



Summation properties of the η_j and Li constants

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ABSTRACT

We find new summatory and other properties of the constants η_j entering the Laurent expansion of the logarithmic derivative of the Riemann zeta function about $s = 1$. We relate these constants to other coefficients and functions appearing in the theory of the zeta function. In particular, connections to the Li equivalence of the Riemann hypothesis are discussed and quantitatively developed. The validity of the Riemann hypothesis is reduced to the condition of the sublinear order of a certain alternating binomial sum.

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1. Introduction

The Riemann hypothesis is equivalent to the Li criterion governing the sequence of real constants $\{\lambda_k\}_{k=1}^{\infty}$, that are certain logarithmic derivatives of the Riemann xi function evaluated at unity. This equivalence results from a necessary and sufficient condition that the logarithmic derivative of the function $\xi[1/(1-z)]$ be analytic in the unit disk, where ξ is the Riemann xi function. The Li equivalence [1] states that a necessary and sufficient condition for the nontrivial zeros of the Riemann zeta function to lie on the critical line $\text{Re } s = 1/2$ is that $\{\lambda_k\}_{k=1}^{\infty}$ is nonnegative for every integer k .

In this paper we determine summation and other properties of the constants η_j entering the Laurent expansion of the logarithmic derivative of the Riemann zeta function about $s = 1$. Such properties are key to our approach of lower bounding the Li constants [2,3], since the η_j 's are prominent in a subcomponent sum S_2 of the Li constants. In fact, should $S_2(n)$ be provably $O(n)$ or smaller, the Riemann hypothesis would follow.

The Li constants are the binomial transform of the sequence $\{\sigma_k\}$, where $\sigma_j = \sum_{\rho} \rho^{-j}$ are sums of reciprocal powers of the nontrivial zeros of the Riemann zeta function. Herein we recall the relation of the η_j coefficients to the σ_k 's, and use it to provide an alternative proof of a summatory relation among the former constants.

It is possible to consider the Li constants as a particular value of differentiable functions defined on the positive real axis. Indeed, Freitas [4] has very recently taken this approach and related the nonnegativity of such functions α_n to zero-free half-plane regions of the zeta function. In this paper, we present an explicit representation of the $\alpha_n(s)$'s in terms of the η_j coefficients. Furthermore, we estimate the resulting polygamma summation term $S_1(n, s)$. All of these developments show the context of the $s = 1$ special case for the Li constants. Since the α_j functions satisfy an infinite set of linear first-order ordinary differential equations, it is also possible to describe their derivatives at $s = 1$ directly in terms of the Li constants. These and related results are also described in a later section of the paper.

After introducing some notation and some definitions, we proceed to the summation results for the η_j constants. Here we make use of the functional equation for the zeta function [5–9] and hence of its logarithmic derivative. Our work makes multiple use of the properties of the polygamma function, including the connection of its reflection formula to derivatives of

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the cotangent function. From such relations we are able to explicitly construct the necessary expansions with overlapping domains of validity.

In this paper, attention is restricted to the classical zeta function. However, the developments carry over to Dirichlet L functions, Hecke L functions, and other generalized zeta functions. The Li constants are defined for such functions [10] and an equivalence relates them to a generalized Riemann hypothesis. For some explicit results and estimations along these lines, Refs. [11,12] may be consulted.

2. Notation and background

The function ξ is determined from ζ by the relation $\xi(s) = (s/2)(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$, where Γ is the Gamma function [7,6,9,5,8], and satisfies the functional equation $\xi(s) = \xi(1-s)$. The sequence $\{\lambda_n\}_{n=1}^\infty$ is defined by

$$\lambda_n = \frac{1}{(n-1)!} \frac{d^n}{ds^n} [s^{n-1} \ln \xi(s)]_{s=1}. \quad (1)$$

The λ_j 's are connected to sums over the nontrivial zeros of $\zeta(s)$ by way of [13,1]

$$\lambda_n = \sum_{\rho} \left[1 - \left(1 - \frac{1}{\rho} \right)^n \right]. \quad (2)$$

