Some results on the $\xi(\mathbf{s})$ and $\Xi(\mathbf{t})$ functions associated with Riemann's $\zeta(\mathbf{s})$ function. *

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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 reexamine 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 $\xi(s)$ 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)

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

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

$$\xi(1-s) = \xi(s).$$
(3)

If we write

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

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¹In 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 $\Xi(t)$.

the property (3) is paraphrased as

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $f'(s) = \frac{df(s)}{ds}$.

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:

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

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

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

Proof. See Kobayashi [8].

2.2 The Product Formula for $\xi(s)$

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

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

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

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

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

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

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

$$B = \log(2\pi) - 1 - \frac{1}{2}\log\pi - \gamma/2 = \frac{1}{2}\log(4\pi) - 1 - \gamma/2 = -0.0230957\dots$$
(20)

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

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

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which, together with (17), yields

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

Thus,

$$B = -\sum_{n} \frac{1}{\rho_n} - \frac{1}{2} \left(\sum_{n} \frac{1}{s - \rho_n} - \sum_{n} \frac{1}{s - (1 - \rho_n)} \right)$$
$$= -\sum_{n} \frac{1}{\rho_n} = -2\sum_{n=1}^{\infty} \frac{\sigma_n}{\sigma_n^2 + t_n^2},$$
(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

$$\xi(s) = \frac{1}{2} \exp\left(-s \sum_{n} \frac{1}{\rho_{n}}\right) \prod_{n} \left(1 - \frac{s}{\rho_{n}}\right) e^{s/\rho_{n}} = \frac{1}{2} \prod_{n} e^{-s/\rho_{n}} \left(1 - \frac{s}{\rho_{n}}\right) e^{s/\rho_{n}}$$
$$= \frac{1}{2} \prod_{n} \left(1 - \frac{s}{\rho_{n}}\right).$$
(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

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

From this and Lemma 2.1, we have

$$\frac{1}{|\xi(s)|} \frac{\partial |\xi(s)|}{\partial \sigma} = \Re\left(\sum_{n} \frac{1}{s - \rho_n}\right) = \sum_{n} \frac{\sigma - \sigma_n}{(\sigma - \sigma_n)^2 + (t - t_n)^2}.$$
(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 σ_{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 $\sigma > \sigma_{\sup} \ge \frac{1}{2}$ 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 $\sigma < 1 - \sigma_{\sup} \le \frac{1}{2}$.

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

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

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

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

$$b(t) = \left. \frac{\partial \Im \left\{ \xi(s) \right\}}{\partial \sigma} \right|_{\sigma = \frac{1}{2}} = \Xi(t) \cdot \sum_{n} \frac{t - t_n}{(t - t_n)^2 + (\frac{1}{2} - \sigma_n)^2}.$$
 (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

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

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

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

where

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

From the Cauchy-Riemann equation we find

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

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

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

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

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

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Lemma 2.2. Let us define

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

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

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

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

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

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

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

Corollary 2.3. Let us define

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

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

Then the following relations hold:

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

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

$$\frac{\partial a(\lambda, t)}{\partial \lambda} = \alpha'(\lambda, t), \qquad \frac{\partial \alpha(\lambda, t)}{\partial \lambda} = -a'(\lambda, t)$$
(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. $\hfill \square$

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

3.1 Integral representation of $\xi(\mathbf{s})$

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 function² Edwards ([3], p. 17) gives the following expression by generalizing Riemann's result, which holds for any complex number s:

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

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

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

By writing

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

with D(x) defined by

$$D(x) = \sum_{n=1}^{\infty} n^2 (n^2 \pi x - \frac{3}{2}) e^{-n^2 \pi x} > 0, \text{ for } x \ge 1,$$
(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

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

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

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

and defining

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

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

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

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

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

3.2 The kernel function $S(\omega)$ as a power spectral function.

The kernel $S(\omega)$ defined by (54) is positive for all $\omega \ge 0$, because D(x) is positive for $x \ge 1$. 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 $\omega \ge 0$, we can readily establish the following proposition:

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

$$\Xi(t)| \le \Xi(0) = 0.4971..., \text{ for all } t.$$
 (58)

Furthermore,

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

Proof. From (55), it readily follows that

$$|\Xi(t)| \le \int_0^\infty |S(\omega)| \, d\omega = \int_0^\infty S(\omega) \, d\omega = \Xi(0).$$
(60)

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

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

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

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

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

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

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

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

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

By setting x = 1 in (64) we obtain

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

(66)

