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AN ASYMPTOTIC FORM FOR THE STIELTJES CONSTANTS $\gamma_k(a)$ AND FOR A SUM $S_\gamma(n)$ APPEARING UNDER THE LI CRITERION

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ABSTRACT. We present several asymptotic analyses for quantities associated with the Riemann and Hurwitz zeta functions. We first determine the leading asymptotic behavior of the Stieltjes constants $\gamma_k(a)$. These constants appear in the regular part of the Laurent expansion of the Hurwitz zeta function. We then use asymptotic results for the Laguerre polynomials L_n^α to investigate a certain sum $S_\gamma(n)$ involving the constants $\gamma_k(1)$ that appears in application of the Li criterion for the Riemann hypothesis. We confirm the sublinear growth of $S_\gamma(n)+n$, which is consistent with the validity of the Riemann hypothesis.

1. INTRODUCTION

Let $\zeta(s)$ be the Riemann zeta function, and the function ξ, satisfying $\xi(s) = \xi(1-s)$, be given by $\xi(s) = (s/2)(s-1)\Gamma(s/2)\pi^{-s/2}\zeta(s)$ [14, 18, 29, 33]. Within the critical strip $0 < \text{Re } s < 1$, the zeros of ζ and ξ coincide. The Li criterion [23] states that the nonnegativity of the quantities

$$\lambda_n = \frac{1}{(n-1)!}\frac{d^n}{ds^n}[s^{n-1}\ln\xi(s)]_{s=1}, \tag{1.1}$$

for each $n \geq 1$ is equivalent to the Riemann hypothesis (RH) that all nontrivial zeros of ζ have real part $1/2$. The λ_n's are connected to sums over the nontrivial zeros ρ_ℓ of $\zeta(s)$ by way of [19, 23]

$$\lambda_n = \sum_\ell \left[1 - \left(1 - \frac{1}{\rho_\ell}\right)^n\right], \tag{1.2}$$

and thus satisfy $\lambda_n = \lambda_{-n}$. For $n > 1$, the series in (1.2) is absolutely convergent, while for $n = 1$ the sum should be taken over complex conjugate pairs of zeros of increasing imaginary part.

The Li/Keiper [19] constants may be written in the form [3, 4, 5, 6]

$$\lambda_n = S_1(n) + S_2(n) + 1 - \frac{n}{2}[\gamma + \ln(4\pi)], \tag{1.3}$$

where S_1 and S_2 are certain alternating binomial sums, and γ is the Euler constant. The sum $S_1(n)$ is relatively easy to estimate. Its leading order is $O(n\log n)$, and this appears to be that of λ_n itself. Although it is not necessarily required to verify the Li

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criterion, a precise estimation of the sum $S_2(n)$ is desirable and remains open. Any subexponential bound for $|S_2(n)|$ would suffice to verify the Riemann hypothesis under the Li criterion. Recently, Coffey has further given the decomposition [11, 10],

$$S_2(n) = [S_{2\Lambda}(n) - n] + [S_\gamma(n) + n], \tag{1.4}$$

where, as the notation suggests, $S_{2\Lambda}$ is a certain summation over the von Mangoldt function Λ. We shall review at the end of section 3 that the sum S_γ is a binomial sum over the classical Stieltjes constants γ_k [31],

$$S_\gamma(n) \equiv \sum_{k=1}^{n} \frac{(-1)^k}{(k-1)!}\binom{n}{k}\gamma_{k-1} = \int_1^\infty \frac{1}{t} L_{n-1}^1(\ln t)\,dP_1(t). \tag{1.5}$$

In this equation, L_n^α is the Laguerre polynomial of degree n and parameter α [32] and $P_1(t)$ is the first periodized Bernoulli polynomial. A key determination of this paper is to provide a detailed asymptotic analysis of $S_\gamma(n) + n$.

Previously Coffey estimated $|S_\gamma(n) + n|$ as $O(n^{1/4})$ [11, 10] by using a known asymptotic form of the Stieltjes constants and the leading order form of the Laguerre polynomial. Here we give a self-contained study that presents detailed asymptotic expressions for $|S_\gamma(n) + n|$. These in turn can be estimated to verify the sublinear growth in n. As we show, $S_\gamma(n) + n = O(n^{3/4})$. It appears that a yet closer estimation would yield a $|S_\gamma(n) + n| = O(n^{1/4+\epsilon})$ result with $\epsilon \geq 0$.

We shall also give asymptotic results for $\gamma_n(a)$, the Stieltjes constants for the Hurwitz zeta function $\zeta(s, a)$. Knowledge of $\gamma_n(a)$ is useful for several areas, including in analytic number theory in the study of $\zeta(s, a)$ and Dirichlet L-functions. Our result for $\gamma_n(a)$ now reduces to the $\gamma_n(1) \equiv \gamma_n$ special case in [21].

The Laguerre polynomials are pervasive in formulating the Li criterion [7]. They provide certain test functions for a Weil inner product whose nonnegativity is equivalent to the Li criterion.

In addition, Laguerre polynomials are widespread in numerous application areas, including random matrix theory, quantum mechanics, and many others. For example, two important problems of quantum mechanics, that are indeed essentially equivalent, the higher-dimensional harmonic oscillator and hydrogen atom, have wavefunctions with Laguerre polynomial factors. Hence, detailed asymptotic forms for these polynomials are of interest.

There have been previous asymptotic analyses of Laguerre polynomials, including [13, 15, 27]. We shall use a 2-term asymptotic result from [12] for $L_n^\alpha(x)$ for $x > 0$, and we also mention a corresponding result for $L_n^\alpha(-z)$ for $z > 0$ in [34].

The paper proceeds as follows. In section 2 we introduce the constants $\gamma_k(a)$, analyze them for $k \gg 1$, and illustrate the main result numerically. In section 3 we perform an asymptotic analysis of $S_\gamma(n) + n$ with the help of various asymptotic results for $L_n^\alpha(x)$ for $x > 0$. Finally, in section 4 we numerically compare the asymptotic expressions with known values of $S_\gamma(n) + n$.

2. An asymptotic form for the Stieltjes constants $\gamma_k(a)$

The Hurwitz zeta function $\zeta(s, a)$ may be analytically continued to the whole complex s-plane. Its only singularity is a pole at $s = 1$ with residue 1. Correspondingly, there is the Laurent series for $s = 1$,

$$\zeta(s, a) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n \gamma_n(a)}{n!}(s-1)^n. \tag{2.1}$$

In this expansion, $\gamma_n(a)$ are called the Stieltjes constants [2, 8, 17, 20, 22, 24, 25, 26, 31, 35, 36][1], and $\gamma_0(a) = -\psi(a)$, where $\psi = \Gamma'/\Gamma$ is the digamma function. For the coefficients corresponding to the Laurent expansion for the Riemann zeta function, one denotes $\gamma_n(1) = \gamma_n$.

In this section, we present the leading asymptotic form of these constants for $n \gg 1$. Throughout we write $f(n) \sim g(n)$ when the limit relation $\lim_{n\to\infty} \frac{f(n)}{g(n)} = 1$ holds. We put

$$C_n(a) \equiv \gamma_n(a) - \frac{1}{a}\log^n a. \tag{2.2}$$

We have

Theorem 1. *Let $v = v(n)$ be the unique solution of the equation*

$$2\pi \exp[v \tan v] = n\frac{\cos v}{v}, \tag{2.3}$$

in the interval $(0, \pi/2)$, with $v \to \pi/2$ as $n \to \infty$. Let $u = v \tan v$ with $u(n) \sim \log n$ as $n \to \infty$. Then we have for $n \gg 1$,

$$\begin{aligned} C_n(a) &\sim \frac{B}{\sqrt{n}} e^{nA}[\cos(2\pi a)\cos(\alpha n + \beta) + \sin(2\pi a)\sin(\alpha n + \beta)] \\ &= \frac{B}{\sqrt{n}} e^{nA}\cos(\alpha n + \beta - 2\pi a), \end{aligned} \tag{2.4}$$

where

$$A = \frac{1}{2}\log(u^2+v^2) - \frac{u}{u^2+v^2},$$
$$B = \frac{2\sqrt{2\pi}\sqrt{u^2+v^2}}{[(u+1)^2+v^2]^{1/4}},$$
$$\alpha = \tan^{-1}\left(\frac{v}{u}\right) + \frac{v}{u^2+v^2},$$

and

$$\beta = \tan^{-1}\left(\frac{v}{u}\right) - \frac{1}{2}\tan^{-1}\left(\frac{v}{u+1}\right). \tag{2.5}$$

Formula (2.4) holds as long as we stay bounded away from zeros of the cosine factor. We note that, in view of (2.3), the functions A, B, α, β depend weakly on n as $\log n$ and $\log\log n$. The leading order is, $A \sim \log\log n$ and $B \sim \frac{\pi}{2}(\log n)^{-1}$.