In the representation [14,15,11]

$$\lambda_n = S_1(n) + S_2(n) - \frac{n}{2}(\gamma + \ln \pi + 2 \ln 2) + 1, \quad (3)$$

where γ is the Euler constant, the sum

$$S_1(n) \equiv \sum_{m=2}^n (-1)^m \binom{n}{m} (1 - 2^{-m}) \zeta(m), \quad n \geq 2, \quad (4)$$

has been bounded [11]:

$$\frac{n}{2} \ln n + (\gamma - 1) \frac{n}{2} + \frac{1}{2} \leq S_1(n) \leq \frac{n}{2} \ln n + (\gamma + 1) \frac{n}{2} - \frac{1}{2}. \quad (5)$$

Further bounds on $S_1(n)$ have been developed by applying Euler–MacClaurin summation to all orders [11]. The summand of the quantity S_1 can be written as a sum over the trivial zeros of ζ :

$$(1 - 2^{-n}) \zeta(n) - 1 = \sum_{m=1}^{\infty} \frac{1}{(2m+1)^n} = \sum_{\substack{j=-\infty \\ \text{even}}}^{-2} \frac{1}{(1-j)^n}. \quad (6)$$

The constants η_j enter the expansion around $s = 1$ of the logarithmic derivative of the zeta function,

$$\frac{\zeta'(s)}{\zeta(s)} = -\frac{1}{s-1} - \sum_{p=0}^{\infty} \eta_p (s-1)^p, \quad |s-1| < 3, \quad (7)$$

the corresponding Dirichlet series valid for $\text{Re } s > 1$ is

$$\frac{\zeta'(s)}{\zeta(s)} = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s}, \quad (8)$$

and these constants are used to form the sum S_2 :

$$S_2(n) \equiv -\sum_{m=1}^n \binom{n}{m} \eta_{m-1}. \quad (9)$$

The constants η_j can be written as [14,16]

$$\eta_k = \frac{(-1)^k}{k!} \lim_{N \rightarrow \infty} \left(\sum_{m=1}^N \frac{1}{m} \Lambda(m) \ln^k m - \frac{\ln^{k+1} N}{k+1} \right). \quad (10)$$

In Eqs. (8) and (10), Λ is the von Mangoldt function [7,6,9,5,8,16], such that $\Lambda(k) = \ln p$ when k is a power of a prime p and $\Lambda(k) = 0$ otherwise.

3. Summation relation for the η_j 's

As part of our program to characterize the η_j constants, we derive an explicit summatory relation. We first demonstrate

Proposition 1. *We have*

$$1 - \sum_{j=0}^{\infty} (-1)^j \eta_j = \ln 2\pi, \quad (11)$$

and for $j \geq 1$

$$[1 + (-1)^j] \eta_j = (-1)^j + \{1 - [1 + (-1)^{j+1}] 2^{-(j+1)}\} \zeta(j+1) + \sum_{k=j+1}^{\infty} (-1)^{k+1} \binom{k}{j} \eta_k. \quad (12)$$

Eq. (11) follows simply by evaluating Eq. (7) at $s = 0$ and using the well known result $\zeta'(0)/\zeta(0) = \ln(2\pi)$. We prove relation (12) in two different ways. The first method is directly based upon the functional equation satisfied by the Riemann zeta function. The second method relies upon the functional equation of the Riemann xi function. The two paths show the consistency of the theory, and several of the intermediate results may be of independent interest themselves.

First approach. From the functional equation satisfied by the classical zeta function, we obtain that of its logarithmic derivative:

$$\frac{\zeta'(s)}{\zeta(s)} = -\psi(1-s) + \ln 2\pi + \frac{\pi}{2} \cot\left(\frac{\pi}{2}s\right) - \frac{\zeta'(1-s)}{\zeta(1-s)}. \quad (13)$$

In this equation, $\psi = \Gamma'/\Gamma$ is the digamma function. We develop each term of Eq. (13) in a power series in $s - 1$. There is a common region of validity of these expansions about $s = 1$, so that the conclusion (12) holds.

