations and Laplace's equation, the above relations can be easily derived. □

3 The Fourier transform representation of $\xi(s)$

3.1 Integral representation of ξ(s)

We begin with the following integral representation of $\xi(s)$ (see Appendix A) found in Edwards [3], p.16.

$$\xi(s)=\frac{1}{2}-\frac{s(1-s)}{2}\int_1^\infty\psi(x)\left(x^{s/2}+x^{(1-s)/2}\right)\frac{dx}{x}, \tag{45}$$

where

$$\psi(x)=\sum_{n=1}^\infty e^{-n^2\pi x} \tag{46}$$

is called the *theta function*. By applying integration by parts to (45) and Jacobi's identity for the theta function[2] Edwards ([3], p. 17) gives the following expression by generalizing Riemann's result, which holds for any complex number s:

$$\xi(s)=4\int_1^\infty\frac{d[x^{3/2}\psi'(x)]}{dx}x^{-1/4}\cosh\left[\tfrac{1}{2}\left(s-\tfrac{1}{2}\right)\log x\right]\,dx. \tag{48}$$

[2] Jacobi's identity for the theta function $\psi(x)$ is

$$2\psi(x)+1=x^{-1/2}\left(2\psi(x^{-1})+1\right). \tag{47}$$

By writing

$$\frac{d[x^{3/2}\psi'(x)]}{dx}x^{-1/4} = \pi x^{1/4}D(x) \tag{49}$$

with $D(x)$ defined by

$$D(x) = \sum_{n=1}^{\infty} n^2(n^2\pi x - \tfrac{3}{2})e^{-n^2\pi x} > 0, \quad \text{for} \quad x \geq 1, \tag{50}$$

we can write (48) as

$$\xi(s) = 4\pi \int_1^{\infty} x^{1/4}D(x)\cos\left(\frac{\tau \log x}{2}\right) dx, \tag{51}$$

where τ is a complex number defined by

$$\tau = t - i\lambda = -i(s - \tfrac{1}{2}), \tag{52}$$

and we used the identity $\cosh(iy) = \cos y$. By changing the variable from x to ω by

$$\omega = \frac{\log x}{2}, \quad x \geq 1, \tag{53}$$

and defining

$$S(\omega) = 8\pi e^{5\omega/2}D(e^{2\omega}), \quad \omega \geq 0 \tag{54}$$

we can write (51) as

$$\xi(s) = \int_0^{\infty} S(\omega)\cos(\omega\tau)\, d\omega, \tag{55}$$

which is a compact expression for

$$\xi(\tfrac{1}{2} + \lambda + it) = \int_0^{\infty} S(\omega)\left(\cos\omega t\cosh(\omega\lambda) + i\sin\omega t\sinh(\omega\lambda)\right)\, d\omega. \tag{56}$$

On the critical line $s = \frac{1}{2} + it$ (i.e., when $\lambda = 0$), the above reduces to a more familiar formula

$$\Xi(t) = \int_0^{\infty} S(\omega)\cos(\omega t)\, d\omega. \tag{57}$$

3.2 The kernel function S(ω) as a power spectral function.

The kernel $S(\omega)$ defined by (54) is positive for all $\omega \geq 0$, because $D(x)$ is positive for $x \geq 1$. Therefore, $S(\omega)$ can qualify as a *spectral density function* of a certain wide-sense stationary (a.k.a. weakly stationary) process, and we can interpret $\Xi(t)$ as its autocorrelation function (see e.g., [10] p. 349). In this context, the Fourier transforms between the spectrum $S(\omega)$ and the function $\Xi(t)$ are what is known as the Wiener-Khinchin theorem (a.k.a. the Wiener-Khinchin-Einstein theorem). The inverse transform to (57), given below by (61), exists when $\Xi(t)$ is absolutely integrable.

