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POLYGAMMA THEORY, THE LI/KEIPER CONSTANTS AND THE LI CRITERION FOR THE RIEMANN HYPOTHESIS

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ABSTRACT. The Riemann hypothesis is equivalent to the Li criterion governing a sequence of real constants, $\{\lambda_k\}_{k=1}^{\infty}$, that are certain logarithmic derivatives of the Riemann xi function evaluated at unity. We present a series of results for associated sets of constants c_n and d_n, $n = 0, 1, \ldots$, and give the precise relation of these to the Li/Keiper constants. In the course of our investigation, we obtain new representations of classical special functions under a Möbius transformation. Among the conclusions is that the leading behavior $(1/2)\ln n$ of λ_n/n is absent in c_n, suggesting that the Riemann hypothesis should hold. In addition, we present a recurrence relation for c_n based upon quantities derivable from elementary functions. The quantitative estimation of this recursion could provide a result stronger than the Riemann hypothesis itself.

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 [**21**] states that a necessary and sufficient condition for the nontrivial zeros of the Riemann zeta function to lie on the critical line $\mathrm{Re}\, s = 1/2$ is that $\{\lambda_k\}_{k=1}^{\infty}$ is nonnegative for every integer k.

This paper is a further contribution to our research program to characterize the Li (Keiper [**19**]) constants [**21**]. We have previously rederived [**5, 6**] an arithmetic formula [**4, 20**] for these constants and described how it could be used to estimate them. Elsewhere, among

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several other results, we have examined summatory properties of the Li and Stieltjes constants and investigated the η_j coefficients appearing in the Laurent expansion of the logarithmic derivative of the zeta function about $s = 1$ [**7**]. In particular, a key feature of the sequence $\{\eta_j\}_{j=0}^{\infty}$ is now known: it possesses strict sign alternation [**7**].

In this article, we investigate a related set of constants [**24**] c_n, $n = 1, 2, \ldots$, that might be thought of as reduced Li/Keiper constants. We show in detail that the leading behavior $(1/2)\ln n$ of λ_n/n is absent in c_n. We present a series of analytic results on c_n and polygammic constants d_n and a conjecture as to the order of c_n as $n \to \infty$. As a significant byproduct of this research, we obtain new representations of classical special functions under the fractional linear transformation $s(z) = 1/(1 - z)$.

The Riemann ξ function, the completed classical zeta function, is determined from the Riemann zeta function ζ by the relation $\xi(s) = s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$, where Γ is the Gamma function [**12, 13, 16–18, 23, 25**] and satisfies the normalization $\xi(0) = 1$ and the functional equation $\xi(s) = \xi(1 - s)$. The sequence $\{\lambda_n\}_{n=1}^{\infty}$ is defined by

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

The λ_js are connected to sums over the nontrivial zeros of $\zeta(s)$ by way of [**19, 21**]

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

Proposition 1. *Let*

$$F(z) = \ln\left[\frac{z}{1-z}\zeta\left(\frac{1}{1-z}\right)\right] = \sum_{n=0}^{\infty} c_n z^n, \tag{1}$$

where $c_0 = 0$ *and* $c_1 = \gamma$, *the Euler constant. Then we have*

$$\frac{\lambda_n}{n} = c_n + \frac{1}{n} - \frac{1}{2}\ln\pi + d_n, \quad n \geq 1, \tag{2}$$

where d_n *is the coefficient of* z^n *in the Maclaurin series of the function* $\ln\Gamma[1/2(1-z)]$. *That is,*

$$d_n = \frac{1}{n!}\frac{d^n}{dz^n}\ln\Gamma\left[\frac{1}{2(1-z)}\right]_{z=0}. \tag{3}$$

Proposition 2 [**4–7, 20**]. *Let*

$$\frac{\lambda_n}{n} = \frac{1}{n}S_1(n) + \frac{1}{n}S_2(n) - \frac{1}{2}(\gamma + \ln \pi + 2\ln 2) + \frac{1}{n}, \tag{4}$$

where

$$S_1(n) \equiv \sum_{m=2}^{n} (-1)^m \binom{n}{m} (1 - 2^{-m})\zeta(m), \quad n \geq 2, \tag{5}$$

$$S_2(n) \equiv -\sum_{m=1}^{n} \binom{n}{m} \eta_{m-1}, \tag{6}$$

the constants η_k *can be written as*

$$\eta_k = \frac{(-1)^k}{k!} \lim_{N\to\infty} \left(\sum_{m=1}^{N} \frac{1}{m}\Lambda(m) \ln^k m - \frac{\ln^{k+1} N}{k+1} \right), \tag{7}$$

and Λ *is the von Mangoldt function* [**13, 17, 18, 23, 25**]. *We recall that, for positive integers* n, $\Lambda(n) = 0$ *unless* $n = p^k$ *is a power of a prime number, in which case* $\Lambda(n) = \ln p$. *Then we have the exact relation*

$$\frac{S_2(n)}{n} = c_n, \quad n \geq 1. \tag{8}$$

Proposition 3. *Let* L_n^α *denote the Laguerre polynomial* [**2**, Section 6.2] *and* ψ *the digamma function. Then we have the integral representation*

$$d_n = \frac{1}{2}\psi\left(\frac{1}{2}\right) - \frac{1}{2n}\int_0^\infty \frac{e^{t/2}}{(e^t - 1)} \left[L_{n-1}^1\left(\frac{t}{2}\right) - n \right] dt, \quad n \geq 2. \tag{9}$$