From the defining relation (7), use of the binomial theorem, and reordering of series, we have

$$\frac{\zeta'(1-s)}{\zeta(1-s)} = \frac{1}{s} - \sum_{n=0}^{\infty} \sum_{j=n}^{\infty} (-1)^j \binom{j}{n} \eta_j (s-1)^n, \quad |s| < 3, \quad (14)$$

where $1/s = \sum_{m=0}^{\infty} (-1)^m (s-1)^m$. For the digamma term in Eq. (13) we obtain [17]

$$\psi(1-s) = -\gamma + \frac{1}{s-1} - \sum_{k=1}^{\infty} \zeta(k+1) (s-1)^k. \quad (15)$$

There are several means by which to expand the cotangent term in Eq. (13). We could use the trigonometric definitions, and obtain the needed Taylor series coefficients at $s = 1$ by applying the Faà di Bruno formula for the n th derivative of a composite function directly to the cotangent function, or to its $-\csc^2$ derivative. However, we avoid this method and invoke polygamma functions. From the reflection formula satisfied by the digamma function, we have

$$\frac{\pi}{2} \cot\left(\frac{\pi}{2}z\right) = \frac{1}{2} \left[\psi\left(1 - \frac{z}{2}\right) - \psi\left(\frac{z}{2}\right) \right], \quad (16)$$

which immediately delivers

$$\frac{\pi}{2} \left(\frac{d}{dz}\right)^n \cot\left(\frac{\pi}{2}z\right) = \frac{1}{2^{n+1}} \left[(-1)^n \psi^{(n)}\left(1 - \frac{z}{2}\right) - \psi^{(n)}\left(\frac{z}{2}\right) \right], \quad (17)$$

where $\psi^{(j)}$ is the polygamma function. Since $\psi^{(n)}(1/2) = (-1)^{n+1} n! (2^{n+1} - 1) \zeta(n+1)$ for $n \geq 1$, we find that

$$\frac{\pi}{2} \cot\left(\frac{\pi}{2}s\right) = \sum_{n=1}^{\infty} [-1 + (-1)^n] [1 - 2^{-(n+1)}] \zeta(n+1) (s-1)^n, \quad |s-1| < 1. \quad (18)$$

From Eqs. (7), (14), (15) and (18), and equating coefficients of like powers of $s - 1$ in Eq. (13), we obtain the relation for $j \geq 1$,

$$\eta_j = (-1)^j + \{1 - [1 + (-1)^{j+1}] 2^{-(j+1)}\} \zeta(j+1) + \sum_{k=j+1}^{\infty} (-1)^{k+1} \binom{k}{j} \eta_k, \quad (19)$$

and the Proposition follows.

Second approach. We consider the sums

$$\sigma_k = \sum_{\rho} \rho^{-k}, \quad (20)$$

where the summation is taken over all the complex zeros of the zeta function. These constants appear in an expansion of the logarithm of the xi function,

$$\ln \xi(s) = -\ln 2 - \sum_{k=1}^{\infty} (-1)^k \frac{\sigma_k}{k} (s-1)^k, \quad (21)$$

and are of interest for a variety of reasons. One of these is the direct binomial transformation to the Li constants: $\lambda_n = -\sum_{j=1}^n (-1)^j \binom{n}{j} \sigma_j$. In Ref. [11], we showed that

$$\sigma_k = (-1)^k \eta_{k-1} - (1-2^{-k})\zeta(k) + 1, \quad k \geq 2, \quad (22)$$

with

$$\sigma_1 = \lambda_1 = -\frac{\ln \pi}{2} + \frac{\gamma}{2} + 1 - \ln 2. \quad (23)$$

Based upon the functional equation $[\xi'(s)/\xi(s)]^{(j)} = -[\xi'(1-s)/\xi(1-s)]^{(j)}$ we find the summatory relation

$$\sigma_{j+1} = (-1)^{j+1} \sum_{k=j}^{\infty} \binom{k}{j} \sigma_{k+1}. \quad (24)$$

We now show that Eq. (12) is implicit in this relation. We insert Eq. (22) into both sides of Eq. (24) and use the sum

$$\begin{aligned} \sum_{k=j}^{\infty} \binom{k}{j} [1 - (1-2^{-(k+1)})\zeta(k+1)] &= -\sum_{k=j}^{\infty} \binom{k}{j} \sum_{m=1}^{\infty} \frac{1}{(2m+1)^{k+1}} \\ &= -\sum_{m=1}^{\infty} \frac{1}{(2m)^{j+1}} = -2^{-(j+1)}\zeta(j+1). \end{aligned} \quad (25)$$

For Eq. (25), we applied the summation [11]

$$\sum_{k=j}^{\infty} \binom{k}{j} q^k = \frac{q^j}{(1-q)^{j+1}}, \quad |q| < 1. \quad (26)$$

Rearrangement of terms gives Eq. (19) and then (12).