The Fourier transform representation (57) has been studied by George Pólya [14] and others (see e.g., Titchmarsh [18], Chapter 10). Dimitrov and Rusev [2] give a comprehensive review of the past work on "zeros of entire Fourier transforms," including Pólya's work.

From the above observation that $S(\omega)$ is positive for $\omega \geq 0$, we can readily establish the following proposition:

Theorem 3.1. *The modulus $|\Xi(t))|$ is maximum at $t=0$, i.e.,*

$$|\Xi(t)| \leq \Xi(0) = 0.4971\ldots, \quad \textit{for all} \ \ t. \tag{58}$$

Furthermore,

$$\int_0^\infty \Xi(t)\,dt = 3\pi\left(\frac{\pi^{1/4}}{\Gamma(3/4)} - 1\right) = 2.8067\ldots. \tag{59}$$

Proof. From (55), it readily follows that

$$|\Xi(t)| \leq \int_0^\infty |S(\omega)|\,d\omega = \int_0^\infty S(\omega)\,d\omega = \Xi(0). \tag{60}$$

Since $\zeta(\frac{1}{2}) = -1.46035\ldots$[3], and $g(\frac{1}{2}) = -\frac{1}{8}\pi^{-1/4}\Gamma(\frac{1}{4}) = -0.3404\ldots$, we have $\Xi(0) = \xi(\frac{1}{2}) = g(\frac{1}{2})\zeta(\frac{1}{2}) = 0.4971\ldots$.

From the Wiener-Khinchin inverse formula, which holds when $\Xi(t)$ is absolutely integrable, we have

$$S(\omega) = \frac{2}{\pi}\int_0^\infty \Xi(t)\cos(\omega t)\,dt. \tag{61}$$

By setting $\omega = 0$, we readily find

$$S(0) = \frac{2}{\pi}\int_0^\infty \Xi(t)\,dt. \tag{62}$$

By setting $\omega = 0$ in (54), we have

$$S(0) = 8\pi D(1) = 8\left(\tfrac{3}{2}\psi'(1) + \psi''(1)\right). \tag{63}$$

The function $\psi(x)$ satisfies the aforementioned Jacobi's identity (47). By differentiating the identity equation, we find

$$2\psi'(x) = -\tfrac{1}{2}x^{-3/2} - x^{-3/2}\psi(1/x) - 2x^{-5/2}\psi'(1/x) \tag{64}$$

By setting $x = 1$ in (64) we obtain

$$\psi'(1) = -\tfrac{1}{8}(1 + 2\psi(1)) \tag{65}$$

$$\tag{66}$$

The value of $\psi(1)$ is known (see e.g., Yi [19], Theorem 5.5 in p. 398)

$$\psi(1) = \tfrac{1}{2}\left(\frac{\pi^{1/4}}{\Gamma(3/4)} - 1\right) = \tfrac{1}{2}\left(\frac{1.3313}{1.2254} - 1\right) = 0.0432\ldots. \tag{67}$$

Hence,

$$\psi'(1) = -\tfrac{1}{8}\frac{\pi^{1/4}}{\Gamma(3/4)} = -0.1358\ldots. \tag{68}$$

The numerical evaluation of $\psi''(1)$ is straightforward, since its series representation converges rapidly:

$$\psi''(1) = \pi^2\sum_{n=1}^{\infty} n^4 e^{-\pi n^2} \approx \pi^2\sum_{n=1}^{2} n^4 e^{-\pi n^2} = 0.4271\ldots. \tag{69}$$

Thus, we finally evaluate

$$\int_0^\infty \Xi(t)\,dt = \frac{\pi}{2}S(0) = 4\pi\left(\tfrac{3}{2}\psi'(1) + \psi''(1)\right) = 2.8067\ldots \tag{70}$$

□

[3] See e.g. `https://oeis.org/A059750`.