Proposition 4. *We have*

$$\frac{S_1(n)}{n} - \frac{\gamma}{2} = d_n + \ln 2, \quad n \geq 1. \tag{10}$$

Proposition 5. *We have the exact expressions*

$$\begin{aligned} d_n &= \frac{1}{2}\psi\left(\frac{1}{2}\right) + \frac{1}{2n}\sum_{j=1}^{n-1}(n-j)\sum_{m=1}^{\infty}\frac{1}{m^2} \\ &\qquad \times \left[2\left(1-\frac{1}{m}\right)^{j-1} - \frac{1}{2}\left(1-\frac{1}{2m}\right)^{j-1}\right] \\ &= \frac{1}{2}\psi\left(\frac{1}{2}\right) \\ &\quad + \frac{1}{2n}\sum_{m=1}^{\infty}\left[2\left(1-\frac{1}{m}\right)^{n} - 2\left(1-\frac{1}{2m}\right)^{n} + \frac{n}{m}\right], \\ &\qquad n \geq 1, \end{aligned} \tag{11}$$

where $\psi(1/2)/2 = -\gamma/2 - \ln 2$.

Proposition 6. *We have* $d_j > 0$ *for all* $j > 3$.

Proposition 7. *Let*

(12a)
$$b_0 \equiv \int_0^\infty \left(\frac{1}{e^t-1} - \frac{1}{t} + \frac{1}{2}\right)e^{-t}dt = \gamma - \frac{1}{2},$$

(12b)
$$b_n \equiv \frac{1}{n}\int_0^\infty \left(\frac{1}{e^t-1} - \frac{1}{t} + \frac{1}{2}\right)e^{-t}\ln t L_{n-1}^1(-\ln t)\, dt, \quad n \geq 1,$$

and

$$g_k \equiv \frac{1}{k!}\,\frac{d^k}{dz^k}\frac{1}{\Gamma[1/(1-z)]}\bigg|_{z=0}, \quad k \geq 0, \tag{13}$$

with $g_0 = 1$ *and* $g_1 = \gamma$. *Put*

$$h_m \equiv \sum_{k=0}^{m} g_k b_{m-k}, \quad m \geq 0, \tag{14}$$

and $a_0 = 1$, $a_1 = \gamma$,

$$a_j = \gamma + \sum_{\ell=1}^{j-1} h_{j-\ell}, \quad j \geq 2. \tag{15}$$

Then we have the recurrence relation

$$c_k = a_k - \frac{1}{k}\sum_{q=1}^{k-1} q c_q a_{k-q}, \quad k \geq 1. \tag{16}$$

We recall that, in the Laurent expansion for the Hurwitz zeta function about the simple pole at $s = 1$,

$$\zeta(s,a) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\gamma_n(a)(s-1)^n,$$

the coefficients $\gamma_n(a)$ are called the Stieltjes constants.

Proposition 8. *The constants b_j, $j \geq 0$ of equation* (12) *are expressible in terms of the Stieltjes constants and vice versa.*

Proposition 9. *Let*

$$d_n(p) = \frac{1}{n!}\frac{d^n}{dz^n}\ln\Gamma\left[\frac{1}{p(1-z)}\right]_{z=0}, \quad p > 0. \tag{17}$$

Then

(18)

$$d_n(p) = \frac{1}{p}\psi\left(\frac{1}{p}\right) - \frac{1}{pn}\int_0^\infty \frac{e^{(1-1/p)t}}{(e^t-1)}\left[L_{n-1}^1\left(\frac{t}{p}\right) - n\right] dt, \quad n \geq 1,$$

$d_0(p) = \ln\Gamma(1/p)$, *and* $d_1(p) = \psi(1/p)/p$. *In particular,*

$$d_n(1) = -\gamma - \frac{1}{n}\int_0^\infty \frac{\left[L_{n-1}^1(t) - n\right]}{(e^t-1)}\, dt, \quad n \geq 1, \tag{19}$$

$d_0(1) = 0$, *and* $d_1(1) = -\gamma$. *Moreover,*

$$d_n(p) = \frac{1}{p}\psi\left(\frac{1}{p}\right) + \frac{1}{n}\sum_{j=0}^{\infty}\left[\frac{n}{pj+1} - 1 + \left(\frac{jp}{jp+1}\right)^n\right], \tag{20a}$$

$$\frac{1}{p}[\psi(n)+\gamma-1]+\frac{1}{p}\psi\left(\frac{1}{p}\right)+\frac{1}{np}+1-\frac{1}{n} \geq d_n(p) \geq \frac{1}{p}[\psi(n)+\gamma-1]+\frac{1}{p}\psi\left(\frac{1}{p}\right)+\frac{1}{np}. \tag{20b}$$

Proposition 10. *Put*

$$\Gamma\left(\frac{1}{1-z}\right)=\sum_{n=0}^{\infty} f_n z^n, \qquad \frac{1}{\Gamma[1/(1-z)]}=\sum_{n=0}^{\infty} g_n z^n, \quad |z|<1. \tag{21}$$

Then (a) $f_0=1$, $f_1=-\gamma=\psi(1)$,

$$f_n=\frac{1}{n}\int_0^{\infty} e^{-t}\ln t L_{n-1}^1(-\ln t)dt, \quad n\geq 1; \tag{22}$$

and (b) $g_0=1/f_0=1$, $g_1=-f_1=\gamma$, *and*

$$g_j=-\sum_{n=1}^{j-1} f_n g_{j-n}-f_j, \quad j\geq 2. \tag{23}$$

Proposition 11. *Put* ([**27**, Section 5])

$$\alpha(z)=\frac{1}{1-z}+\frac{\ln(1-z)}{z}\left(\frac{1}{1-z}-\frac{1}{2}\right)+\frac{1}{z}\ln\Gamma\left(\frac{1}{1-z}\right)=\sum_{n=0}^{\infty}\alpha_n z^n, \quad |z|<1, \tag{24}$$

with $\alpha_0=-b_0=1/2-\gamma$. *Then*

(a)

$$\alpha_j=1+\frac{1}{2(j+1)}-\gamma-\psi(j+2)+d_{j+1}(1); \tag{25}$$

(b) α_j *is bounded for all* $j\geq 0$, $|\alpha_j|\leq|\alpha_0|$;
(c) α_j *is expressible in terms of the integrals* b_k *of equation* (12); *and*
(d) $\alpha(z)$ *may be analytically continued to the whole complex plane.*

