Some results on the $\xi(s)$ and $\Xi(t)$ functions associated with Riemann’s $\zeta(s)$ 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 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 $\xi(s)$ and its properties

The Riemann zeta function is defined by

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

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 $\xi(s)$ defined by (see Appendix A)

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

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

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

If we write

$$s = \sigma + it = \frac{1}{2} + \lambda + it,$$
the property (3) is paraphrased as
\[ \Re \{ \xi \left( \frac{1}{2} + \lambda + it \right) \} = \Re \{ \xi \left( \frac{1}{2} - \lambda + it \right) \}, \]
\[ \Im \{ \xi \left( \frac{1}{2} + \lambda + it \right) \} = -\Im \{ \xi \left( \frac{1}{2} - \lambda + it \right) \}, \]
(4)

(5)

By setting \( \lambda = 0 \) in (5), we find
\[ \Im \{ \xi \left( \frac{1}{2} + it \right) \} = 0, \quad \text{for all } t, \]
(6)

which implies that \( \xi(s) \) is real on the “critical line.” Thus, if we define a real-valued function
\[ \Xi(t) = \xi \left( \frac{1}{2} + it \right) = \Re \{ \xi \left( \frac{1}{2} + it \right) \}, \]
(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
\[ \frac{\partial^2 \Im \{ \xi(s) \}}{\partial \lambda^2} \bigg|_{\lambda=0} = 0. \]
(8)

Thus, it follows that \( \Im \{ \xi(s) \} \) must be a polynomial in \( \lambda \) of degree 1 in the vicinity of \( \lambda = 0 \), viz.,
\[ \Im \{ \xi(s) \} \approx b(t) \lambda, \quad \text{for } \lambda \approx 0, \]
(9)

where \( b(t) \) is a function of \( t \) only, independent of \( \lambda \).

Similarly, by applying Laplace’s equation to \( \Re \{ \xi(s) \} \) and using the Cauchy-Riemann equation:
\[ \frac{\partial \Re \{ \xi(s) \}}{\partial t} = -\frac{\partial \Im \{ \xi(s) \}}{\partial \lambda}. \]
(10)

and using (9), we find that the real part of \( \xi(s) \) is a polynomial in \( \lambda \) of degree 2:
\[ \Re \{ \xi(s) \} \approx \frac{b'(t)}{2} \lambda^2, \quad \text{for } \lambda \approx 0, \]
(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
\[ \frac{1}{|f(s)|} \cdot \frac{\partial |f(s)|}{\partial \sigma} = \Re \left\{ \frac{f'(s)}{f(s)} \right\}, \]
\[ \frac{1}{|f(s)|} \cdot \frac{\partial |f(s)|}{\partial t} = -\Im \left\{ \frac{f'(s)}{f(s)} \right\}, \]
(12)
(13)

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

**Proof.** See Kobayashi [5].

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:

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

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

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

Proof. See Kobayashi [8]. \qed

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

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

\[
\xi(s) = \frac{i}{2} e^{B s} \prod_n \left[ \left( 1 - \frac{s}{\rho_n} \right) e^{\pi i / \rho_n} \right],
\]

using Weierstrass'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 $\rho_n$'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

\[
\frac{\xi'(s)}{\xi(s)} = B + \sum_n \left( -\frac{1}{s - \rho_n} + \frac{1}{\rho_n} \right).
\]

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

\[
\frac{\xi'(s)}{\xi(s)} = \frac{1}{s} + \frac{1}{s - 1} - \frac{\log \pi}{2} + \Psi\left(\frac{s}{2}\right) + \frac{\zeta'(s)}{\zeta(s)},
\]

where

\[
\Psi(s) = \frac{\Gamma'(s)}{\Gamma(s)}
\]

is the digamma function.

We equate (17) to (13), use the identity $\Psi\left(\frac{s}{2} + 1\right) = \frac{1}{s} + \frac{1}{2} \Psi\left(\frac{s}{2}\right)$, and set $s = 0$, obtaining

\[
B + \sum_n \left( -\frac{1}{\rho_n} + \frac{1}{\rho_n} \right) = -1 - \frac{1}{2} + \frac{1}{2} \Psi(1) + \frac{\zeta'(0)}{\zeta(0)}.
\]

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

\[
B = \log(2\pi) - 1 - \frac{1}{2} \log \pi - \gamma/2 = \frac{1}{2} \log(4\pi) - 1 - \gamma/2 = -0.0230957\ldots.
\]

Davenport (11) pp. 81-82) derives an alternative expression for $B$. The reflective property of $\xi(s)$ gives the identity

\[
\frac{\xi'(s)}{\xi(s)} = -\frac{\xi'(1 - s)}{\xi(1 - s)}.
\]
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 \( \rho_n \) 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]. Matiyasevich et al. [11] also discuss the monotonicity of the \(\xi(s)\) and other functions.