The variable t of the complex variable $s = \sigma + it = \frac{1}{2} + \lambda + it$ is often called the *height* in the zeta function related literature. In view of the Wiener-Khinchin theorem (57) and (61), it may be appropriate to interpret t as "time" and the variable ω of $S(\omega)$ as the "(angular) frequency." Then, we may refer to the complex number τ defined by (52) as "complex-time." Use of the complex-time τ allow the compact representation (55) given earlier, viz.

$$\xi(s) = \int_0^\infty S(\omega)\cos(\omega\tau)\,d\omega. \tag{71}$$

This interpretation of Riemann's result (48) will shed some new light to the Fourier transform representation of the $\xi(s)$ function. We will further discuss this in a later section.

4 Further results on the Fourier transform representation

4.1 Decomposition of $\mathbf{S}(\omega)$

In the Fourier transform representation (55) the kernel function $S(\omega)$ can be expressed as

$$S(\omega) = \sum_{n=1}^{\infty} S_n(\omega), \tag{72}$$

with

$$S_n(\omega) = 8\pi e^{5\omega/2} D_n(e^{2\omega}), \tag{73}$$

where

$$D_n(x) = n^2(n^2\pi x - \tfrac{3}{2})e^{-n^2\pi x}. \tag{74}$$

The Fourier transform can therefore be written as a summation of infinite components, i.e.,

$$\xi(s) = \sum_{n=1}^{\infty} f_n(s), \tag{75}$$

with

$$\begin{aligned} f_n(s) &= \int_0^\infty S_n(\omega)\cos(\omega\tau)\,d\omega \\ &= 8\pi \int_0^\infty e^{5\omega/2} D_n(e^{2\omega})\cos(\omega\tau)\,d\omega. \end{aligned} \tag{76}$$

The switching in the order between the summation over n and the integration over ω, as used in (76) and (75), can be justified, because the series $\sum_{n=1}^{N} S_n(\omega)$ uniformly converges to $S(\omega)$ as $N \to \infty$ in the entire range $\omega \geq 0$. Note also that in the range $\omega \geq 0$, $S(\omega)$ is predominantly determined by its first components $S_1(\omega)$, leaving $S_n(\omega), n \geq 2$ negligibly smaller. However, any attempt to replace $S(\omega)$ by $S_1(\omega)$ in an effort to prove the Riemann hypothesis would fail, as argued by Titchmarsh (see [18], Chapter 10, p. 256).

4.2 The Fourier transform of $\mathbf{S}(\omega)$ in $-\infty < \omega < \omega$.

Now let us consider the Fourier transform of $S(\omega)$ defined over the entire real line $-\infty < \omega < \infty$, instead of the positive line $\omega \geq 0$. Note that the kernel $S(\omega)$ of (54) extended to the range $-\infty < \omega < \infty$ is symmetric, i.e.,

$$S(-\omega) = S(\omega), \quad -\infty < \omega < \infty, \tag{77}$$

which can be shown using Jacobi's identity (47). See [9] for a derivation of (77).

The Fourier transform representation (55) can then be rewritten as

$$\xi(s) = \tfrac{1}{2}\int_{-\infty}^{\infty} S(\omega)e^{i\omega\tau}\,d\omega = \tfrac{1}{2}\int_{-\infty}^{\infty} S(\omega)e^{\omega(s-\frac{1}{2})}\,d\omega. \tag{78}$$

Since the kernel $S(\omega)$ is a symmetric real function, we can readily derive the reflective property $\xi(1-s) = \xi(s)$ and thus $\xi(s)$ is real on the critical line.