Conjecture.

$$|c_n| = O\left(\frac{1}{n^{1/2-\varepsilon}}\right), \tag{26}$$

where $\varepsilon > 0$ *but is otherwise arbitrary.*

Propositions 3 and 7–11 have not been presented before, while the others represent a condensation and reorganization of a subset of results that were previously described in [**8**].

Proofs of propositions. Here we outline the proofs of the propositions above, leaving to the references relevant background material.

Proposition 1. From equation (1) and the definition of the xi function, we have

$$\ln\xi\left(\frac{1}{1-z}\right) = F(z) - \ln(1-z) + \frac{1}{2(z-1)}\ln\pi + \ln\Gamma\left[\frac{1}{2(1-z)}\right]. \tag{27}$$

Since we have [**21**]

$$\ln\xi\left(\frac{1}{1-z}\right) = \sum_{n=1}^{\infty}\frac{\lambda_n}{n}z^n, \tag{28}$$

the expansion of equation (27) in powers of z readily yields equation (2).

Proposition 2. From equation (1) it follows that $c_n = (1/n!) \times (d^n/dz^n)F(z)|_{z=0}$, and from the definition of the xi function and [**21**]

$$\lambda_n = \frac{1}{(n-1)!}\frac{d^n}{ds^n}[s^{n-1}\ln\xi(s)]_{s=1}, \tag{29}$$

we have

$$\begin{aligned} S_2(n) &= \frac{1}{(n-1)!}\frac{d^n}{ds^n}\left[s^{n-1}\ln[(s-1)\zeta(s)]\right]_{s=1} \\ &= \sum_{m=1}^{n}\binom{n}{m}\frac{1}{(m-1)!}\frac{d^m}{ds^m}\ln\left[(s-1)\zeta(s)\right]_{s=1}. \end{aligned} \tag{30}$$

Under the mapping $s(z) = 1/(1-z)$, derivatives transform as $d/dz = s^2(d/ds)$, and Proposition 2 follows.

Proposition 3. We have [**8**]

(31a)
$$\frac{d^n}{dz^n}\ln\Gamma\left[\frac{1}{2(1-z)}\right] = \frac{1}{2}\frac{d^{n-1}}{dz^{n-1}}\frac{1}{(1-z)^2}\psi\left[\frac{1}{2(1-z)}\right]$$

(31b)
$$= \frac{1}{2}\sum_{j=0}^{n-1}\binom{n-1}{j}\frac{(n-j)!}{(1-z)^{n-j+1}}\frac{d^j}{dz^j}\psi\left[\frac{1}{2(1-z)}\right]$$

(31c)
$$= \frac{1}{2}\left\{\frac{n!}{(1-z)^{n+1}}\psi\left[\frac{1}{2(1-z)}\right] + \sum_{j=1}^{n-1}\binom{n-1}{j}\frac{(n-j)!}{(1-z)^{n+1}}\sum_{\ell=1}^{j}\binom{j}{\ell}\frac{(j-1)!}{(\ell-1)!} \times\frac{1}{2^\ell(1-z)^\ell}\psi^{(\ell)}\left[\frac{1}{2(1-z)}\right]\right\},$$

where ψ is the digamma function and $\psi^{(j)}$ is the polygamma function. The idea of the proof is to use equation (3), equation (31b) and a certain integral representation of $\psi^{(j)}[1/2(1-z)]$. By using an integral representation of the digamma function, e.g., [**1**, page 259] or [**15**, page 943],

(32a)
$$\psi(z) = -\gamma + \int_0^\infty \frac{e^{-t} - e^{-st}}{1-e^{-t}}\,dt, \quad \operatorname{Re} s > 0,$$

and making use of a standard exponential generating function for L_m^β [**2, 15**],

(32b)
$$\sum_{n=0}^\infty L_n^\alpha(x)z^n = \frac{1}{(1-z)^{\alpha+1}}e^{xz/(z-1)}, \quad |z| < 1,$$

we determine that

(32c)
$$\frac{d^j}{dz^j}\psi\left[\frac{1}{2(1-z)}\right] = \frac{1}{2}\sum_{n=0}^\infty\int_0^\infty \frac{tL_{n+j-1}^1(t/2)}{1-e^{-t}}e^{-t/2}\,dt(n+j-1)(n+j-2)\cdots(n+1)z^n, \quad j \geq 1,$$

so that

(32d)
$$\frac{d^j}{dz^j}\psi\left[\frac{1}{2(1-z)}\right]\bigg|_{z=0} = \frac{(j-1)!}{2}\int_0^\infty \frac{tL_{j-1}^1(t/2)}{1-e^{-t}}e^{-t/2}\,dt, \quad j \geq 1.$$

From equation (31b) we then have

$$d_n = \frac{1}{2}\psi\left(\frac{1}{2}\right) + \frac{1}{4}\sum_{j=1}^{n-1}\frac{1}{j}\left(1-\frac{j}{n}\right)\int_0^\infty \frac{tL_{j-1}^1(t/2)}{1-e^{-t}}e^{-t/2}dt. \tag{33}$$