4. Extension of the Li constants

Very recently, Freitas [4] has introduced the coefficients

$$\alpha_n(\tau) = \frac{1}{(n-1)!} \frac{d^n}{d\tau^n} [\tau^{n-1} \ln \xi(\tau)], \quad \tau > 0, n = 1, 2, \dots, \quad (27)$$

such that $\alpha_n(1) = \lambda_n$, that allow the formulation of either the Riemann hypothesis or a weakened form. In particular, for $\tau > 1/2$, the half-plane $\text{Re } s > \tau/2$ is a zero-free region of the zeta function if and only if $\alpha_n(\tau) \geq 0$ for each $n = 1, 2, \dots$ [4]. By using the Weierstrass product form of the xi function, it is easy to show the relation of $\alpha_n(\tau)$ to sums over the nontrivial zeros ρ of the zeta function:

$$\alpha_n(\tau) = \frac{1}{\tau} \sum_{\rho} \left[1 - \left(\frac{\rho}{\rho - \tau} \right)^n \right]. \quad (28)$$

We have determined explicit representations for the coefficient functions of Eq. (27), including:

Proposition 2. For $\tau > 0$,

$$\begin{aligned} \alpha_n(\tau) &= \frac{1}{\tau} + \frac{n}{2} \left[\psi\left(\frac{\tau}{2}\right) - \ln \pi \right] + \sum_{m=2}^n \binom{n}{m} \frac{\tau^{m-1}}{(m-1)!} \frac{\psi^{(m-1)}(\tau/2)}{2^m} \\ &\quad - \sum_{m=1}^n \tau^{m-1} \binom{n}{m} \sum_{p=m}^{\infty} \binom{p-1}{m-1} \eta_{p-1} (\tau-1)^{p-m}. \end{aligned} \quad (29)$$

While other forms could be written, we have used the expansion (7). As it should, Eq. (29) properly reduces to the decomposition (3) of the Li constants when $\tau = 1$.

The procedure for deriving Eq. (29) is very close to that previously used for determining Eq. (3). Since this is described in Refs. [15,11], we omit the details.

By using an integral representation for the polygamma function [17,18], we may rewrite a term on the right side of Eq. (29):

$$\begin{aligned} S_1(n, \tau) &\equiv \sum_{m=2}^n \binom{n}{m} \frac{\tau^{m-1}}{(m-1)!} \frac{\psi^{(m-1)}(\tau/2)}{2^m} = -\frac{1}{2} \int_0^1 \frac{t^{\tau/2-1}}{1-t} \left[L_{n-1}^1 \left(-\frac{\tau}{2} \ln t \right) - n \right] dt \\ &= -\frac{1}{\tau} \int_0^\infty \frac{e^{-v}}{1-e^{-2v/\tau}} \left[L_{n-1}^1(v) - n \right] dv, \end{aligned} \quad (30)$$

where L_n^α is a Laguerre polynomial.

In fact, we may present an elegant integral form of the sum S_1 that exhibits its dominant behavior. We show

Proposition 3. For $\tau > 0$ we have

$$S_1(n, \tau) = \frac{n}{2} [\psi(n) + \gamma - 1] + \frac{1}{2} + \frac{1}{2\tau} (n-1) + \frac{1}{2} \int_0^\infty \left[\frac{1}{1-e^{-t}} - \frac{1}{t} - \frac{1}{2} \right] \left[n - L_{n-1}^1 \left(\frac{t\tau}{2} \right) \right] e^{-t\tau/2} dt. \quad (31)$$