**Theorem 2.1** (Monotonicity of Modulus Function \(|\xi(s)|\)). Let \(\sigma_{\text{sup}}\) be the supremum of the real parts of all zeros:
\[ \sigma_{\text{sup}} = \sup_n \{\sigma_n\}. \]

Then the modulus \(|\xi(\sigma + it)|\) is a monotone increasing function of \(\sigma\) in the region \(\sigma > \sigma_{\text{sup}}\) for all real \(t\). Likewise, the modulus is a monotone decreasing function of \(\sigma\) in the region \(\sigma < \sigma_{\text{inf}}\), where
\[ \sigma_{\text{inf}} = \inf_n \{\sigma_n\} = 1 - \sigma_{\text{sup}}. \]

**Proof.** It is apparent from (26) that \(|\xi(s)|\) is a monotone increasing function of \(\sigma\) in the range \(\sigma > \sigma_{\text{sup}} \geq \frac{1}{2}\) for all \(t\). Because of the reflective property \([9]\) it then readily follows that \(|\xi(s)|\) is a monotone decreasing function of \(\sigma\) in the range \(\sigma < 1 - \sigma_{\text{sup}} \leq \frac{1}{2}\). \(\square\)

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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 $\sigma$ in the right half plane, $\sigma > \frac{1}{2}$. Likewise, the modulus is a monotone decreasing function of $\sigma$ in the left half plane, $\sigma < \frac{1}{2}$.

**Proof.** The above discussion that has led to this corollary should suffice as a proof. \hfill \Box

### 2.3 Functions $a(\lambda, t)$, $b(\lambda, t)$, $\alpha(\lambda, t)$, $\beta(\lambda, t)$ 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

$$
\frac{1}{\xi(s)} \frac{\partial^3 \xi(s)}{\partial \sigma^3} \bigg|_{\sigma=\frac{1}{2}} = \sum_{n} \frac{t - t_n}{(t - t_n)^2 + (\frac{1}{2} - \sigma_n)^2}.
$$

(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)

and

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

(29)

Differentiate (28) 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

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

(31)

where

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

(32)

From the Cauchy-Riemann equation we find

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

(33)

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

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

(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
\[ 2a(\lambda, t) = \frac{\partial^2 \Re \{\xi(s)\}}{\partial \lambda^2} = -\Re \{\xi''(t)\}, \]  
\[ b(\lambda, t) = \frac{\partial \Im \{\xi(s)\}}{\partial \lambda}, \]  
where \( \xi''(s) \) is the second partial derivative of \( \xi(s) \) with respect to \( t \). Then, the following relations hold:
\[ a(\lambda, t) = \frac{1}{2} b'(\lambda, t), \]  
\[ b(\lambda, t) = -\Re \{\xi'(t)\}. \]  

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
\[ 2\alpha(\lambda, t) = \frac{\partial^2 \Im \{\xi(s)\}}{\partial \lambda^2} = -\Im \{\xi''(s)\}, \]  
\[ \beta(\lambda, t) = \frac{\partial \Re \{\xi(s)\}}{\partial \lambda}. \]  
Then the following relations hold:
\[ \alpha(\lambda, t) = -\frac{1}{2} \beta'(\lambda, t), \]  
\[ \beta(\lambda, t) = \Re \{\xi'(s)\}. \]  
\[ \frac{\partial a(\lambda, t)}{\partial \lambda} = \alpha'(\lambda, t), \quad \frac{\partial b(\lambda, t)}{\partial \lambda} = -\beta'(\lambda, t). \]  

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 \( \xi(s) \)

We begin with the following integral representation of \( \xi(s) \) (see Appendix A) found in Edwards [3], p.16.
\[ \xi(s) = \frac{1}{2} - \frac{s(1-s)}{2} \int_1^\infty \psi(x) \left(x^{3/2} + x^{(1-s)/2}\right) \frac{dx}{x}, \]  
where
\[ \psi(x) = \sum_{n=1}^\infty e^{-n^2 \pi x} \]  
is called the theta function. By applying integration by parts to [45] and Jacobi’s identity for the theta function [5] Edwards [3], p. 17 gives the following expression by generalizing Riemann’s result, which holds for any complex number \( s \):
\[ \xi(s) = 4 \int_1^\infty \frac{d[x^{3/2}\psi'(x)]}{dx} x^{-1/4} \cosh \left[ \frac{1}{2} \left( s - \frac{1}{2} \right) \log x \right] \ dx. \]  

[2] Jacobi’s identity for the theta function \( \psi(x) \) is
\[ 2\psi(x) + 1 = x^{-1/2} \left( 2\psi(x^{-1}) + 1 \right). \]  