Upon performing the summations on the right side of this equation, we find that

$$\begin{aligned} d_n = \frac{1}{2}\psi\left(\frac{1}{2}\right) &- \frac{1}{4n}\int_0^\infty \frac{tL_{n-2}^2(t/2)}{1-e^{-t}}e^{-t/2}dt \\ &- \frac{1}{2}\int_0^\infty \frac{[L_{n-1}(t/2)-1]}{1-e^{-t}}e^{-t/2}dt. \end{aligned} \tag{34}$$

In particular, we have used [**15**, page 1038] $\sum_{m=1}^{n+1} L_{m-1}^\alpha(x) = L_n^{\alpha+1}(x)$, together with

$$\sum_{j=1}^n \frac{L_{j-1}^1(x)}{j} = \frac{1}{x}[1-L_n(x)]. \tag{35}$$

A direct proof of this relation follows by interchanging sums:

$$\begin{aligned} \sum_{j=1}^n \frac{L_{j-1}^1(x)}{j} &= \sum_{j=1}^n \frac{1}{j}\sum_{m=1}^j (-1)^{m-1}\binom{j}{m}\frac{x^{m-1}}{(m-1)!} \\ &= \sum_{m=1}^n (-1)^{m-1}\frac{x^{m-1}}{(m-1)!}\sum_{j=m}^n \frac{1}{j}\binom{j}{m} \\ &= \sum_{m=1}^n (-1)^{m-1}\binom{n}{m}\frac{x^{m-1}}{m!} = \frac{1}{x}[1-L_n(x)]. \end{aligned} \tag{36}$$

We then apply the recursion relations [**15**, page 1037]

(37a)
$$(t/2)L_{n-2}^2(t/2) = nL_{n-2}^1(t/2) - (n-1)L_{n-1}^1(t/2),$$

and

$$L_{n-2}^1(t/2) = L_{n-1}^1(t/2) - L_{n-1}(t/2), \tag{37b}$$

to obtain Proposition 3.

Proposition 4. This follows from the use of Propositions 1 and 2. Else, we may start with [**6**]:

$$\begin{aligned} S_1(n) &= \frac{1}{2}\int_0^\infty \left[n + L_{n-1}^1(t/2) - 2L_{n-1}^1(t)\right]\frac{dt}{(e^t-1)} \\ &= \frac{1}{2}I + \frac{1}{2}\int_0^\infty \frac{L_{n-1}^1(t/2) - L_{n-1}^1(t)}{e^t-1}\,dt, \end{aligned} \tag{38a}$$

where

$$I \equiv \int_0^\infty \frac{[n - L_{n-1}^1(t)]}{e^t-1}\,dt. \tag{38b}$$

By termwise integration, using the power series form of L_{n-1}^1 [**15**, page 1037], we find that

$$\begin{aligned} &\int_0^\infty \frac{L_{n-1}^1(t/2) - L_{n-1}^1(t)}{e^t-1}\,dt \\ &\quad = \sum_{m=2}^n (-1)^{m-1}\binom{n}{m}\frac{1}{(m-1)!}\int_0^\infty \frac{[(t/2)^{m-1} - t^{m-1}]}{e^t-1}\,dt \\ &\quad = \sum_{m=2}^n (-1)^m \binom{n}{m}(1-2^{1-m})\zeta(m) \equiv S. \end{aligned} \tag{39}$$

On the other hand, by changing variable in equation (9) and using partial fractions we have

$$\begin{aligned} d_n - \frac{1}{2}\psi\left(\frac{1}{2}\right) &= -\frac{1}{n}\int_0^\infty \frac{e^w}{e^{2w}-1}[L_{n-1}^1(w) - n]\,dw \\ &= -\frac{1}{2n}\int_0^\infty \left[\frac{1}{e^w-1} + \frac{1}{e^w+1}\right][L_{n-1}^1(w) - n]\,dw \\ &= \frac{1}{2n}I - \frac{1}{2n}\int_0^\infty \frac{L_{n-1}^1(w) - n}{e^w+1}\,dw \\ &= \frac{1}{2n}I + \frac{1}{2n}S, \end{aligned} \tag{40}$$

thereby reproving Proposition 4. The last step here follows from another termwise integration:

(41)
$$\begin{aligned}\int_0^\infty \frac{L_{n-1}^1(w)-n}{e^w+1}\,dw &= \int_0^\infty \left[\sum_{m=1}^n (-1)^{m-1}\binom{n}{m}\frac{w^{m-1}}{(m-1)!}-n\right]\frac{dw}{e^w+1}\\ &= \sum_{m=2}^n (-1)^{m-1}\binom{n}{m}\int_0^\infty \frac{w^{m-1}}{(m-1)!}\frac{dw}{(e^w+1)} = -S.\end{aligned}$$

Proposition 5. This follows from equation (31c) evaluated at $z=0$, with the second line coming from application of finite geometric series. Here, we recall that

(42)
$$\begin{aligned}\psi^{(n)}\left(\frac{1}{2}\right) &= (-1)^{n+1}n!\sum_{k=0}^\infty \frac{1}{(k+1/2)^{n+1}}\\ &= (-1)^{n+1}n!(2^{n+1}-1)\zeta(n+1), \quad n\geq 1.\end{aligned}$$

Else, we may rewrite the result of Proposition 3 by expanding $(1-e^{-t})^{-1}$ as a geometric series,

(43a)
$$d_n = \frac{1}{2}\psi\left(\frac{1}{2}\right)-\frac{1}{2n}\int_0^\infty \frac{e^{-t/2}}{(1-e^{-t})}\left[L_{n-1}^1\left(\frac{t}{2}\right)-n\right]dt, \quad n\geq 2,$$

(43b)
$$= \frac{1}{2}\psi\left(\frac{1}{2}\right)-\frac{1}{n}\sum_{j=0}^\infty\int_0^\infty e^{-(2j+1)u}\left[-\frac{d}{du}L_n(u)-n\right]du, \quad n\geq 2.$$

Then, using integration by parts and the Laplace transform of a Laguerre polynomial [**15**, page 844], gives a form equivalent to equation (11).