The case of $\gamma_n(1)$ has been recently investigated by us in [21]. The additional oscillation of the asymptotic form of $\gamma_n(a)$ in the parameter a has been anticipated in Proposition 5 of [8]. Although Theorem 1 is predicated on $n \gg 1$, we find that it provides a useful approximation for even small values of n. As was true for the special case $a = 1$, the result (2.4) captures the rapid exponential growth in magnitude with n. It additionally contains the oscillatory behavior with respect to both n and a. The form (2.4) explicitly exhibits the 1/2-antiperiodicity of $C_n(a)$ for large n, i.e., for $n \gg 1$ we have $C_n(a) \approx -C_n(a + 1/2)$.

[1] It appears that in (5) and several later equations in Sections 2-4 of [25] a factor of $n!$ is missing.

Proof. Here we indicate the proof of Theorem 1, concentrating on the extensions to the argument of [21]. We start with the integral representation ([36], pp. 153-154) for $n \geq 1$,

$$C_n(a) = \int_1^\infty P_1(x-a)\frac{\log^{n-1} x}{x^2}(n - \log x)dx, \tag{2.6}$$

where $P_1(x) = B_1(x-[x]) = x-[x]-1/2$ is the first periodic Bernoulli polynomial. With the change of variable $t = \log x$, we have

$$C_n(a) = \int_0^\infty P_1(e^t - a)t^n e^{-t}\left(\frac{n}{t} - 1\right) dt. \tag{2.7}$$

Since P_1 has the Fourier representation [1] (pp. 805),

$$P_1(x) = -\sum_{L=1}^{\infty} \frac{\sin(2\pi Lx)}{\pi L}, \tag{2.8}$$

we may write

$$C_n(a) = -\mathrm{Im}\left\{\sum_{L=1}^{\infty} \frac{1}{L\pi}\int_0^\infty \exp[2\pi i L e^t + n\log t]e^{-2\pi i La}e^{-t}\left(\frac{n}{t} - 1\right) dt\right\}. \tag{2.9}$$

We shall show below that the series over L is absolutely and uniformly convergent, which justifies exchanging the order of summation and integration in going from (2.7) to (2.9). We shall show that for $n \to \infty$ the $L = 1$ term in (2.9) dominates the others (see also [21]). As in [21] we put

$$h(t) \equiv 2\pi i L e^t + n \log t, \tag{2.10}$$

and the saddle points occur for $h'(t) = 0$. Therefore, they satisfy

$$te^t = \frac{ni}{2L\pi}, \tag{2.11}$$

and are asymptotically given by $t \sim \log n - \log\log n + \gamma + \delta$. For integers M, we have $\gamma = \left(2M + \frac{1}{2}\right)\pi i - \log(2L\pi)$ and $\delta = \log\log n/\log n - \gamma/\log n = o(1)$. This gives

$$\begin{aligned} t_M &= \log n - \log\log n - \log(2L\pi) \\ &\quad + \left(2M + \frac{1}{2}\right)\pi i + \frac{\log\log n}{\log n}[1 + o(1)], \;\; M = 0, \pm 1, \pm 2, \ldots . \end{aligned} \tag{2.12}$$

We find that $|e^{h(t_M)}|$ as a function of M is maximized at $M = 0$, and as a function of L, at $L = 1$.

More precisely, we have the estimate

$$\begin{aligned} \log|e^{h(t_M)}| &= \mathrm{Re}[h(t_M)] = n\log\log n \\ &\quad - \frac{n}{\log n}[\log\log n + 1 + \log(2L\pi)] - \frac{1}{2}\frac{n}{\log^2 n}\left(2M + \frac{1}{2}\right)^2 \pi^2 \\ &\quad + \frac{1}{2}\frac{n}{\log^2 n}[\log\log n + \log(2L\pi)]^2 + O_R\left(\frac{n}{\log^3 n}\right), \end{aligned} \tag{2.13}$$

where the O_R "rough" error term may omit some factors of $\log\log n$. From the right-hand side of (2.13) we see that the terms in (2.9) with $L \geq 2$ are roughly exponentially smaller than the first term. In terms of M, (2.13) is largest at $M = 0$, but we can also easily show that the original contour ($t \in [0, \infty)$) can be deformed to a steepest descent contour that passes only through the saddle t_0. In Figure 1 we plot the curves $\mathrm{Re}[h'(t)] = 0$ and $\mathrm{Im}[h'(t)] = 0$ in the (x, y) plane, with $L = 1$ and $t = x + iy$. The intersection points of these curves are the saddle points, and the figure captures 3 saddles in the range $y = \mathrm{Im}(t) \in [-2\pi, 3\pi]$ (here we used $n = 1,000$). The steepest descent (SD) curve through the saddle $t_0 = u_0 + iv_0$ is given by $\mathrm{Im}[h(t)] = \mathrm{Im}[h(t_0)]$ so that

$$n \tan^{-1}\left(\frac{y}{x}\right) + 2\pi e^x \cos y = \frac{nv_0}{u_0^2 + v_0^2} + n \tan^{-1}\left(\frac{v_0}{u_0}\right). \tag{2.14}$$

The right side of (2.14), for $n \to \infty$, is approximately $n\pi/(2\log n)$ so that the SD contour starts at the origin roughly at the slope $y/x = \pi/(2\log n)$, traverses the saddle in a nearly horizontal direction (since $h''(t_0)$ is to leading order real and negative) and winds up at $t = \infty + i\pi/2$. In Figure 2 we sketch the SD contour when $n = 1,000$, along with the steepest ascent (SA) contour that is also a branch of (2.14), and which orthogonally intersects the SD contour at the saddle t_0 (here $t_0 \approx 3.706 + 1.246i$).

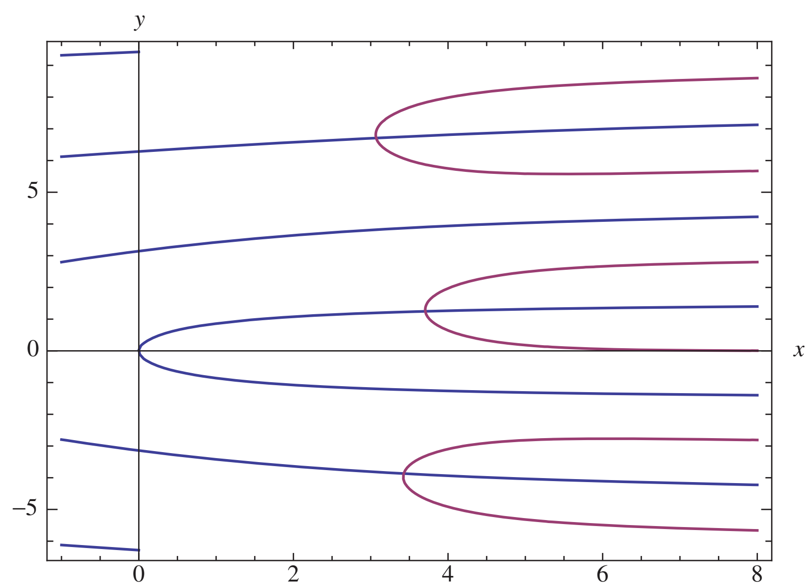

FIGURE 1. The real and imaginary parts of the saddle point equation $h'(t) = 0$ are plotted in the (x, y) plane, with $L = 1$ and $t = x + iy$. Three saddle points are present in the range $y = \mathrm{Im}(t) \in [-2\pi, 3\pi]$. Here, $n = 1,000$ in (2.11).

The saddle point calculation can also be used to estimate the Lth term in (2.9) for n fixed and $L \to \infty$, and this shows the rapid decay with L of the summand in (2.9), and the absolute and uniform convergences of the series.