The kernel $S_n(\omega)$ of (73) can be written as

$$S_n(\omega) = 8\pi n^2 e^{\frac{5\omega}{2}} D_1(n^2 e^{2\omega}) \tag{79}$$

with

$$D_1(x) = (\pi x - \tfrac{3}{2})e^{-\pi x}. \tag{80}$$

Furthermore, we can write $S_n(\omega)$ in terms of $S_1(\omega)$ as follows:

$$S_n(\omega) = \frac{1}{\sqrt{n}} S_1(\omega + \log n), \quad n = 1, 2, 3, \ldots. \tag{81}$$

By substituting (72) and (81) into the above, we obtain

$$\begin{aligned}\xi(s) &= \tfrac{1}{2}\int_{-\infty}^{\infty}\sum_{n=1}^{\infty} S_n(\omega)e^{i\omega\tau}\,d\omega = \tfrac{1}{2}\int_{-\infty}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\sqrt{n}}S_1(\omega+\log n)e^{i\omega\tau}\,d\omega \\ &= \tfrac{1}{2}\int_{-\infty}^{\infty} S_1(\omega')e^{i\omega'\tau}\,d\omega' \sum_{n=1}^{\infty}\frac{1}{\sqrt{n}}e^{-i\tau\log n},\end{aligned} \tag{82}$$

where we set $\omega + \log n = \omega'$ in the above derivation. The summed term is nothing but the zeta function $\zeta(s)$, i.e.,

$$\sum_{n=1}^{\infty}\frac{1}{\sqrt{n}}e^{-i\tau\log n} = \sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}+i\tau}} = \zeta\left(\tfrac{1}{2}+i\tau\right) = \zeta(s), \tag{83}$$

The result (82) can be compactly expressed as

$$\xi(s) = \xi_1(s)\zeta(s). \tag{84}$$

By writing

$$g(s) = \frac{s(s-1)}{2}\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right), \tag{85}$$

we can state the following proposition by referring to (2):

Theorem 4.1. *(The Fourier transform of* $\mathbf{S_1}(\omega)$*)*
The function $g(s)$ (85) that transforms $\zeta(s)$ into $\xi(s)$ by multiplication is the Fourier transform of $S_1(\omega)$ to the domain τ, i.e.,

$$g(s) = \tfrac{1}{2}\int_{-\infty}^{\infty} S_1(\omega)e^{i\omega\tau}\,d\omega = \xi_1(s), \tag{86}$$

where $\tau = t - i\lambda = t - i(\sigma - \frac{1}{2}) = -i(s - \frac{1}{2})$.

Proof. See [9]. □

Let us denote the Fourier transform of $S_n(\omega)$ as $\xi_n(s)$:

$$\xi_n(s) = \tfrac{1}{2}\int_{-\infty}^{\infty} S_n(\omega)e^{i\omega\tau}\,d\omega = \xi_1(s)n^{-s}, \tag{87}$$

and

$$\xi(s) = \sum_{n=1}^{\infty} \xi_n(s). \tag{88}$$

Note that the functions $\xi_n(s)$ are individually complex functions even on the critical line, since $S_n(\omega)$ are not symmetric functions, thus $\xi_n(s)$'s do not enjoy the reflective property that their sum $\xi(s)$ does. If we define

$$\overline{\xi}_n(s) = \tfrac{1}{2}[\xi_n(s) + \xi_n(1-s)] = \tfrac{1}{2}[g_n(s)n^{-s} + g_n(1-s)n^{s-1}], \tag{89}$$

this function is reflective and

$$\xi(s) = \sum_{n=1}^{\infty} \overline{\xi}_n(s). \tag{90}$$

4.3 Properties of the g(s) function

In this section we discuss some properties of $g(s)$ defined by (85), and its relations to the Riemann-Siegel function and Hardy's Z-function.

We set $s = \frac{1}{2} + it$ in $g(s)$ and define real functions $a(t)$ and $b(t)$:

$$\begin{aligned} a(t) &= \Re\left\{\log\Gamma\left(\tfrac{1}{4} + \tfrac{it}{2}\right)\right\}, \\ b(t) &= \Im\left\{\log\Gamma\left(\tfrac{1}{4} + \tfrac{it}{2}\right)\right\}. \end{aligned} \tag{91}$$

Then, we can write

$$g\left(\tfrac{1}{2} + it\right) = -\tfrac{1}{2}\left(t^2 + \tfrac{1}{4}\right)\pi^{-1/4}e^{-i\frac{t}{2}\log\pi}e^{a(t)+ib(t)}. \tag{92}$$