Proposition 6. We indicate three methods of proof of this result. The first is to make use of the monotonically increasing lower bound of $d_n(2)=d_n$ given in equation (20b). We find that this lower bound is positive and increasing for all values of $n \geq 11$. Then the separate cases d_n for $n = 4, \ldots, 10$ may be separately checked for positivity.

As a variation on the first method, we may note in equation (20b) the harmonic number $H_{n-1} = \psi(n) + \gamma$, and various inequalities for these numbers have been well studied, e.g., [**28**]. For instance, we have

$$\frac{1}{2n + (1/(1-\gamma)) - 2} \leq H_n - \ln n - \gamma \leq \frac{1}{2n + 1/3}, \tag{44}$$

the constants $1/(1-\gamma) - 2 \simeq 0.3652721$ and $1/3$ are the best possible, and equality holds only for $n = 1$. Therefore, positivity for d_n may be obtained for all n above a modest value n_0 and the initial values of d_n examined individually.

Thirdly, there are several ways in which to obtain highly accurate approximations to d_n for even moderate values of n [**8**]. One result is

$$\ln \Gamma \left[\frac{1}{2(1-z)} \right] \simeq \frac{1}{2} \ln \pi + \frac{1}{2} \sum_{j=1}^{\infty} \left[\psi(j) + \gamma - \ln 2 - 1 \right] z^j. \tag{45}$$

That is, for $j \gg 1$, we have

$$d_j = \frac{1}{2} \left[\ln j - \frac{1}{2j} - \frac{1}{12j^2} + \gamma - \ln 2 - 1 + O\left(\frac{1}{j^4}\right) \right]. \tag{46}$$

The first few d_j's are written explicitly in the Appendix, and directly from equation (46) we have that $d_j > 0$ for all sufficiently large j.

Proposition 7. Per an integral representation of the zeta function coming from Euler-Maclaurin summation [**25**, page 24]

$$\zeta(s) = \frac{1}{2} + \frac{1}{s-1} + \frac{1}{\Gamma(s)} \int_0^{\infty} \left(\frac{1}{e^t - 1} - \frac{1}{t} + \frac{1}{2} \right) e^{-t} t^{s-1}\, dt, \quad \operatorname{Re} s > -1, \tag{47}$$

we obtain

$$\zeta\left(\frac{1}{1-z}\right) = \frac{1}{z} - \frac{1}{2} + \frac{1}{\Gamma[1/(1-z)]} \times \int_0^{\infty} \left(\frac{1}{e^t - 1} - \frac{1}{t} + \frac{1}{2} \right) e^{-t} \left[1 + \ln t \sum_{n=1}^{\infty} \frac{1}{n} L_{n-1}^1(-\ln t) z^n \right] dt. \tag{48}$$

In view of equations (1) and (12)–(14), we may then write

$$\zeta\left(\frac{1}{1-z}\right) = \frac{1}{z} - \frac{1}{2} + \sum_{k=0}^{\infty} g_k z^k \sum_{n=0}^{\infty} b_n z^n$$

$$(49) \qquad = \frac{1}{z} - \frac{1}{2} + \sum_{m=0}^{\infty} h_m z^m$$

$$= \frac{(1-z)}{z} \exp\left[\sum_{n=0}^{\infty} c_n z^n\right].$$

Performing some elementary manipulations and then carrying out the exponentiation of power series in equation (49) then gives the recursion (16).

Proposition 8. The Stieltjes constants $\gamma_k(y)$ are the coefficients of the Laurent expansion of the Hurwitz zeta function $\zeta(s,y)$ about $s=1$ [**9, 10**]. In particular, by convention, one puts $\gamma_k(1)=\gamma_k$. Then directly from equation (47) we have for nonnegative integers j,

$$\int_0^\infty \left(\frac{1}{e^t-1} - \frac{1}{t} + \frac{1}{2}\right) e^{-t} t^a \ln^j t \, dt$$

(50a)

$$= \frac{d^j}{da^j}\left\{\Gamma(a+1)\left[\zeta(a+1) - \frac{1}{a} - \frac{1}{2}\right]\right\}, \quad \operatorname{Re} a > -2,$$

(50b)

$$= \frac{d^j}{da^j}\Gamma(a+1)\left[\gamma - \frac{1}{2} + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!}\gamma_k a^k\right], \quad \operatorname{Re} a > -2.$$

Therefore, by the linearity of integration and definition (12), the integrals b_k may be put in closed form in terms of γ_ℓ by using equation (50b) evaluated at $a=0$. The relation between b_k and the Stieltjes constants may be inverted, so that γ_ℓ may be written in terms of a sum over the integrals b_j.

Since $\gamma_0=\gamma$, $b_0=\gamma-1/2$ as given in equation (12a). When $n=1$, $L_{n-1}^1(w)=1$ and then $b_1=-\gamma^2-\gamma_1+\gamma/2\approx 0.0282457541267245$.