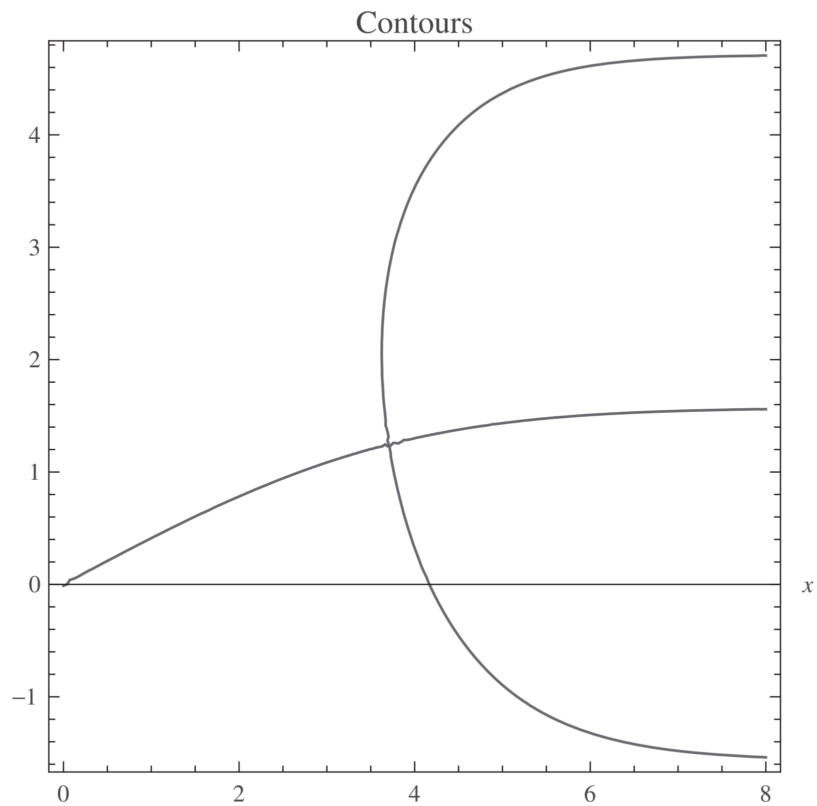

FIGURE 2. The steepest descent and ascent contours intersecting at the saddle point t_0 are shown. Here, $n = 1,000$.

We have $h''(t) = 2L\pi i e^t - n/t^2$, so that $h''(t_0) = -n/t_0 - n/t_0^2$. We put $A(n) = \mathrm{Re}[\log t_0 - 1/t_0]$ and $\alpha(n) = \mathrm{Im}[\log t_0 - 1/t_0]$ and find

$$e^{h(t_0)} = \exp\left[n\left(\log t_0 - \frac{1}{t_0}\right)\right] = e^{n[A(n)+i\alpha(n)]}. \tag{2.15}$$

We then have from (2.9),

$$\begin{aligned} C_n(a) &\sim -\sqrt{\frac{2n}{\pi}} e^{nA(n)} \mathrm{Im}\left[\frac{e^{-t_0}}{\sqrt{t_0+1}} e^{in\alpha(n)} e^{-2\pi i a}\right], \\ &= 2\sqrt{\frac{2\pi}{n}} e^{nA(n)} \mathrm{Im}\left[\frac{it_0}{\sqrt{t_0+1}} e^{in\alpha(n)} e^{-2\pi i a}\right], \end{aligned} \tag{2.16}$$

where the saddle point relation (2.11) at $L = 1$ has been used. Therefore, we have

$$\begin{aligned} C_n(a) \sim 2\sqrt{\frac{2\pi}{n}} e^{nA(n)} \Bigg[&-\mathrm{Re}\left(\frac{it_0}{\sqrt{t_0+1}} e^{in\alpha(n)}\right) \sin(2\pi a) \\ &+ \mathrm{Im}\left(\frac{it_0}{\sqrt{t_0+1}} e^{in\alpha(n)}\right) \cos(2\pi a)\Bigg]. \end{aligned} \tag{2.17}$$

We now use, with the definitions (2.5), the relations

$$\begin{aligned}\text{Re}\left(\frac{it_0}{\sqrt{t_0+1}}e^{in\alpha(n)}\right) &= -\text{Im}\left(\frac{t_0}{\sqrt{t_0+1}}e^{in\alpha(n)}\right)\\ &= -\frac{1}{2\sqrt{2\pi}}B\sin[n\alpha(n)+\beta(n)],\end{aligned} \tag{2.18a}$$

and

$$\begin{aligned}\text{Im}\left(\frac{it_0}{\sqrt{t_0+1}}e^{in\alpha(n)}\right) &= \text{Re}\left(\frac{t_0}{\sqrt{t_0+1}}e^{in\alpha(n)}\right)\\ &= \frac{1}{2\sqrt{2\pi}}B\cos[n\alpha(n)+\beta(n)].\end{aligned} \tag{2.18b}$$

Then (2.4) results from (2.17).

Putting $t_0 = u + iv$ in the saddle point relation (2.10) at $L = 1$, and eliminating u, results in the equation (2.3) solely for v. □

Remarks. The representation (2.6) may be readily verified by substitution in the defining relation (1.1). Then we obtain

$$\zeta(s,a) = \frac{a^{1-s}}{s-1} + \frac{a^{-s}}{2} - s\int_0^\infty \frac{P_1(x)}{(x+a)^{s+1}}dx, \ \text{Re } s > -1. \tag{2.19}$$

Some discussion on how to add higher order corrections to the saddle point method employed above is provided in [21]. In particular, only the $L = 1$ term is still required, but the Taylor expansion of $h(t)$ should be extended, as well as a more detailed treatment of the factors $e^{-t}(n/t-1)$ in (2.7).

We have noted the near anti-periodicity of $C_n(a)$ for large n. A simple explicit example of this is the special case $C_n(1/2) \sim \gamma_n(1/2) \sim -\gamma_n = -C_n(1)$ for $n \gg 1$.

Our asymptotic result also has relevance for determing the asymptotic form of expansion coefficients of other important functions of analysis and analytic number theory. We briefly describe applications to the Lerch zeta function $\Phi(z,s,a)$ and to Dirichlet L functions.

For instance, we may consider the Lipshitz-Lerch transcendent

$$L(x,s,a) = \sum_{n=0}^\infty \frac{e^{2\pi inx}}{(n+a)^s} = \Phi(e^{2\pi ix},s,a), \tag{2.20}$$

for complex a different from a negative integer. If we take here x real and nonintegral, the sum in (2.12) converges for Re $s > 0$. (For x an integer in (2.20), we can reduce to the Hurwitz zeta function.) A case of interest is $x = 1/2$. Then we obtain the alternating Hurwitz zeta function,

$$L\left(\frac{1}{2},s,a\right) = \sum_{n=0}^\infty \frac{(-1)^n}{(n+a)^s} = 2^{-s}\left[\zeta\left(s,\frac{a}{2}\right) - \zeta\left(s,\frac{a+1}{2}\right)\right]. \tag{2.21}$$

Therefore, expansion at $s = 1$ can be made in terms of a combination of *differences* of Stieltjes constants $\gamma_k(a/2) - \gamma_k[(a+1)/2]$. More specifically, we have, with the superscript denoting differentiation with respect to the second argument of L,

$$L^{(j)}\left(\frac{1}{2},s,a\right) = (-1)^j 2^{-s}\sum_{\ell=0}^j (-1)^\ell \binom{j}{\ell}\log^{\ell-j}(2)\left[\zeta^{(\ell)}\left(s,\frac{a}{2}\right) - \zeta^{(\ell)}\left(s,\frac{a+1}{2}\right)\right], \tag{2.22}$$

yielding

$$L^{(j)}\left(\frac{1}{2},1,a\right) = \frac{(-1)^j}{2}\sum_{\ell=0}^{j}\binom{j}{\ell}\log^{\ell-j}(2)\left[\gamma_\ell\left(\frac{a}{2}\right)-\gamma_\ell\left(\frac{a+1}{2}\right)\right]. \tag{2.23}$$

Dirichlet L-functions $L(\chi,s)$ are known to be expressible as linear combinations of Hurwitz zeta functions. We have for Dirichlet characters χ of modulus k,

$$L(\chi,s) = \sum_{n=1}^{\infty}\frac{\chi(n)}{n^s} = \frac{1}{k^s}\sum_{m=1}^{k}\chi(m)\zeta\left(s,\frac{m}{k}\right),\ \text{Re } s>1. \tag{2.24}$$

This equation holds for at least Re $s>1$. If χ is a nonprincipal character, then (2.24) converges for Re $s>0$. Again, derivatives at $s=1$ may be obtained as combinations of Stieltjes constants.

Numerical results. Formulas (2.2)-(2.5) are easily implemented for numerical computations. In Figure 3 the exact values of $C_5(a)$ from Mathematica V7 are plotted versus a for $0<a\le 1$. In Figure 4, values of $C_5(a)$ obtained from (2.4) are plotted versus a in the same range. Already for the small value of $n=5$, Theorem 1 gives a very good numerical approximation.

In Figure 5, the ratio R_n of the exact values of $C_n(1/3)$ to the values obtained from (2.4) is plotted for $n=10,15,20,\ldots,150$. Over this range of n, C_n oscillates and its magnitude varies from less than 1.2×10^{-4} to greater than 2.1×10^{36}. This range of values of $|C_n(1/3)|$ illustrates the rapid growth of the Stieltjes constants with n. The only points where R_n deviates significantly from 1 is near the zeros of the expression in (2.4), as we would expect.