By defining two real functions $r(t)$ and $\vartheta(t)$

$$\begin{aligned} r(t) &= -\tfrac{1}{2}\left(t^2 + \tfrac{1}{4}\right)\pi^{-1/4}e^{a(t)}, \\ \vartheta(t) &= b(t) - \tfrac{t}{2}\log\pi = \Im\left\{\log\Gamma\left(\tfrac{1}{4} + \tfrac{it}{2}\right)\right\} - \tfrac{t}{2}\log\pi, \end{aligned} \tag{93}$$

we can rewrite (92) as

$$g\left(\tfrac{1}{2} + it\right) = r(t)e^{i\vartheta(t)}. \tag{94}$$

The function $\vartheta(t)$ of (93) is called the Riemann-Siegel theta function, and the function $Z(t)$ defined by

$$Z(t) = \zeta\left(\tfrac{1}{2} + it\right)e^{i\vartheta(t)}, \tag{95}$$

is often referred to as Hardy's Z-function [6], which is real for real t and has the same zeros as $\zeta(s)$ at $s = \frac{1}{2} + it$, with t real. Thus, locating the Riemann zeros on the critical line reduces to locating zeros on the real line of $Z(t)$. Furthermore,

$$|Z(t)| = |\zeta(\tfrac{1}{2} + it)|.$$

Consider the following Stirling approximation formula for $\Gamma(s)$:

$$\log\Gamma(s) \approx \tfrac{1}{2}\log\frac{2\pi}{s} + s(\log s - 1). \tag{96}$$

Then

$$\log\Gamma(s/2) \approx \left(1-\tfrac{s}{2}\right)\log 2 + \tfrac{1}{2}\log\pi + \left(\tfrac{s-1}{2}\right)\log s - \tfrac{s}{2}. \tag{97}$$

By evaluating the above at $s = \frac{1}{2} + it$, we have

$$\begin{aligned}\log\Gamma\left(\tfrac{1}{4}+\tfrac{it}{2}\right) &= a(t) + ib(t)\\ &\approx \tfrac{3}{4}\log 2 + \tfrac{1}{2}\log\pi - \left(\tfrac{1}{4}+\tfrac{t\theta(t)}{2}\right) - \tfrac{1}{8}\log\left(t^2+\tfrac{1}{4}\right) + i\left[\tfrac{t}{4}\log\left(t^2+\tfrac{1}{4}\right) - \tfrac{t}{2} - \tfrac{t}{2}\log 2 - \tfrac{\theta(t)}{4}\right],\end{aligned} \tag{98}$$

where

$$\theta(t) = tan^{-1}2t. \tag{99}$$

Thus, we obtain

$$\begin{aligned} r(t) &\approx -2^{-\frac{1}{4}}\pi^{\frac{1}{4}}\left(t^2+\tfrac{1}{4}\right)^{\frac{7}{8}} e^{-\frac{1}{4}-\frac{\theta(t)t}{2}}\\ \vartheta(t) &\approx \tfrac{t}{2}\log\tfrac{t}{2\pi e} - \tfrac{\theta(t)}{4} + \tfrac{t}{4}\log\left(1+\tfrac{1}{4t^2}\right).\end{aligned} \tag{100}$$

If we set

$$A(t) = -r(t), \quad \text{and} \quad \varphi(t) = \vartheta(t) + \pi, \tag{101}$$

then,

$$g\left(\tfrac{1}{2}+it\right) = A(t)e^{i\varphi(t)}. \tag{102}$$

We denote the real and imaginary parts of $g\left(\frac{1}{2}+it\right)$ by $G(t)$ and $\hat{G}(t)$, respectively, viz:

$$g\left(\tfrac{1}{2}+it\right) = G(t) + i\hat{G}(t). \tag{103}$$

Then it is apparent that

$$G(t) = A(t)\cos\varphi(t), \quad \text{and} \quad \hat{G}(t) = A(t)\sin\varphi(t). \tag{104}$$