Proposition 9. The first part follows by the method of Proposition 3, and equation (20) follows from the methods of [**6**]. In particular, we recall the comparison integral that forms the basis of the bounds in (20b):

$$\begin{aligned}(51)\quad \int_0^\infty \left[\frac{n}{px+1} - 1 + \left(\frac{px}{px+1}\right)^n\right] dx \\ &= \frac{1}{p}\int_1^\infty \left[\frac{n}{y} - 1 + \left(\frac{y-1}{y}\right)^n\right] dy \\ &= \frac{n}{p}\int_0^1 \left[1-(1-v)^{n-1}\right]\frac{dv}{v} + \frac{1}{p}(1-n) \\ &= \frac{n}{p}\int_0^1 \frac{1-t^{n-1}}{1-t}\,dt + \frac{1}{p}(1-n) \\ &= \frac{n}{p}\left[\psi(n)+\gamma-1\right] + \frac{1}{p}.\end{aligned}$$

Herein, we changed variables, integrated by parts and applied [**15**, page 943].

Remark. By using the first correction term of Euler-Maclaurin summation, the lower bound of (20b) can be used to write the approximation $d_n(p) \simeq [\psi(n)+\gamma-1+\psi(p)+1/n]/p + (1/2)(1-1/n)$, and in particular, $d_n(1) \simeq \psi(n) + (1/2)(1/n-1)$.

Alternatively, we give a demonstration of the equivalence of equations (18) and (20a), especially as some of the intermediate expressions appear to be of interest in their own right. From (20a), binomial expansion and the interchange of two sums, we have

$$\begin{aligned}d_n(p) - \frac{1}{p}\psi\left(\frac{1}{p}\right) &= \frac{1}{n}\sum_{j=0}^\infty \left[\frac{n/p}{j+1/p} - 1 + \left(\frac{j}{j+1/p}\right)^n\right] \\ &= \frac{1}{n}\sum_{j=1}^\infty \left[\frac{n/p}{j+1/p-1} - 1 + \left(\frac{j-1}{j+1/p-1}\right)^n\right] \\ &= \frac{1}{n}\sum_{j=1}^\infty \sum_{\ell=2}^n \left(-\frac{1}{p}\right)^\ell \binom{n}{\ell}\frac{1}{(j+1/p-1)^\ell}\end{aligned}$$

$$= \frac{1}{n} \sum_{\ell=2}^{n} \left(-\frac{1}{p} \right)^{\ell} \binom{n}{\ell} \zeta(\ell, 1/p)$$
$$= \frac{1}{n} \sum_{\ell=2}^{n} \left(-\frac{1}{p} \right)^{\ell} \binom{n}{\ell} \frac{1}{(\ell-1)!} \int_0^{\infty} \frac{t^{\ell-1} e^{(1-1/p)t}}{e^t - 1}\, dt$$
$$= -\frac{1}{pn} \int_0^{\infty} \frac{e^{(1-1/p)t}}{(e^t-1)} \left[L_{n-1}^1 \left(\frac{t}{p} \right) - n \right] dt, \quad n \geq 1.$$

Above, we applied a standard integral representation for the Hurwitz zeta function, e.g., [**15**, page 1072].

Remark. This alternative proof shows the explicit connection of $d_n(p)$ with divided differences of the Riemann zeta function when p is either a positive integer or a positive half integer.

Proposition 10. Part (a) follows from the standard integral representation of Γ,

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t}\, dt, \quad \operatorname{Re} z > 0, \tag{52}$$

and the conventional exponential generating function of L_{n-1}^1 [**2, 15**] given in (32b). The recursion relation of part (b) follows upon the long division of power series.

Proposition 11. For part (a) we manipulate power series and use the definition of $d_n(1)$ of (17). We find that

$$\alpha_j = 1 + \frac{1}{2(j+1)} - \sum_{k=0}^{j} \frac{1}{k+1} + d_{j+1}(1). \tag{53}$$

We then use [**1, 15**] $\psi(j+1)+\gamma = \sum_{k=0}^{j-1} 1/(k+1) = H_j$, the harmonic number, to obtain (25). Alternatively, we may employ the generating function $-(1-z)^{-1}\ln(1-z) = \sum_{n=1}^{\infty} H_n z^n$.

The well-known asymptotic form of the digamma function is $\psi(z) = \ln z - 1/2z + O(1/z^2)$ as $z \to \infty$. By Proposition 9 and its proof, it is then obvious that the leading behavior $\ln(j+1)$ of $d_{j+1}(1)$ is canceled by $\psi(j+2) = \psi(j+1) + 1/(j+1)$ in equation (25). Therefore, α_j remains bounded for all $j \geq 0$, giving part (b). Furthermore, since $d_{j+1}(1) = \ln(j+1) + C_p + O(1/j)$, where C_p is a constant depending only upon p, as follows from Proposition 9, we find that the terms $O(1/j)$ also cancel in α_j, and that $|\alpha_j| \leq |\alpha_0|$ for all $j \geq 0$. Alternatively, this result follows from

Lemma. *We have*

$$\frac{1}{2x} < \ln x - \psi(x) = \int_0^\infty \left(\frac{1}{1-e^{-t}} - \frac{1}{t}\right) e^{-xt}\, dt < \frac{1}{x}, \quad x > 0.$$

The middle equality is simply a standard Binet formula for the digamma function. The function $f(x) = x(\ln x - \psi(x))$ satisfies $\lim_{x\to 0} f(x) = 1$ and $\lim_{x\to\infty} f(x) = 1/2$. Furthermore, [**14**, page 824],

$$f(x) = \frac{1}{2} + \frac{1}{12x} - \frac{\theta}{120x^3}, \quad 0 < \theta < 1,$$

and f is strictly decreasing on $(0, \infty)$.