In order to prove Eq. (31), we make use of a classical Binet formula for the digamma function [18]. Upon repeated differentiation, we find

$$\psi^{(n)}(z) = (-1)^{n-1} \frac{(n-1)!}{z^n} - \frac{(-1)^n n!}{2z^{n+1}} - (-1)^n \int_0^\infty \left[\frac{1}{1-e^{-t}} - \frac{1}{t} - \frac{1}{2} \right] t^n e^{-tz} dt, \quad \operatorname{Re} z > 0. \quad (32)$$

Based upon this expression, we insert $\psi^{(m-1)}(\tau/2)$ into the definition of $S_1(n, \tau)$, interchange summation and integration, apply the power series definition of L_{n-1}^1 and the binomial theorem, and obtain the Proposition.

Furthermore, it is possible to transform S_1 into an alternative exact summation:

Proposition 4. We have

$$S_1(n, \tau) = \frac{1}{\tau} \sum_{k=0}^\infty \left[\frac{n\tau}{2k+\tau} - 1 + \frac{2^n k^n}{(2k+\tau)^n} \right], \quad \tau > 0. \quad (33)$$

One proof of Eq. (33) rests on the connection of the polygamma function with the Hurwitz zeta function $\zeta(s, a)$, $\psi^{(n)}(z) = (-1)^{n+1} n! \zeta(n+1, z) = (-1)^{n+1} n! \sum_{k=0}^\infty (k+z)^{-(n+1)}$. Introducing this relation in the definition of $S_1(n, \tau)$, interchanging summations, and applying the binomial expansion gives the Proposition.

Eq. (33) can also be obtained from the integral representation (30). The method is to change variable and write the integrand factor $(1-e^{-u})^{-1}$ as a geometric series. Then performing term-by-term integration [17] and manipulating the result gives a second proof of Eq. (33). In more detail, we have from Eq. (30)

$$\begin{aligned} S_1(n, \tau) &= -\frac{1}{\tau} \sum_{j=0}^\infty \int_0^\infty e^{-(1+2j/\tau)v} [L_{n-1}^1(v) - n] dv \\ &= -\frac{1}{\tau} \sum_{j=0}^\infty \int_0^\infty e^{-(1+2j/\tau)v} L_{n-1}^1(v) dv + \frac{n}{\tau} \sum_{j=0}^\infty \frac{1}{1+\frac{2j}{\tau}}. \end{aligned} \quad (34)$$

The remaining integral may be performed by integrating by parts [17]:

$$\begin{aligned} \int_0^\infty e^{-(1+2j/\tau)v} L_{n-1}^1(v) dv &= \left(1 + \frac{2j}{\tau} \right) \int_0^\infty e^{-(1+2j/\tau)v} L_n(v) dv + 1 \\ &= 1 - \frac{2^n j^n}{(2j+\tau)^n}. \end{aligned} \quad (35)$$

Combining the results of Eqs. (34) and (35) then returns the Proposition of Eq. (33).

Very similarly to the methods of our Ref. [11], one may develop a number of comparison integrals for S_1 . We illustrate this approach, as it puts into context the $\tau = 1$ special case. Defining

$$I_1(n, \tau) \equiv \frac{1}{\tau} \int_0^\infty \left[\frac{n\tau}{2k+\tau} - 1 + \frac{2^n k^n}{(2k+\tau)^n} \right] dk, \quad \tau > 0, \quad (36)$$

with a change of variable we have

$$I_1(n, \tau) = \frac{1}{2\tau} \int_{\tau}^{\infty} \left[\frac{n\tau}{x} - 1 + \frac{(x - \tau)^n}{x^n} \right] dx. \quad (37)$$

With another change of variable,

$$I_1(n, \tau) = \frac{1}{2} \int_0^1 \left[ny - 1 + (1 - y)^n \right] \frac{dy}{y^2}, \quad (38)$$

an integration by parts yields

$$I_1(n, \tau) = \frac{n}{2} \int_0^1 \left[1 - (1 - y)^{n-1} \right] \frac{dy}{y} - \frac{1}{2}(n - 1) = \frac{n}{2} [\psi(n) + \gamma - 1] + 1/2. \quad (39)$$

When $\tau = 1$, the remaining integral evaluates in terms of $\psi(n) + \gamma$, readily leading to the $O(n \ln n)$ dominant order of the Li constants [11]. Our result (39) shows how this special case emerges. We have lower bounded S_1 and may write

Proposition 5.

$$S_1(n, \tau) \geq \frac{n}{2} \ln n + (\gamma - 1) \frac{n}{2} + \frac{1}{2}. \quad (40)$$

Similarly, improved such bounds may be derived, as well as upper bounds. For example, we very quickly have $S_1(n, \tau) \leq (n/2) \ln n + (\gamma + 1)(n/2) - 1/2$.