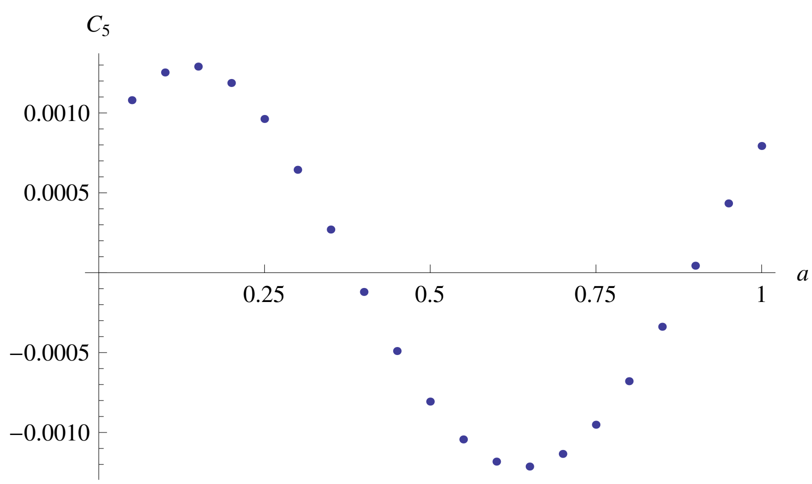

FIGURE 3. Exact values of $C_5(a)$ are plotted versus $0<a\le 1$.

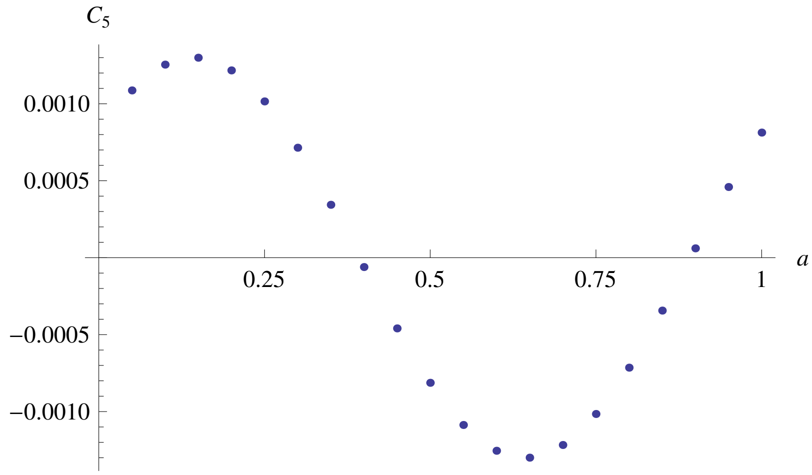

FIGURE 4. Values of $C_5(a)$ obtained from (2.4) are plotted versus a in the same range.

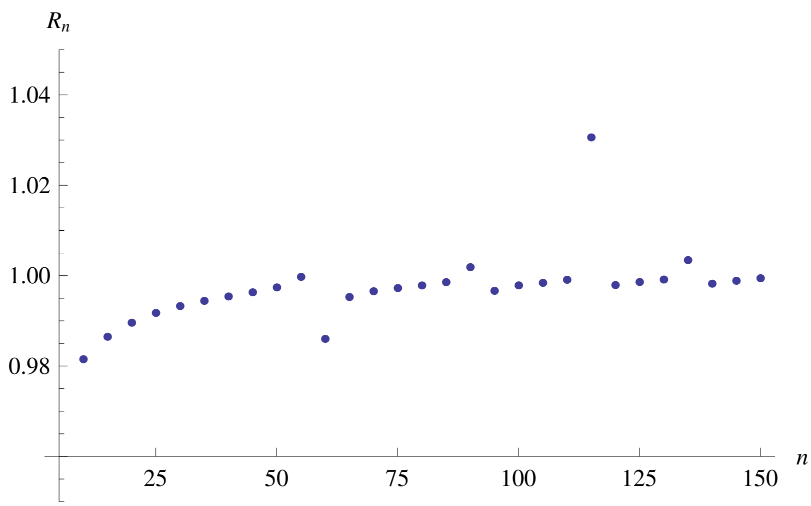

FIGURE 5. The ratio of the exact values of $C_n(1/3)$ to the values obtained from (2.4) is plotted versus $n = 10, 15, 25, \ldots, 150$.

3. Asymptotics of $S_\gamma(n) + n$

First, we present a result going beyond Theorem 8.22.5 of [32], which is given in [12], and can be obtained using integral representations and the saddle point method. We have

Lemma 1. *For $x > 0$ and $\alpha > -1$ we have*

$$L_n^\alpha(x) = \frac{1}{\sqrt{\pi}} \left(\frac{n}{x}\right)^{\alpha/2} \frac{e^{x/2}}{(nx)^{1/4}} \left\{ \sin\left[2\sqrt{nx} - \alpha\frac{\pi}{2} + \frac{\pi}{4}\right] + \cos\left[2\sqrt{nx} - \alpha\frac{\pi}{2} + \frac{\pi}{4}\right] \frac{\mathcal{M}}{\sqrt{nx}} + O(n^{-1}) \right\}, \tag{3.1}$$

where

$$\mathcal{M} = \mathcal{M}(x;\alpha) = (\alpha+1)\frac{x}{2} - \frac{x^2}{12} + \frac{\alpha^2}{4} - \frac{1}{16}. \tag{3.2}$$

This applies for $n \to \infty$ with a fixed x and $0 < x < \infty$.

For $n \to \infty$ the sum in (1.5) behaves as $S_\gamma(n) \sim -n$ and here we seek to estimate $S_\gamma(n) + n$, which we will show to be at most of the order $O(n^{3/4})$, with significant oscillations. We first express (1.5) in terms of Laguerre functions, and obtain the following.

Lemma 2. *We have, with $N = n - 1$,*

$$S_\gamma(n) + n = \sum_{m=1}^{\infty} F(m; N+1), \tag{3.3}$$

where

$$F(m; N+1) \equiv \int_{\log m}^{\log(m+1)} L_N^1(y)dy - \frac{1}{m+1} L_N^1[\log(m+1)], \tag{3.4}$$

and also

$$F(m; N+1) = \frac{1}{2\pi i} \oint \frac{z^{-n}}{(1-z)^2} \left\{ \frac{z-1}{z} \left[(m+1)^{\frac{z}{z-1}} - m^{\frac{z}{z-1}}\right] - (m+1)^{\frac{1}{z-1}} \right\} dz, \tag{3.5}$$

where the contour is a small counterclockwise loop about $z = 0$.

Proof. By the definition of P_1, from (1.5) we have

$$S_\gamma(n) = \int_1^\infty \frac{1}{t} L_{n-1}^1(\log t)dt - \sum_{m=1}^{\infty} \frac{1}{m} L_{n-1}^1(\log m). \tag{3.6}$$

Then using $L_{n-1}^1(0) = n$ we obtain

$$S_\gamma(n) + n = \sum_{m=1}^{\infty} \left[\int_m^{m+1} \frac{1}{t} L_{n-1}^1(\log t)dt - \frac{1}{m+1} L_{n-1}^1[\log(m+1)] \right]. \tag{3.7}$$

The change of variable $y = \log t$ then yields (3.3) with F as given in (3.4). To obtain (3.5) we apply the contour integral representation

$$e^{-x} L_{n-1}^\alpha(x) = \frac{1}{2\pi i} \oint \frac{z^{-n}}{(1-z)^{\alpha+1}} \exp\left(\frac{x}{z-1}\right) dz, \tag{3.8}$$

and let $x = \log t$ in (3.7). Then integrating over t, using

$$\int_m^{m+1} t^{\frac{1}{z-1}} dt = \frac{z-1}{z}\, t^{\frac{z}{z-1}} \Big|_{t=m}^{t=m+1}, \tag{3.9}$$

we obtain (3.5).