For part (c), we may verify, as outlined below, that

$$\zeta(s) = \frac{s}{s-1} - \frac{1}{2} - s\sum_{n=0}^\infty (-1)^n \binom{s-1}{n} \alpha_n. \tag{54}$$

We may then note from (47) and the relations

$$-s\sum_{n=0}^\infty (-1)^n \binom{s-1}{n} \alpha_n = \frac{1}{\Gamma(s)} \int_0^\infty \left(\frac{1}{e^t - 1} - \frac{1}{t} + \frac{1}{2}\right) e^{-t} t^{s-1}\, dt, \tag{55}$$

and $t^{s-1} = \exp[(s-1)\ln t]$ that, by expanding in powers of $s-1$, α_n is expressible in terms of b_k of (12). In fact, it is also clear that the expansion of the factor $1/\Gamma(s)$ about $s = 1$ introduces polygamma factors $\psi^{(j)}(1)$, and these may be written in terms of Riemann zeta values at integer argument. Equivalently, α_n may be written in terms of the Stieltjes constants with the aid of Stirling numbers of the first kind s_k^ℓ [**1, 27**].

The representation (54) is part of a family that we elaborate elsewhere [**11**]. We consider series representations of the form

$$\zeta(s) = \frac{qs^q}{s^q-1} + qf(s) - s^q \sum_{k=0}^{\infty} (-1)^k \binom{s-1}{k} t_k, \tag{56}$$

where $q \geq 1$ is an integer, the real coefficients t_k depending upon q are to be determined, and the function f is such that $\zeta(s) - 1/(s-1)$ is regular in C. We are interested here in the case $q = 1$, when very simply $f = 0$. Due to a property of the binomial coefficient, when $s = n$ is a positive integer in equation (56), we have

$$\zeta(n) - \frac{qn^q}{n^q-1} - qf(n) = -n^q \sum_{k=0}^{n-1} (-1)^k \binom{n-1}{k} t_k. \tag{57}$$

Putting $n \to n+1$ in this equation, we may rewrite it as

$$\frac{q}{(n+1)^q-1} + \frac{qf(n+1)}{(n+1)^q} - \frac{\zeta(n+1)}{(n+1)^q} = t_0 + \sum_{k=1}^{n} (-1)^k \binom{n}{k} t_k. \tag{58}$$

We now multiply both sides of this equation by $(-1)^n \binom{m}{n}$ and sum on $1 \leq n \leq m$, using the orthogonality of binomial coefficients,

$$\sum_{n=1}^{m} (-1)^n \binom{m}{n} \binom{n}{k} = (-1)^m \delta_{m,k}, \tag{59}$$

where $\delta_{n,j}$ is the Kronecker delta, obtaining

(60)

$$t_m = t_0 + \sum_{n=1}^{m} (-1)^n \binom{m}{n} \left[\frac{q}{(n+1)^q-1} + \frac{qf(n+1)}{(n+1)^q} - \frac{\zeta(n+1)}{(n+1)^q} \right], \ m \geq 1.$$

For simplicity, we now specialize to $q = 1$, when

$$t_m = t_0 + \sum_{n=1}^{m} (-1)^n \binom{m}{n} \left[\frac{1}{n} - \frac{\zeta(n+1)}{(n+1)} \right], \quad m \geq 1. \tag{61}$$

Since $\lim_{s\to 1}[\zeta(s) - 1/(s-1)] = \gamma$, we find $t_0 = 1 - \gamma$. We now have that for $q = 1$, the difference of $\zeta(s)$ and the right side of (56) vanishes on the positive integers, and we apply Carlson's theorem [**26**, Section 5.81]. This difference function g is of exponential type and satisfies $|g(z)| < C\exp(k|z|)$ for $\mathrm{Re}\, z \geq 0$, where $k = \pi/2 < \pi$. Therefore, it is identically zero and the series representation (56) with $q = 1$ and t_m as in equation (61) follows.

For large n, we have $t_n \to 1/2(n+1)$ and accordingly we put $\alpha_n = t_n - 1/2(n+1)$, giving (54). In addition, by the use of [**1**, page 256], we find the generating function of (24). This completes part (c).

The upshot of part (d) is that we may remove the initial restriction $|z| < 1$ in equation (24). By part (b) we now know that the power series on the right side of this equation converges for at least $|z| < 1/|\alpha_0|$, i.e., beyond the unit circle on which any singularity in the finite complex plane of $\alpha(z)$ would have to exist. Therefore, $\alpha(z)$ may be analytically continued to all of C.

Remark. Equation (61) together with our work (above equation (52) when $p = 1$) give another way to prove equation (25). We have

$$\begin{aligned} t_m - t_0 &= \sum_{n=1}^{m} (-1)^n \binom{m}{n} \left[\frac{1}{n} - \frac{\zeta(n+1)}{(n+1)}\right], \quad m \geq 1, \\ &= -\gamma - \psi(m+1) - \sum_{n=1}^{m} (-1)^n \binom{m}{n} \frac{\zeta(n+1)}{(n+1)}. \end{aligned} \tag{62}$$

We note that

$$\binom{m}{n} \frac{1}{n+1} = \frac{1}{m+1} \binom{m+1}{n+1}, \tag{63}$$

giving

$$t_m - t_0 = -\gamma - \psi(m+1) + \frac{1}{m+1} \sum_{n=2}^{m+1} (-1)^n \binom{m+1}{n} \zeta(n). \tag{64}$$

This equation provides

$$t_m - t_0 = d_{m+1}(1) - \psi(m+1), \tag{65}$$

that is equivalent to equation (25).