We give yet another exact representation of the sum S_1 in the

Proposition 6. For $\tau > 0$ we have

$$\begin{aligned} S_1(n, \tau) &= \frac{n}{2} [\psi(n) + \gamma - 1] + \frac{1}{2} + \frac{1}{2\tau} (n - 1) \\ &\quad + \frac{n}{2} \int_0^{\infty} \frac{P_1(x)}{x(x + \tau/2)^2} \left\{ \frac{\tau}{2} + (x + \tau/2) \left[-1 + \left(\frac{2x}{2x + \tau} \right)^n \right] \right\} dx, \end{aligned} \quad (41)$$

where P_1 is a periodized Bernoulli polynomial, $P_1(x) \equiv B_1(x - [x]) = x - [x] - 1/2$.

The proof of Eq. (41) uses an integral representation for the digamma function coming from Euler–Maclaurin summation [7]. In turn, we have

$$\psi^{(n)}(z) = (-1)^{n-1} \frac{(n-1)!}{z^n} - \frac{(-1)^n n!}{2z^{n+1}} + (-1)^n (n+1)! \int_0^{\infty} \frac{P_1(x)}{(x+z)^{n+2}} dx. \quad (42)$$

The use of Eq. (42) in the definition of S_1 , interchange of summation and integration, and evaluation of the resulting sums yields the Proposition.

The functions α_n satisfy an infinite system of linear differential equations [4],

$$\frac{\tau}{n} \alpha'_n(\tau) + \frac{(n+1)}{n} \alpha_n(\tau) = \alpha_{n+1}(\tau), \quad n \geq 1. \quad (43)$$

Clearly, the term $1/\tau$ of the representation (29) is the homogeneous solution of this set of equations. We have that $\alpha_{n+1}(0) = \alpha_n(0) - \sigma_1$, and by the functional equation of the xi function, $\alpha_1(0) = -\lambda_1$. Therefore, $\alpha_n(0) = -n\lambda_1 < 0$. From the differential equation (43), we have $\alpha'_n(1) = n\lambda_{n+1} - (n+1)\lambda_n$. Taking the $(j-1)$ th derivative of Eq. (43) gives

$$\frac{\tau}{n} \alpha_n^{(j)}(\tau) + \left(1 + \frac{j}{n} \right) \alpha_n^{(j-1)}(\tau) = \alpha_{n+1}^{(j-1)}(\tau), \quad n \geq 1. \quad (44)$$

This allows all derivatives of α_n to be recursively calculated (algebraically) at $\tau = 1$ solely in terms of the Li constants. For instance, we have $\alpha''_n(1) = (n+1)\lambda_{n+2} - (n+1)(n+2)\lambda_{n+1} - (n+1)(n+2)\lambda_n$. Furthermore, since we know the leading order of the Li constants, we then know that of all the derivatives of α_n at $\tau = 1$. Since $\lambda_n = O(n \ln n)$, we know, for instance, that $\alpha'_n(1)$ is positive and linearly increasing with n : $\alpha'_n(1) \sim n + 1 > 0$. Since the combination $\alpha_{n+1}(0) - (1 + 1/n)\alpha_n(0) = 0$, the sign of $\alpha'_n(0)$ (or possible vanishing of) remains indeterminate to us at present.

5. Summary

In this paper we have investigated properties of the particular Laurent expansion coefficients η_j of the logarithmic derivative of the Riemann zeta function. In addition, we have derived new expressions and properties of $\alpha_n(\tau)$, an extension of the Li constants λ_n . Concerning recent progress on decomposing the sum $S_2(n)$, Ref. [19] may be consulted.

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