For sufficiently large $t \gg 1$, $\theta(t) \approx \frac{\pi}{2}$. Thus, $A(t)$ and $\varphi(t)$ can be approximated by

$$\begin{aligned} A(t) &\approx (2e\pi)^{-\frac{1}{4}} e^{-\frac{\pi t}{4}} t^{\frac{7}{4}}, \quad \text{for} \quad t \gg 1,\\ \varphi(t) &\approx \frac{t}{2}\log\frac{t}{2e\pi} + \frac{7\pi}{8}, \quad \text{for} \quad t \gg 1.\end{aligned} \tag{105}$$

The function $A(t)$ is strictly positive for all t, hence $G(t)$ becomes zero only when $\varphi(t) = n\pi + \frac{\pi}{2}$ for some integer n. Similarly, $\hat{G}(t)$ crosses zero only when $\varphi(t) = n\pi$ for integer n. Thus, the number of zeros $N(T)$ of $G(t)$ in $(0,T)$ is given by

$$N(T) = \frac{\varphi(T)}{\pi} \approx \frac{T}{2\pi}\log\frac{T}{2\pi e} + \frac{7}{8}, \quad T > T(\epsilon). \tag{106}$$

The same result should hold for the number of zeros $N(T)$ of $\hat{G}(T)$ in $(0,T)$. The above $N(T)$ agrees to the asymptotic "Riemann-von Mangoldt formula" for the number of zeros of $\zeta\left(\frac{1}{2}+it\right)$ (and hence the number of zeros of $\xi\left(\frac{1}{2}+it\right)$, as well), which Riemann conjectured in his 1859 lecture and proved by von Mangoldt in 1905 (see e.g.,[3, 12]).

Gram [4] observed in 1909 that zeros of $Z(t)$ and zeros of $\sin\vartheta(t)$ alternate on the t axis, with some few exception (see Edwards [3] p. 125). His observation is consistent with our analysis given above that the number of zeros $\hat{G}(t) = A(t)\sin\varphi(t) = -A(t)\sin\vartheta(t)$ in the interval $[0,t]$ is asymptotically equivalent to that of $\zeta(\frac{1}{2}+it)$ (and hence that of $\Xi(t)$ as well). If we define the complex function

$$z(s) = \frac{\xi(s)}{r(t)}, \tag{107}$$

then $z(s)$ is reflective. Furthermore $z\left(\frac{1}{2}+it\right) = Z(t)$, because (94) and (95) imply

$$Z(t) = \frac{\Xi(t)}{r(t)}. \tag{108}$$

Let $G_n(t)$ denote the value on the critical line of $\overline{\xi}_n(s)$ defined in (89), i.e.,

$$\begin{aligned} G_n(t) = \overline{\xi}_n\left(\tfrac{1}{2}+it\right) &= \tfrac{1}{2}[g(s)n^{-s} + g(1-s)n^{s-1}]\big|_{s=\frac{1}{2}+it} = \tfrac{1}{2}\left[(G(t)+i\hat{G}(t))n^{-\frac{1}{2}-it} + (G(t)-i\hat{G}(t))n^{-\frac{1}{2}+it}\right] \\ &= G(t)n^{-\frac{1}{2}}\cos(t\log n) + \hat{G}(t)n^{-\frac{1}{2}}\sin(t\log n) = A(t)n^{-\frac{1}{2}}\cos(\varphi(t) - t\log n). \end{aligned} \tag{109}$$

Thus, we find

$$\Xi(t) = \sum_{n=1}^{\infty} G_n(t) = A(t)\sum_{n=1}^{\infty} n^{-\frac{1}{2}}\cos(\varphi(t) - t\log n), \tag{110}$$

where $A(t) = -r(t)$ and $\varphi(t) = \vartheta(t) + \pi$ are defined in (101), and

$$g\left(\tfrac{1}{2}+it\right) = G(t) + i\hat{G}(t) = A(t)e^{i\varphi(t)} = -r(t)e^{i\vartheta(t)}. \tag{111}$$