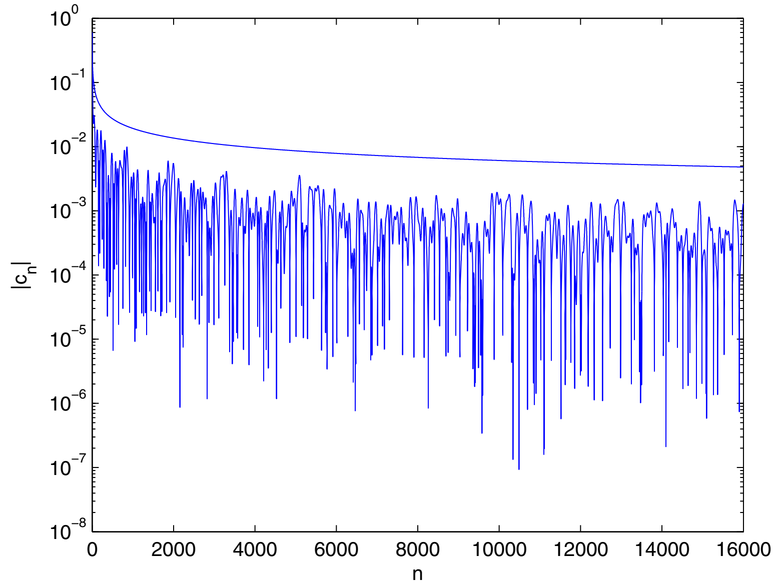

FIGURE 1. In this semi-logarithmic plot, the upper curve corresponds to values of $6/\pi^2\sqrt{n}$ versus n, and the lower to values of $|c_n|$ versus n.

Discussion. We have previously conjectured $|S_2(n)| = O(n^{1/2+\varepsilon})$ for $\varepsilon > 0$, leading to our conjecture (26). That is, we anticipate that the magnitudes $|c_n|$ decrease nearly as the square root of n for large n. In Figure 1 we compare such a decrease with available numerical evidence [**6, 22, 24**]. Figure 1 contains a semi-logarithmic plot of $|c_n|$ versus n, together with a curve corresponding to $6/\pi^2\sqrt{n}$. For this limited set, after a few initial values, the latter curve appears to provide a consistent upper bound. In light of the von Koch result on the Riemann hypothesis that $\psi_0(x) = x + O(x^{1/2}\ln^2 x)$ [**16, 29**], where $\psi_0(x) = \sum_{n\le x}\Lambda(n)$ is the Chebyshev function, we suspect that the optimal order of $|c_n|$ is very close to $O(\ln n/n^{1/2})$. In regard to these magnitudes, any subexponential bound on $|c_n|$ would serve to verify the Riemann hypothesis [**4, 24**]. Indeed, the Riemann hypothesis fails only if a λ_k becomes negative and exponentially large in k, cf. [**4**, Theorem 1, criterion (c)]. By our work, this could only occur if a c_k becomes exponentially large.

The Li equivalence is by itself a qualitative reformulation of the Riemann hypothesis. The Riemann hypothesis does not of itself dictate the exact nature of the Li/Keiper constants. In fact, one can easily formulate conjectures on the nature and order of the Li/Keiper constants that are then stronger than the Riemann hypothesis. These observations indicate that the Riemann hypothesis may be verifiable without knowing the optimal order or other properties of the Li/Keiper constants that would more fully characterize them. Details of the distribution of the complex zeta zeros are beyond the Riemann hypothesis. We emphasize therefore that our conjecture (26) is a stronger statement than the celebrated Riemann hypothesis itself. For according to the criterion just cited [**4**], if *any* bound of the form $|c_n| = O(n^p)$, with $p < \infty$ holds, then the Riemann hypothesis follows. However, reiterating, the detailed bound of (26) does not follow from the Li criterion for the Riemann hypothesis.

Proposition 8 is not surprising and shows the consistency of the theory, in that there are many equivalent representations of the Stieltjes constants [**8, 9**]. A key result of this article is Proposition 7. In overall terms, the constants b_j increase exponentially with j (approximately $\propto \exp(\sqrt{j})$ for large j), while the polygammic constants g_ℓ oscillate, i.e., occasionally change sign, leading to cancelation in h_m. The result is that a_j oscillates about unity, and therefore, we conjecture, c_k remains bounded. We have effectively reduced verification of the Riemann hypothesis to the asymptotic estimation of the quantities a_j and c_k in equation (16).

In regard to Proposition 11, we may note the close similarity of representations of the Riemann zeta function between [**27**, Section 5] (66)

$$\zeta(s) = \frac{s}{s-1} - s\sum_{n=0}^{\infty} t_n P_n(s) \equiv \frac{s}{s-1} - s\sum_{n=0}^{\infty}\left[\frac{1}{2(n+1)} + \alpha_n\right] P_n(s),$$

and [**3**]

$$\zeta(s) = \frac{1}{s-1}\sum_{k=0}^{\infty} A_k P_k\left(\frac{s}{2}\right), \tag{67}$$

where $P_k(s) \equiv (-1)^k \binom{s-1}{k}$ and $A_0 = \zeta(2)$. That α_j decreases faster than any power of $1/j$ then follows from the corresponding property for A_k. In fact, we suspect that both A_j and α_j decrease exponentially quickly with j.

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APPENDIX

Examples of d_n. The first few values of $k!d_k$ are given by

$$d_0 = \frac{1}{2}\ln\pi, \tag{A.1}$$

$$d_1 = -\gamma/2 - \ln 2, \tag{A.2}$$

$$2!d_2 = -\gamma + \frac{1}{8}\pi^2 - 2\ln 2, \tag{A.3}$$

$$3!d_3 = -3\gamma + \frac{3}{4}\pi^2 - 6\ln 2 - \frac{7}{4}\zeta(3), \tag{A.4}$$

$$4!d_4 = -12\gamma + \frac{9}{2}\pi^2 + \frac{\pi^4}{16} - 24\ln 2 - 21\zeta(3), \tag{A.5}$$

and

$$5!d_5 = -60\gamma + 30\pi^2 + \frac{5}{4}\pi^4 - 120\ln 2 - 210\zeta(3) - \frac{93}{4}\zeta(5). \tag{A.6}$$

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