We proceed to evaluate the summand in (3.3) for N and/or $m \to \infty$. This will involve separately treating several ranges of m and N, and we first consider $m \to \infty$ with $N = O(1)$. $\square$

Lemma 3. *Let*

$$F(m; N+1; \alpha) \equiv \int_{\log m}^{\log(m+1)} L_N^\alpha(y)dy - \frac{1}{m+1} L_N^\alpha[\log(m+1)]. \tag{3.10}$$

Then for $N = O(1)$ as $m \to \infty$ we have

$$F(m; N+1; \alpha) = \frac{1}{2m^2} L_N^{\alpha+1}(\log m) \left[1 + O\left(\frac{1}{m}\right)\right]. \tag{3.11}$$

Proof. We let $y_2 = \log(m+1)$, $y_1 = \log m$ and since $(d/dx)L_{N+1}^\alpha(x) = -L_N^{\alpha+1}(x)$, we have

$$\begin{aligned} F(m; N+1; \alpha) &= \int_{y_1}^{y_2} L_N^\alpha(x)dx - e^{-y_2} L_N^\alpha(y_2) \\ &= L_{N+1}^{\alpha-1}(y_1) - L_{N+1}^{\alpha-1}(y_2) - e^{-y_2} L_N^\alpha(y_2) \\ &= L_{N+1}^{\alpha-1}(y_2 + \Delta) - L_{N+1}^{\alpha-1}(y_2) - e^{-y_2} L_N^\alpha(y_2), \end{aligned} \tag{3.12}$$

where $\Delta \equiv y_1 - y_2 = -1/m + 1/(2m^2) + O(1/m^3)$. Then expanding Δ for $m \to \infty$ we have

$$\begin{aligned} F(m; N+1; \alpha) &= -(\Delta + e^{-y_2}) L_N^\alpha(y_2) + \frac{\Delta^2}{2} L_{N-1}^{\alpha+1}(y_2) + O(\Delta^3) L_{N-2}^{\alpha+2}(y_2) \\ &= \left[\frac{1}{2m^2} + O\left(\frac{1}{m^3}\right)\right] L_N^\alpha(y_2) + \left[\frac{1}{2m^2} + O\left(\frac{1}{m^3}\right)\right] L_{N-1}^{\alpha+1}(y_2) + O(\Delta^3) L_{N-2}^{\alpha+2}(y_2) \\ &= \left[\frac{1}{2m^2} + O\left(\frac{1}{m^3}\right)\right] [L_N^\alpha(y_2) + L_{N-1}^{\alpha+1}(y_2)] \\ &= \left[\frac{1}{2m^2} + O\left(\frac{1}{m^3}\right)\right] L_N^{\alpha+1}(y_2) \\ &= \frac{1}{2m^2} L_N^{\alpha+1}(\log m) \left[1 + O\left(\frac{1}{m}\right)\right]. \end{aligned} \tag{3.13}$$

Here, we used the recursion $L_N^\alpha(x) + L_{N-1}^{\alpha+1}(x) = L_N^{\alpha+1}(x)$. $\square$

Lemma 4. *Let $F(m; n)$ be as defined in (3.4) and let $\beta = (\log m)/n$. Let Ai denote the Airy function (e.g., [28]). Then we have the following β-dependent asymptotic forms:*

(i) *For $\beta > 4$ we have*

$$F(m; n) \sim \frac{(-1)^{n+1}}{2m} \frac{1}{\beta} \frac{1}{\sqrt{n}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{-z_*}} \frac{1}{\sqrt{\beta - 2\sqrt{\beta}\sqrt{-z_*}}} (-z_*)^{-n} m^{\frac{1}{z_* - 1}}, \tag{3.14}$$

where

$$z_* = \frac{1}{2}[2 - \beta + \sqrt{\beta}\sqrt{\beta - 4}] = -\frac{1}{4}(\sqrt{\beta - 4} - \sqrt{\beta})^2. \tag{3.15}$$

(ii) *For $\beta \approx 4$, we let $\beta = 4 + n^{-2/3}\alpha$, with $\alpha = O(1)$. Then we have*

$$F(m; n) \sim \frac{1}{16} \frac{(-1)^{n+1}}{m^{3/2}} \left(\frac{4}{n}\right)^{1/3} Ai\left(\frac{\alpha}{4^{2/3}}\right). \tag{3.16}$$

(iii) *For $0 < \beta < 4$, we have*

$$F(m;n) \sim \frac{1}{m^{3/2}} \frac{1}{\sqrt{2\pi n}} \frac{\beta^{-5/4}}{(4-\beta)^{1/4}} \sin[nf(\beta) + g(\beta)], \tag{3.17}$$

where

$$z_+ = \frac{1}{2}[2 - \beta + i\sqrt{\beta}\sqrt{4-\beta}], \tag{3.18}$$

$$f(\beta) = \frac{1}{2}\sqrt{\beta}\sqrt{4-\beta} + arg[2-\beta + i\sqrt{\beta(4-\beta)}], \tag{3.19}$$

$$g(\beta) = arg[(1-z_+)^3] - \frac{\pi}{2} + \frac{1}{2} arg\left(\frac{z_+ + 1}{z_+^2(1-z_+)}\right). \tag{3.20}$$

The values of arg are such that arg $\in \left(\frac{\pi}{2}, \frac{5\pi}{2}\right)$, with the left endpoint corresponding to $\beta \to 4$ and the right endpoint to $\beta \to 0$. The value arg $= \pi$ corresponds to $\beta = 2 + \sqrt{2}$.

(iv) *For m, $n \to \infty$ with ξ fixed, where $\xi = \xi(m,n)$ is defined by*

$$\xi = \frac{\sqrt{n}}{(m+1)\sqrt{\log(m+1)}}, \tag{3.21}$$

we have

$$\begin{aligned} F(m;n) \sim \frac{1}{\sqrt{\pi}} \frac{[\log(m+1)]^{-1/2}}{\sqrt{\xi}} &\left\{(\cos\xi - 1)\sin\left[2\sqrt{n}\sqrt{\log(m+1)} + \frac{\pi}{4}\right]\right. \\ &\left. +(\xi - \sin\xi)\cos\left[2\sqrt{n}\sqrt{\log(m+1)} + \frac{\pi}{4}\right]\right\}. \end{aligned} \tag{3.22}$$

(v) *For $n \to \infty$ with $m = O(1)$, we have*

$$F(m;n) \sim \frac{n^{1/4}}{\sqrt{\pi}\sqrt{m+1}[\log(m+1)]^{3/4}} \cos\left[2\sqrt{n}\sqrt{\log(m+1)} + \frac{\pi}{4}\right]. \tag{3.23}$$

Proof. We merely sketch the main points. Note that some of these results also follow from the uniform asymptotic results for the Laguerre function in [15]. But, here we wish to give the expressions for $F(m;n)$ in the simplest possible forms.

From Lemma 3 with $\alpha = 1$ and the representation (3.8) we have

$$\begin{aligned} F(m;N) &= \frac{1}{2m^2} L_N^2(\log m)\left[1 + O\left(\frac{1}{m}\right)\right] \\ &\sim \frac{1}{2m}\frac{1}{2\pi i}\oint \frac{1}{(1-z)^3} e^{-n\log z} e^{\frac{\log m}{z-1}}\, dz. \end{aligned} \tag{3.24}$$

The latter expression is suitable for a steepest-descents expansion, and the saddle points occur for

$$-\frac{n}{z} - \frac{\log m}{(z-1)^2} = 0, \tag{3.25}$$

or $z^2 + (\beta-2)z + 1 = 0$. This equation has real roots for $\beta^2 - 4\beta > 0$, or $\beta > 4$. The root inside the unit circle is given by (3.15), so that $1 - z_* = (\beta - \sqrt{\beta^2 - 4\beta})/2$. The steepest descent method gives

$$F \sim \frac{1}{2m}\frac{(-1)^{n+1}}{(1-z_*)^3}(-z_*)^{-n} m^{\frac{1}{z_*-1}} \left[\frac{n}{z_*^2} + \frac{2\beta n}{(z_*-1)^3}\right]^{-1/2}, \tag{3.26}$$

leading to (3.14).

From (3.15) we have that the saddle point $z_* \to -1$ as $\beta \to 4$. So for $\beta \approx 4$ we expand the integrand of (3.24) about $z = -1$. We introduce the scaling $z + 1 = n^{-1/3} w$ and $\beta - 4 = n^{-2/3}\alpha$ and determine that

$$F \sim \frac{1}{16} \frac{(-1)^n}{m^{3/2}} \frac{n^{-1/3}}{2\pi i} \int_L \exp\left(\frac{w^3}{12} - \frac{1}{4}\alpha w\right) dw, \tag{3.27}$$

where the path L extends from $w = \infty e^{i\pi/3}$ to $w = \infty e^{-i\pi/3}$. By applying a standard contour integral representation [28], (pp. 53) for the Airy function, we obtain (3.16).