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Appendix A: Derivation of (2) and (45)

Although the essence of both equations is found in Riemann's original paper, we follow Edwards [3] and Matsumoto [12]. We begin with the integral representation of the gamma function

$$\Gamma(s) = \int_0^\infty u^{s-1} e^{-u}\, du. \tag{A.1}$$

By setting $u = \pi n^2 x$, we have

$$\Gamma(s) = \pi^s n^{2s} \int_0^\infty x^{s-1} e^{-\pi n^2 x}\, dx. \tag{A.2}$$

Then,

$$\Gamma(s/2) = \pi^{s/2} n^s \int_0^\infty x^{\frac{s}{2}-1} e^{-\pi n^2 x}\, dx, \tag{A.3}$$

from which we obtain

$$\pi^{-s/2}\Gamma(s/2) n^{-s} = \int_0^\infty x^{\frac{s}{2}-1} e^{-\pi n^2 x}\, dx. \tag{A.4}$$

By summing up over n from 1 to infinity, we obtain

$$\pi^{-s/2}\Gamma(s/2)\zeta(s) = \int_0^\infty x^{\frac{s}{2}-1} \psi(x)\, dx, \tag{A.5}$$

where $\psi(x)$ is given defined in (46).

Let us write (A.5) as $\nu(s)$, and the split the integration interval of the RHS into the two subintervals, $[0, 1)$ and $[1, \infty)$, viz:

$$\begin{aligned} \nu(s) = \pi^{-s/2}\Gamma(s/2)\zeta(s) &= \int_0^\infty x^{\frac{s}{2}-1} \psi(x)\, dx \\ &= \int_0^1 x^{\frac{s}{2}-1} \psi(x)\, dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x)\, dx. \end{aligned} \tag{A.6}$$

By substituting Jacobi's identity for $\psi(x)$ given by (47) into the first integrand, we find

$$\begin{aligned}\nu(s) &= \int_0^1 x^{\frac{s}{2}-1}\left(x^{-1/2}\psi(x^{-1}) + \tfrac{1}{2}x^{-1/2} - \tfrac{1}{2}\right)dx + \int_1^\infty x^{\frac{s}{2}-1}\psi(x)\,dx \\ &= -\frac{1}{1-s} - \frac{1}{s} + \int_1^\infty \left(x^{\frac{s}{2}-1} + x^{\frac{1-s}{2}-1}\right)\psi(x)\,dx. \end{aligned} \tag{A.7}$$

It is apparent that $\nu(s)$ satisfies the reflective property, i.e.,

$$\nu(1-s) = \nu(s).$$

The function $\nu(s)$ is not an entire function since it has $s = 0$ and $s = 1$ as poles. By multiplying $\nu(s)$ by $-\dfrac{s(1-s)}{2}$, we define $\xi(s)$, viz.

$$\xi(s) = -\tfrac{1}{2}s(1-s)\nu(s) = \tfrac{1}{2}s(s-1)\pi^{-s/2}\Gamma(s/2)n^{-s}\zeta(s), \tag{A.8}$$

which is (2).

The function $\xi(s)$ should satisfy the reflective property (3) since both $\nu(s)$ and $-\dfrac{s(1-s)}{2}$ are reflective. From (A.7), we obtain

$$\xi(s) = \tfrac{1}{2} - \tfrac{1}{2}s(1-s)\int_1^\infty \left(x^{\frac{s}{2}} + x^{\frac{1-s}{2}}\right)\psi(x)\,\frac{dx}{x}, \tag{A.9}$$

which is (45). From the last expression, it is apparent that $\xi(0) = \xi(1) = \frac{1}{2}$.