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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
\[
D(x) = \sum_{n=1}^{\infty} n^2(n^2\pi x - \frac{3}{2})e^{-n^2\pi x} > 0, \text{ for } x \geq 1,
\] (50)
we can write (48) as
\[
\xi(s) = 4\pi \int_{1}^{\infty} x^{1/4}D(x) \cos \left(\frac{\tau \log x}{2}\right) dx,
\] (51)
where \(\tau\) is a complex number defined by
\[
\tau = t - i\lambda = -i(s - \frac{1}{2}),
\] (52)
and we used the identity \(\cosh(iy) = \cos y\). By changing the variable from \(x\) to \(\omega\) by
\[
\omega = \frac{\log x}{2}, \text{ } x \geq 1,
\] (53)
and defining
\[
S(\omega) = 8\pi e^{5\omega/2}D(e^{2\omega}), \text{ } \omega \geq 0
\] (54)
we can write (51) as
\[
\xi(s) = \int_{0}^{\infty} S(\omega) \cos(\omega \tau) d\omega,
\] (55)
which is a compact expression for
\[
\xi\left(\frac{1}{2} + \lambda + it\right) = \int_{0}^{\infty} S(\omega) \left(\cos \omega t \cosh(\omega \lambda) + i \sin \omega t \sinh(\omega \lambda)\right) d\omega.
\] (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 \(\omega \geq 0\), 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-Khintchin theorem (a.k.a. the Wiener-Khintchin-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.,

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

Furthermore,

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

Proof. From (55), it readily follows that

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

Since $\zeta(\frac{1}{2}) = -1.46035\ldots$ 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

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

$$S(0) = 8\pi D(1) = 8 \left( \frac{5}{4}\psi'(1) + \psi''(1) \right).$$ (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 (54) we obtain

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

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

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

Hence,

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

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

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

Thus, we finally evaluate

$$\int_0^\infty \Xi(t) \, dt = \frac{\pi}{2} S(0) = 4\pi \left( \frac{5}{4}\psi'(1) + \psi''(1) \right) = 2.8067\ldots$$ (70)

$^3$See e.g. [https://oeis.org/A059750](https://oeis.org/A059750)

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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 $\omega$ of $S(\omega)$ as the “(angular) frequency.” Then, we may refer to the complex number $\tau$ defined by (52) as “complex-time.” Use of the complex-time $\tau$ allow the compact representation (55) given earlier, viz.

$$\xi(s) = \int_{0}^{\infty} S(\omega) \cos(\omega \tau) \, d\omega.$$  \hfill (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

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

with

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

where

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

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

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

with

$$f_n(s) = \int_{0}^{\infty} S_n(\omega) \cos(\omega \tau) \, d\omega = 8\pi \int_{0}^{\infty} e^{5\omega/2} D_n(e^{2\omega}) \cos(\omega \tau) \, d\omega.$$  \hfill (76)

The switching in the order between the summation over $n$ and the integration over $\omega$, 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 $S(\omega)$ in $-\infty < \omega < \infty$.

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.,

$$S(-\omega) = S(\omega), \quad -\infty < \omega < \infty.$$  \hfill (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

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

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

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

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

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

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

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

$$= \frac{1}{2} \int_{-\infty}^{\infty} S_1(\omega') e^{i\omega' \tau} d\omega' \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} e^{-\tau \log n}, \quad (82)$$

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

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

The result (82) can be compactly expressed as

$$\xi(s) = \xi_1(s) \zeta(s). \quad (84)$$

By writing

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

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

**Theorem 4.1.** (The Fourier transform of $S_1(\omega)$)

The function $g(s)$ that transforms $\zeta(s)$ into $\xi(s)$ by multiplication is the Fourier transform of $S_1(\omega)$ to the domain $\tau$, i.e.,

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

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 $\xi_n(s)$:

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

and

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

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

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

this function is reflective and

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

### 4.3 Properties of the $g(s)$ function

In this section we discuss some properties of $g(s)$ defined by $\xi_n(s)$, 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 $b(t)$:

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

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

Then, we can write

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

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

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

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

we can rewrite (92) as

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

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

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

is often referred to as Hardy’s $Z$-function, 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,

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

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

$$\log \Gamma(s) \approx \frac{1}{2} \log \frac{2\pi}{s} + s(\log s - 1). \quad (96)$$
Then
\[
\log \Gamma(s/2) \approx (1 - \frac{1}{s}) \log 2 + \frac{1}{2} \log \pi + \left(\frac{4}{s^2}\right) \log s - \frac{\gamma}{2}.
\] (97)