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

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

Hence,

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

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

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

Thus, we finally evaluate

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

 $^{^3\}mathrm{See}~\mathrm{e.g.}$ 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 $S(\omega)$

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

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

$$f_n(s) = \int_0^\infty S_n(\omega) \cos(\omega\tau) \, d\omega$$
$$= 8\pi \int_0^\infty e^{5\omega/2} D_n(e^{2\omega}) \cos(\omega\tau) \, d\omega.$$
(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 $\omega \ge 0$. Note also that in the range $\omega \ge 0$, $S(\omega)$ is predominantly determined by its first components $S_1(\omega)$, leaving $S_n(\omega), n \ge 2$ 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 $S(\omega)$ 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 $\omega \ge 0$. 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

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

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

with

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

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

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

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

$$\xi(s) = \frac{1}{2} \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} S_n(\omega) e^{i\omega\tau} d\omega = \frac{1}{2} \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} S_1(\omega + \log n) e^{i\omega\tau} d\omega$$
$$= \frac{1}{2} \int_{-\infty}^{\infty} S_1(\omega') e^{i\omega'\tau} d\omega' \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} e^{-i\tau \log n},$$
(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.,

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

The result (82) can be compactly expressed as

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

By writing

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

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

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 $\xi_n(s)$:

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

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

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

this function is reflective and

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

$$a(t) = \Re \left\{ \log \Gamma \left(\frac{1}{4} + \frac{it}{2} \right) \right\},$$

$$b(t) = \Im \left\{ \log \Gamma \left(\frac{1}{4} + \frac{it}{2} \right) \right\}.$$
(91)

Then, we can write

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

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

$$r(t) = -\frac{1}{2} \left(t^2 + \frac{1}{4} \right) \pi^{-1/4} e^{a(t)},$$

$$\vartheta(t) = b(t) - \frac{t}{2} \log \pi = \Im \left\{ \log \Gamma \left(\frac{1}{4} + \frac{it}{2} \right) \right\} - \frac{t}{2} \log \pi,$$
(93)

we can rewrite (92) as

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

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

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

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,

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

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

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

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Then

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

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

$$\log \Gamma\left(\frac{1}{4} + \frac{it}{2}\right) = a(t) + ib(t)$$

$$\approx \frac{3}{4}\log 2 + \frac{1}{2}\log \pi - \left(\frac{1}{4} + \frac{t\theta(t)}{2}\right) - \frac{1}{8}\log\left(t^2 + \frac{1}{4}\right) + i\left[\frac{t}{4}\log\left(t^2 + \frac{1}{4}\right) - \frac{t}{2} - \frac{t}{2}\log 2 - \frac{\theta(t)}{4}\right],$$
(98)

where

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

Thus, we obtain

$$r(t) \approx -2^{-\frac{1}{4}} \pi^{\frac{1}{4}} \left(t^2 + \frac{1}{4} \right)^{\frac{t}{8}} e^{-\frac{1}{4} - \frac{\theta(t)t}{2}} \vartheta(t) \approx \frac{t}{2} \log \frac{t}{2\pi e} - \frac{\theta(t)}{4} + \frac{t}{4} \log \left(1 + \frac{1}{4t^2} \right).$$
(100)

If we set

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

then,

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

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

Then it is apparent that

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

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

$$A(t) \approx (2e\pi)^{-\frac{1}{4}} e^{-\frac{\pi t}{4}} t^{\frac{7}{4}}, \text{ for } t \gg 1,$$

$$\varphi(t) \approx \frac{t}{2} \log \frac{t}{2e\pi} + \frac{7\pi}{8}, \text{ for } t \gg 1.$$
(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

$$N(T) = \frac{\varphi(T)}{\pi} \approx \frac{T}{2\pi} \log \frac{T}{2\pi e} + \frac{7}{8}, \quad T > T(\epsilon).$$
(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 $\zeta(\frac{1}{2} + it)$ (and hence the number of zeros of $\xi(\frac{1}{2} + it)$, 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

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

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

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

Thus, we find

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

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

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

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

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

$$\nu(s) = \int_0^1 x^{\frac{s}{2}-1} \left(x^{-1/2} \psi(x^{-1}) + \frac{1}{2} x^{-1/2} - \frac{1}{2} \right) dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x) dx$$
$$= -\frac{1}{1-s} - \frac{1}{s} + \int_1^\infty \left(x^{\frac{s}{2}-1} + x^{\frac{1-s}{2}-1} \right) \psi(x) dx.$$
(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 $-\frac{s(1-s)}{2}$, we define $\xi(s)$, viz.

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

which is (2).

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

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

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