Next, we consider when $0 < \beta < 4$. In this case we obtain the oscillations in F. Now the two saddle points,

$$z_\pm = \frac{1}{2}[2 - \beta \pm i\sqrt{\beta}\sqrt{4-\beta}], \tag{3.28}$$

are complex conjugates lying on the unit circle. For $0 < \beta < 2$ we have $\mathrm{Re}(z_\pm) > 0$ and for $2 < \beta < 4$ we have $\mathrm{Re}(z_\pm) < 0$. The function $h(z) = -n \log z + \beta n/(z-1)$ has

$$\frac{d^2}{dz^2} h(z) = n\left[\frac{1}{z^2} + \frac{2\beta}{(z-1)^3}\right], \tag{3.29}$$

so that at $z = z_+$, using relation (3.25) we have

$$\frac{1}{n} h''(z_+) = -\frac{1}{z_+^2} \frac{z_+ + 1}{(z_+ - 1)} = \rho e^{i\phi_+}. \tag{3.30}$$

The steepest-descent method gives

$$F(m;n) \sim \frac{1}{m} \frac{1}{\sqrt{2\pi n}} \frac{1}{\sqrt{\rho}} \mathrm{Im}\left[e^{-n\log z_+} \exp\left(\frac{\beta n}{z_+ - 1}\right) e^{-i\phi_+/2} e^{-i\pi/2}\right]. \tag{3.31}$$

Here,

$$\rho = \left|\frac{z_+ + 1}{z_+ - 1}\right| = \sqrt{\frac{4-\beta}{\beta}}, \tag{3.32}$$

and also from (3.29),

$$\phi_+ = \arg\left(\frac{z_+ + 1}{z_+^2(1 - z_+)}\right). \tag{3.33}$$

We obtain from (3.31)

$$F(m;n) \sim \frac{1}{m^{3/2}} \frac{1}{|1 - z_+|^3} \frac{1}{\sqrt{2\pi n}} \frac{\beta^{1/4}}{(4-\beta)^{1/4}} \sin[n f(\beta) + g(\beta)], \tag{3.34}$$

where $|1 - z_+| = \sqrt{\beta}$, and f and g are given in (3.19) and (3.20). Therefore, (3.17) results.

We can easily verify that as $\beta \uparrow 4$, (3.17) asymptotically matches to (3.16) as $\alpha \to -\infty$. Similarly, as $\beta \downarrow 4$ in (3.14), the result matches to (3.16) as $\alpha \to \infty$, in view of the asymptotic form

$$\mathrm{Ai}(z) \sim \frac{1}{2\sqrt{\pi}} z^{-1/4} e^{-\frac{2}{3} z^{3/2}}, \ z \to \infty. \tag{3.35}$$

To obtain (3.23) in Lemma 4 we simply use the leading term in (3.1) and note that for $m = O(1)$,

$$
\begin{aligned}
F(m;n) &= L_n[\log m] - L_n[\log(m+1)] - \frac{1}{m+1} L^1_{n-1}[\log(m+1)] \\
&\sim -\frac{1}{m+1} L^1_{n-1}[\log(m+1)] \\
&\sim -\frac{1}{(m+1)} \frac{n^{1/4}}{[\log(m+1)]^{3/4}} \frac{\sqrt{m+1}}{\sqrt{\pi}} \sin\left[2\sqrt{n}\sqrt{\log(m+1)} - \frac{\pi}{4}\right]. \qquad (3.36)
\end{aligned}
$$

Then using $-\sin(x - \pi/4) = \cos(x + \pi/4)$ yields the results.

Now observe that the expression in (3.23) is not summable over m, as the amplitude decays only as $m^{-1/2}$ for $m \to \infty$. Furthermore, as $m \to \infty$, (3.23) does not match to (3.17) as $\beta \to 0$. Indeed, as $\beta \to 0$, (3.16) behaves as

$$
\begin{aligned}
&-\frac{1}{m^{3/2} 2\sqrt{\pi n}} \beta^{-5/4} \sin\left[2n\sqrt{\beta} + \frac{\pi}{4}\right] \\
&\quad = -\frac{n^{3/4}}{2\sqrt{\pi}} \frac{1}{m^{3/2}(\log m]^{5/4}} \sin\left[2\sqrt{n}\sqrt{\log m} + \frac{\pi}{4}\right]. \qquad (3.37)
\end{aligned}
$$

This means that another scale must be found between $n \to \infty$ with $m = O(1)$, and n, $m \to \infty$ with $\beta = (\log m)/n > 0$. We analyze this new scale below, and this will lead to the expression in (3.22).

To establish (3.22) we first use Lemma 1 to obtain a two-term asymptotic approximation to $F(m;n)$. □

Lemma 5. *We have the following refined asymptotic approximation for the summand of* (3.3). *We adopt the notation*

$$
\sin_m = \sin[2\sqrt{n}\sqrt{\log m} + \pi/4], \;\; \cos_m = \cos[2\sqrt{n}\sqrt{\log m} + \pi/4]. \qquad (3.38)
$$

Then $F(m;n) \sim \mathcal{F}(m;n)$ *where*

$$
\begin{aligned}
\mathcal{F}(m;n) &= \frac{\sqrt{m}}{n^{1/4}\sqrt{\pi}} \frac{1}{(\log m)^{1/4}} \left[\sin_m + \frac{1}{\sqrt{n}\sqrt{\log m}} \left(\frac{\log m}{2} - \frac{\log^2 m}{12} - \frac{1}{16}\right) \cos_m\right] \qquad (3.39) \\
&- \frac{\sqrt{m+1}}{n^{1/4}\sqrt{\pi}} \frac{1}{\log(m+1)]^{1/4}} \left[\sin_{m+1} + \frac{1}{\sqrt{n}\sqrt{\log(m+1)}} \left(\frac{\log(m+1)}{2} - \frac{\log^2(m+1)}{12} - \frac{1}{16}\right) \cos_{m+1}\right] \\
&+ \frac{n^{1/4}}{\sqrt{\pi}\sqrt{m+1}} \frac{1}{[\log(m+1)]^{3/4}} \left[\cos_{m+1} + \frac{1}{\sqrt{n}\sqrt{\log(m+1)}} \left(\frac{\log^2(m+1)}{12} - \frac{3}{16}\right) \sin_{m+1}\right].
\end{aligned}
$$

This expression is $O(m^{-3/2})$ *as* $m \to \infty$. *For* $m = 1$ *the first term in* $\mathcal{F}$ *(involving* $\sin_m$ *and* $\cos_m$*) must be replaced by* 1.

Proof. We let $\Delta(m;n)$ denote the 2-term asymptotic form of $L_n(\log m)$ coming from Lemma 1. Using Lemma 4 we arrive at

(3.40)

$$
\Delta(m;n) \sim \frac{\sqrt{m}}{n^{1/4}\sqrt{\pi}} \frac{1}{(\log m)^{1/4}} \left[\sin_m + \frac{1}{n^{1/2}(\log m)^{1/2}} \left(\frac{\log m}{2} - \frac{\log^2 m}{2} - \frac{1}{16}\right) \cos_m\right].
$$

From Lemma 1 we also have

$$-\frac{L^1_{n-1}[\log(m+1)]}{m+1} = -\frac{1}{\sqrt{\pi}\sqrt{m+1}}\frac{(n-1)^{1/4}}{[\log(m+1)]^{3/4}}\left[\sin\left(2\sqrt{n-1}\sqrt{\log(m+1)}-\frac{\pi}{4}\right)\right.$$
$$\left.+\mathcal{M}(\log(m+1);1)\cos\left(2\sqrt{n-1}\sqrt{\log(m+1)}-\frac{\pi}{4}\right)\right]$$
$$= -\frac{n^{1/4}}{\sqrt{\pi}}[1+O(n^{-1})]\frac{1}{\sqrt{m+1}}\frac{1}{[\log(m+1)]^{3/4}}\left\{-\cos\left(2\sqrt{n-1}\sqrt{\log(m+1)}+\frac{\pi}{4}\right)\right.$$
$$\left.+\sin\left(2\sqrt{n}\sqrt{\log(m+1)}+\frac{\pi}{4}\right)\frac{1}{\sqrt{n}\sqrt{\log(m+1)}}\left[\frac{3}{16}+\log(m+1)-\frac{\log^2(m+1)}{12}\right]+\dots\right\}.$$

Expanding the cosine factor, using $\sqrt{n-1}=\sqrt{n}-1/(2\sqrt{n})+\dots$, then gives

$$-\frac{L^1_{n-1}[\log(m+1)]}{m+1} = \frac{n^{1/4}}{\sqrt{\pi}\sqrt{m+1}}\frac{1}{[\log(m+1)]^{3/4}}\left[\cos[2\sqrt{n}\sqrt{\log(m+1)}+\pi/4]\right.$$
$$\left.+\frac{1}{\sqrt{n}\sqrt{\log(m+1)}}\left(\frac{\log^2(m+1)}{12}-\frac{3}{16}\right)\sin[2\sqrt{n}\sqrt{\log(m+1)}+\pi/4]\right]. \tag{3.41}$$

The use of (3.40) and (3.41) gives Lemma 5.