By evaluating the above at \( s = \frac{1}{2} + it \), we have
\[
\log \Gamma \left(\frac{1}{2} + \frac{it}{2}\right) = a(t) + ib(t)
\]
\[
\approx \frac{i}{4} \log 2 + \frac{i}{4} \log \pi - \left(\frac{1}{4} + \frac{\theta(t)}{2}\right) - \frac{1}{2} \log \left(t^2 + \frac{1}{4}\right) + i \left[\frac{1}{4} \log \left(t^2 + \frac{1}{4}\right) - \frac{1}{2} \log 2 - \frac{\theta(t)}{4}\right],
\] (98)

where
\[
\theta(t) = \tan^{-1} 2t.
\] (99)

Thus, we obtain
\[
r(t) \approx -2^{\frac{1}{2}} \pi^{\frac{1}{2}} \left(t^2 + \frac{1}{4}\right)^\frac{1}{4} e^{-\frac{1}{4} \theta(t)}
\]
\[
\varphi(t) \approx \frac{i}{4} \log \frac{2}{2\pi} - \frac{\theta(t)}{4} + \frac{i}{4} \log \left(1 + \frac{1}{4^t}\right).
\] (100)

If we set
\[
A(t) = -r(t), \quad \text{and} \quad \varphi(t) = \theta(t) + \pi,
\] (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:
\[
g \left(\frac{1}{2} + it\right) = G(t) + i\hat{G}(t).
\] (103)

Then it is apparent that
\[
G(t) = A(t) \cos \varphi(t), \quad \text{and} \quad \hat{G}(t) = A(t) \sin \varphi(t).
\] (104)

For sufficiently large \( t \gg 1, \theta(t) \approx \frac{t}{2} \). Thus, \( A(t) \) and \( \varphi(t) \) can be approximated by
\[
A(t) \approx (2\pi)^{-\frac{1}{4}} e^{-\frac{\pi}{4} t^2}, \quad \text{for} \ t \gg 1,
\]
\[
\varphi(t) \approx \frac{t}{2} \log \frac{t}{2\pi} + \frac{7\pi}{8}, \quad \text{for} \ t \gg 1.
\] (105)

The function \( A(t) \) is strictly positive for all \( t \), hence \( G(t) \) becomes zero only when \( \varphi(t) = n\pi + \frac{\pi}{4} \) 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 \( \zeta \left(\frac{1}{2} + it\right) \) (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

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

then $z(s)$ is reflective. Furthermore $z \left( \frac{1}{2} + it \right) = Z(t)$, because (114) and (115) imply

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

Let $G_n(t)$ denote the value on the critical line of $\frac{1}{2}(s)$ defined in (89), i.e.,

$$G_n(t) = \frac{1}{2} \left[ (G(t) + i\hat{G}(t))n^{-\frac{1}{2}} + (G(t) - i\hat{G}(t))n^{-\frac{1}{2}+it} \right] \Xi(t) = G(t)n^{-\frac{1}{2}} \cos(t \log n) + \hat{G}(t)n^{-\frac{1}{2}} \sin(t \log n) = A(t)n^{-\frac{1}{2}} \cos(\varphi(t) - t \log n).$$

Thus, we find

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

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

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

\[ \Gamma(s) = \int_0^\infty u^{s-1} e^{-u} \, du. \]  

(A.1)

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

\[ \Gamma(s) = \pi^{s/2} \int_0^\infty x^{s-1} e^{-\pi n^2 x} \, dx. \]  

(A.2)

Then,

\[ \Gamma(s/2) = \pi^{s/2} \int_0^\infty x^{s-1} e^{-\pi n^2 x} \, dx, \]  

(A.3)

from which we obtain

\[ \pi^{-s/2} \Gamma(s/2) n^{-s} = \int_0^\infty x^{s-1} e^{-\pi n^2 x} \, dx. \]  

(A.4)

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

\[ \pi^{-s/2} \Gamma(s/2) \zeta(s) = \int_0^\infty x^{s-1} \psi(x) \, dx, \]  

(A.5)

where \( \psi(x) \) is given defined in [40].

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Let us write \( \nu(s) \) 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

\[
\nu(s) = \int_0^1 x^{\frac{s}{2}-1} \left( x^{-1/2} \psi(x^{-1}) + \frac{1}{2} x^{-1/2} - \frac{1}{2} \right) \, dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x) \, dx \\
= -\frac{1}{1-s} - \frac{1}{s} + \int_1^\infty \left( x^{\frac{s}{2}-1} + x^{\frac{1-s}{2}} \right) \psi(x) \, dx.
\]

(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 since both \( \nu(s) \) and \( \frac{-s(1-s)}{2} \) are reflective.

From (A.7), we obtain

\[
\xi(s) = \frac{1}{2} - \frac{1}{2} s(1-s) \int_1^\infty \left( x^{\frac{s}{2}} + x^{\frac{1-s}{2}} \right) \psi(x) \frac{dx}{x},
\]

(A.9)

which is (3). From the last expression, it is apparent that \( \xi(0) = \xi(1) = \frac{1}{2} \).