We observe that for $m\to\infty$,

$$\Delta(m;n)-\Delta(m+1;n) = -\frac{1}{\sqrt{\pi}}\frac{n^{1/4}}{\sqrt{m}(\log m)^{3/4}}\cos_m$$
$$-\frac{1}{\sqrt{\pi}}\frac{n^{-1/4}}{\sqrt{m}(\log m)^{5/4}}\left[\frac{\log^2 m}{12}-\frac{3}{16}\right]\sin_m + O_n(n^{-3/4})+O_m(m^{-3/2}). \tag{3.42}$$

Here the symbol O_n (O_m) is used to denote the order of magnitude for n $(m)\to\infty$; but the above is the same as the negative of (3.41) with $m+1$ replaced by m therein. Thus for $m\to\infty$ (3.39) behaves as the second difference $\Delta(m;n)-2\Delta(m+1;n)+\Delta(m+2;n)+O(m^{-3/2})$ which is of the same order as $\frac{d^2}{dm^2}\Delta(m;n)$, and this is, apart from some logarithmic factors, $O(m^{-3/2})$. Thus (3.39) is summable over m.

We next simplify (3.39) and obtain (3.22) in Lemma 4. We write

$$\sin_m = \sin\left[2\sqrt{n}\sqrt{\log(m+1)}+\frac{\pi}{4}+\delta\right]$$
$$= \sin_{m+1}\cos\delta+\cos_{m+1}\sin\delta \tag{3.43}$$

where, for m large,

$$\delta \equiv 2\sqrt{n}\sqrt{\log m}-2\sqrt{n}\sqrt{\log(m+1)}$$
$$\sim -\frac{\sqrt{n}}{m\sqrt{\log m}} \sim -\frac{\sqrt{n}}{(m+1)\sqrt{\log(m+1)}} \equiv -\xi. \tag{3.44}$$

Thus we replace $\sin_m$ in (3.39) by $\sin_{m+1}\cos\xi-\cos_{m+1}\sin\xi$ and note that, for m large,

$$\frac{\sqrt{m}}{n^{1/4}(\log m)^{1/4}} \sim \frac{1}{\sqrt{\log(m+1)}}\frac{1}{\sqrt{\xi}}. \tag{3.45}$$

Then retaining only the leading order terms in (3.39) leads to the approximation in (3.22). This applies for n, $m\to\infty$ with $\xi=O(1)$. But in fact it remains valid for $n\to\infty$ with $m=O(1)$, and reduces to (3.23) in Lemma 4 in this limit. Note that for $m=O(1)$ and n large, $\xi\to\infty$ and $\xi-\sin\xi\sim\xi$, and this dominates $\cos\xi-1$, which remains $O(1)$. Thus (3.22) reduces to $\pi^{-1/2}[\log(m+1)]^{-1/2}\sqrt{\xi}\cos_{m+1}$ which is precisely (3.23). Also, for $m \gg O(\sqrt{n})$ (3.22) asymptotically matches (3.17), since it agrees with (3.37). Now we have $\xi \to 0$ so that $\xi - \sin\xi = O(\xi^3)$ while $\cos\xi - 1 \sim -\xi^2/2$ and thus (3.22) becomes

$$-\frac{1}{\sqrt{\pi}}\frac{\xi^{3/2}}{2\sqrt{\log(m+1)}}\sin\left[2\sqrt{n}\sqrt{\log(m+1)}+\frac{\pi}{4}\right]$$

which agrees with (3.37) for ξ (hence δ) $\to 0$. We have thus shown that (3.22) provides an asymptotically correct approximation to $F(m;n)$ for $n \to \infty$, both for $m = O(1)$ and for $m = O(\sqrt{n})$. Also, for $m \to \infty$, $\xi \to 0$ and (3.22) is $O(\xi^{3/2}) = O(m^{-3/2})$ so the expression is summable over m. $\square$

Next, we return to our main goal, which is to approximate $S_\gamma(n) + n$ in (3.3). The approximations to the summand F are given in Lemmas 4 and 5. Expressions (3.14), (3.16), and (3.17) apply for $\beta > 0$ so that $m = e^{\beta n}$ is exponentially large in n. But in this range the order in m of F changes from $O(m^{-3/2})$ (cf. (3.17)) to (roughly) $O(m^{-2})$ (cf. (3.11)) and thus the summand is uniformly exponentially small in n when $\beta > 0$. Hence only the terms in m that have $m = O(1)$ or $m = O(\sqrt{n})$ contribute to the leading term of $S_\gamma(n) + n$ and we have

Theorem 2. *For $n \to \infty$ and away from the zeros of $S_\gamma(n) + n$ we have*

$$S_\gamma(n)+n \sim \sum_{m=1}^{\infty}\frac{1}{\sqrt{\pi}}\frac{1}{[\log(m+1)]^{1/2}}\frac{1}{\sqrt{\xi}}\left\{(\cos\xi-1)\sin\left[2\sqrt{n}\sqrt{\log(m+1)}+\frac{\pi}{4}\right]\right.$$
$$\left. +(\xi-\sin\xi)\cos\left[2\sqrt{n}\sqrt{\log(m+1)}+\frac{\pi}{4}\right]\right\} \tag{3.46}$$

where $\xi = \sqrt{n}/[(m+1)\sqrt{\log(m+1)}]$. An alternative asymptotic form is

$$S_\gamma(n)+n \sim \sum_{m=1}^{\infty}\mathcal{F}(m;n), \tag{3.47}$$

where $\mathcal{F}$ is given by (3.39)*, and if $m = 1$, the term in* (3.39) *proportional to* $\sin_m$ *and* $\cos_m$ *must be replaced by* 1.

In section 4 we test the numerical accuracy of both (3.46) and (3.47). We can also obtain the simple upper bound below.

Theorem 3. *For n sufficiently large,*

$$|S_\gamma(n)+n| \le \frac{s_0}{\sqrt{2\pi}}n^{3/4}, \tag{3.48}$$

where

$$s_0 \equiv \sum_{m=1}^{\infty}\frac{1}{[\log(m+1)]^{5/4}}\frac{1}{(m+1)^{3/2}} \simeq 1.0819964. \tag{3.49}$$

Proof. To establish (3.48) we use the elementary inequality $|A\sin\varphi + B\cos\varphi| \leq \sqrt{A^2+B^2}$. Then denoting the summand in (3.46) as $F_*(m;n)$ we have

$$\sqrt{\pi}|F_*| \leq \frac{1}{\sqrt{\log(m+1)}}\frac{1}{\sqrt{\xi}}\sqrt{(\cos\xi-1)^2+(\xi-\sin\xi)^2}. \tag{3.50}$$

But

$$\begin{aligned}(\cos\xi-1)^2+(\xi-\sin\xi)^2 &= 2(1-\cos\xi-\xi\sin\xi)+\xi^2\\ &= \int_0^\xi 2x(1-\cos x)dx \leq \int_0^\xi 2x\left(\frac{x^2}{2}\right)dx = \frac{\xi^4}{4}\end{aligned} \tag{3.51}$$

so that $\sqrt{\pi}|F_*| \leq 2^{-1/2}[\log(m+1)]^{-1/2}\xi^{3/2} = n^{3/4}(m+1)^{-3/2}[\log(m+1)]^{-5/4}$ and Theorem 3 follows.

However, the numerical studies in section 4 suggest that the actual order of magnitude of $S_\gamma(n)+n$ is smaller than $O(n^{3/4})$, as Theorem 3 does not take into account the oscillations of the summands in Theorem 2. The numerical studies suggest that (3.48) is valid also for moderate n, and we conjecture that (3.48) is true for all $n \geq 5$.

We conclude by establishing the first equality in (1.5). We have that for $0 < \mathrm{Re}\ s < 1$,

$$\lim_{N\to\infty}\left[\sum_{m=1}^{N} m^{-s} - \frac{N^{1-s}}{1-s}\right] = \zeta(s). \tag{3.52}$$

Therefore, we find that

$$\lim_{N\to\infty}\left[\sum_{m=1}^{N-1}\frac{z-1}{z}\left[(m+1)^{\frac{z}{z-1}} - m^{\frac{z}{z-1}}\right] - (m+1)^{\frac{1}{z-1}}\right] = \frac{1}{z} - \zeta\left(\frac{1}{1-z}\right). \tag{3.53}$$

Having interchanged summation and integration in (3.3) with (3.5), it follows that

$$\begin{aligned}S_\gamma(n)+n &= \frac{1}{2\pi i}\oint \frac{z^{-n}}{(1-z)^2}\left[\frac{1}{z} - \zeta\left(\frac{1}{1-z}\right)\right]dz\\ &= \frac{1}{2\pi i}\int_C \left(\frac{w}{w-1}\right)^n\left[\frac{w}{w-1} - \zeta(w)\right]dw,\end{aligned} \tag{3.54}$$

where C is a vertical contour to the right of $\mathrm{Re}(w) = 1/2$. By employing the Laurent expansion of $\zeta(w)$, we recover the defining binomial expansion in (1.5) for $S_\gamma(n)$:

$$\begin{aligned}S_\gamma(n)+n &= \frac{1}{2\pi i}\int_C \left(\frac{w}{w-1}\right)^n\left[1 - \sum_{\ell=0}^{\infty}\frac{(-1)^\ell}{\ell!}\gamma_\ell(w-1)^\ell\right]dw\\ &= \frac{1}{2\pi i}\int_C \left(\frac{w}{w-1}\right)^n dw - \sum_{\ell=0}^{n-1}\frac{(-1)^\ell}{\ell!}\gamma_\ell\binom{n}{\ell+1}\\ &= n + \sum_{\ell=1}^{n}\frac{(-1)^\ell}{(\ell-1)!}\gamma_{\ell-1}\binom{n}{\ell}.\end{aligned} \tag{3.55}$$

□

4. Numerical studies. As we have discussed, $S_\gamma(n)+n$ exhibits oscillations, taking on both negative and positive values as n increases. This oscillation contains some local substructure, such as the pairs of nearby maxima and minima near $n=500$, 1100 and 1550 in Figure 6. Also plotted there are the corresponding results using the forms (3.46) and (3.47). At this level of graphical resolution, the refined result (3.47) is virtually indistinguishable from the exact values.

Known and reliable values of $S_\gamma(n)+n$ may be obtained based upon the high precision values of γ_k due to R. Kreminski [22]. The first 2000 of these values of γ_k are valid to 5000 decimal digits. Further values of γ_k are less accurate, with γ_{5000} valid to 1419 decimal digits, and γ_{10000} valid to about 862 decimal digits. These were computed using a variation of the published algorithm in [22]; but instead of using Newton Cotes integration a slightly faster approach using numerical differentiation ideas was used. Accordingly, R. Smith has now calculated $S_\gamma(n)+n$ for n up to 10^4 [30]. This result is shown in Figure 7, along with the corresponding values from (3.46) and (3.47). The numerical results of Smith, obtained with the aid of Mathematica® 7, were simply calculated to 10 significant figures.

The expression (3.46) is usually a lower bound for the exact values of $S_\gamma(n)+n$, while the refined result (3.47) virtually coincides with the exact values, in particular, well capturing the local substructure in both curvature and magnitude. Included in Figure 8 are values of $S_\gamma(n)+n$ and the results of (3.46) and (3.47), as well as the upper bounding curve $\sqrt{2}n^{1/4}+1$ and the lower bounding curve $-\sqrt{2}n^{1/4}$. It does appear that the values of $|S_\gamma(n)+n|$ are very close to $O(n^{1/4})$, in place of the conservative upper bound of Theorem 3.

The inequality in (3.48) of Theorem 3 begins to hold as soon as $n\geq 5$. As this onset is dependent upon the value of s_0, we briefly comment on it. From (3.49) we have

$$\begin{aligned} s_0 &= \frac{1}{\log^{5/4} 2}\frac{1}{2^{3/2}}+\sum_{m=2}^{\infty}\frac{1}{[\log(m+1)]^{5/4}}\frac{1}{(m+1)^{3/2}} \\ &< \frac{1}{\log^{5/4} 2}\frac{1}{2^{3/2}}+\sum_{m=2}^{\infty}\frac{1}{(m+1)^{3/2}} \\ &= \frac{1}{\log^{5/4} 2}\frac{1}{2^{3/2}}+\zeta(3/2)-1-\frac{1}{2\sqrt{2}}. \end{aligned} \tag{4.1}$$

Therefore, we have the simple lower and upper bounds

$$\begin{aligned} &\frac{1}{\log^{5/4} 2}\frac{1}{2^{3/2}}+\frac{1}{\log^{5/4} 3}\frac{1}{3^{3/2}}+\frac{1}{\log^{5/4} 4}\frac{1}{4^{3/2}}<s_0 \\ &\qquad < \frac{1}{\log^{5/4} 2}\frac{1}{2^{3/2}}+\zeta(3/2)-1-\frac{1}{2\sqrt{2}}, \end{aligned} \tag{4.2}$$

i.e., $0.813218 < s_0 < 1.81784$.

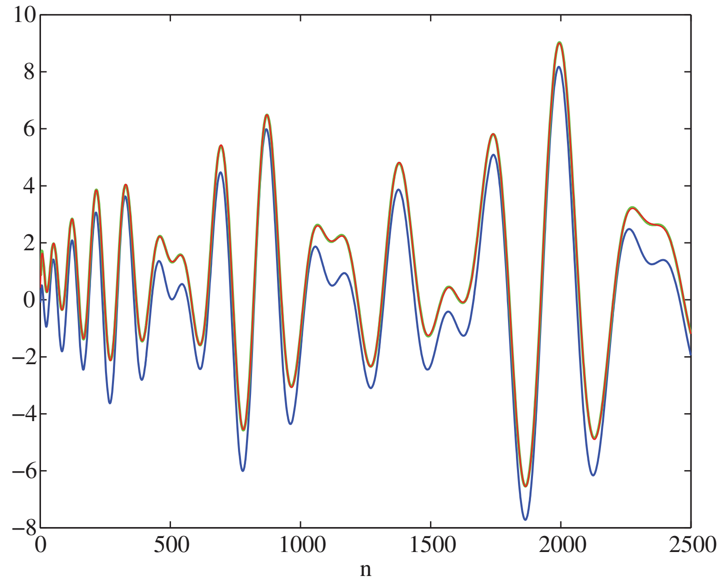

FIGURE 6. Exact values of $S_\gamma(n) + n$, (4.44), and (4.45) for n up to 2500.

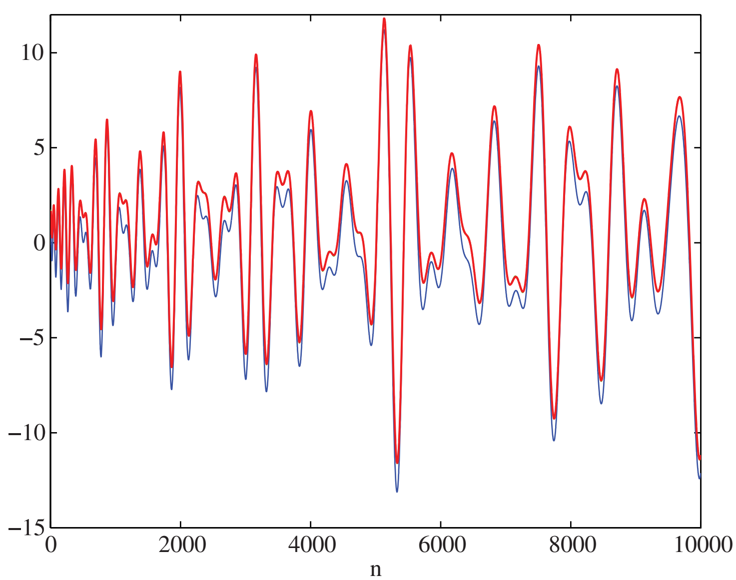

FIGURE 7. Values of $S_\gamma(n) + n$, (4.44), and (4.45) for n up to 10^4.

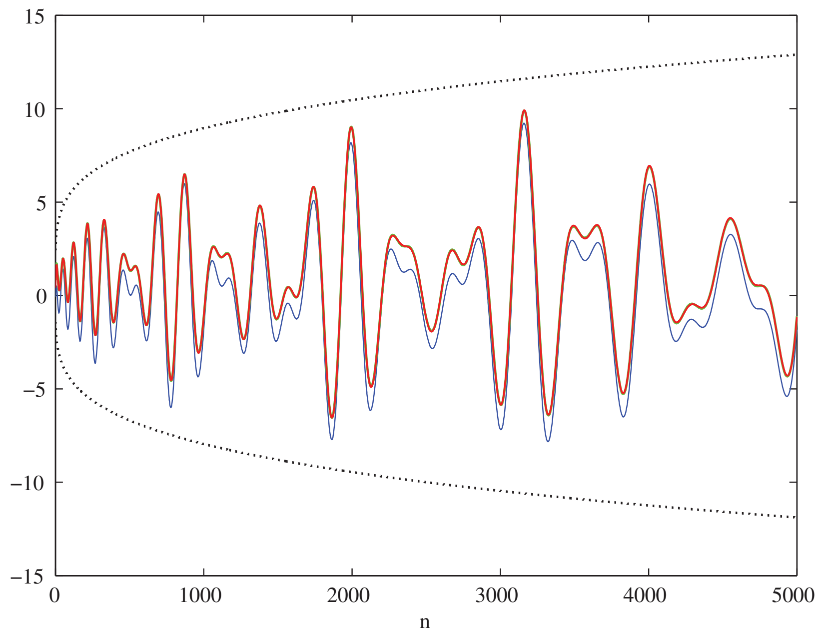

FIGURE 8. Values of $S_\gamma(n)+n$, (4.44), (4.45), and bounding curves varying as $\pm\sqrt{2}n^{1/4}$ (in black, dashed) for n up to 5000.

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