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Comments on and Extensions to Criteria of Keiper and Li for the Riemann Hypothesis

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Abstract

Keiper [1] and Li [2] published independent investigations of the connection between the Riemann hypothesis and the properties of sums over powers of zeros of the Riemann zeta function. Here we comment on these papers, and propose some extensions of their results. Key results are obtained using generalised Lambert functions.

Acknowledgements

We would like to thank Bruno Salvy, Jacques Gelinas and Lindsay Botten for their valuable communications.

1 Relevant equations from the literature

The function $\xi(s)$ is even under $s \rightarrow 1 - s$ and is defined as

$$\xi(s) = \frac{1}{2}s(s-1)\frac{\Gamma(s/2)\zeta(s)}{\pi^{s/2}} = \frac{1}{2}s(s-1)\xi_1(s). \quad (1)$$

We will be interested in mappings which move the location of lines along which zeros are located onto circles in the complex plane. For the case of functions putatively satisfying the Riemann hypothesis, a convenient mapping from the critical line $\Re(s) = \sigma = 1/2$ onto the unit circle is

$$w = u + iv = 1 - \frac{1}{s} = \frac{s-1}{s}. \quad (2)$$

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The inverse transformation is

$$s = \frac{1}{1-w}. \quad (3)$$

We commence with the expansion of $\xi(s + 1/2)$, based on the work of Pustyl'nikov [3, 4] and Hadamard [5]:

$$\xi\left(s + \frac{1}{2}\right) = \sum_{r=0}^{\infty} \xi_r s^{2r}, \quad (4)$$

where the coefficients ξ_r can be obtained in integral form from

$$\xi_r = \frac{2^{-(2r+2)}}{(2r)!} \mathcal{I}_{2r}, \quad (5)$$

with

$$\mathcal{I}_r = \int_1^{\infty} [\log(x)^{r-2}] [16r(r-1) - \log(x)^2] x^{-3/4} \omega(x) dx \quad (6)$$

and $\omega(x) = \sum_{n=1}^{\infty} \exp(-\pi n^2 x)$ being related to the elliptic theta function ϑ_3 . Pustyl'nikov [4] establishes in his Theorem 1 that all even order derivatives of $\xi(s)$ at $s = 1/2$ are strictly positive. His Theorem 2 is that Theorem 1 provides a necessary condition for the Riemann hypothesis to hold. Asymptotic analysis of the integral (4) may be found in Pustyl'nikov [3], and supplementary comments with numeric results are available in [6] and in a valuable communication to the author from Jacques G elinas [7]. The latter reference contains extensions to the asymptotics of Pustyl'nikov, which give an accurate exponent and first digit for the ξ_r . Recent publications [8, 9] contain formulae which substantially improve the asymptotic formulae, such that 16-18 decimal digits are given for r in the range 2000-20000.

Keiper [1] considers two sets of sums over powers of zeros ρ of $\xi(s)$ The first set σ_k occurs in the expansion of $\log[\xi(s)/\xi(0)]$:

$$\log[2\xi(s)] = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{\sigma_k^K}{k} (s-1)^k. \quad (7)$$

(The superscript K here indicates sums as defined by Keiper; we will also discuss similar sums in the work of Li, to be denoted σ_k^L , with $\sigma_k^L = k\sigma_k^K$.) The derivative of (7) is

$$\frac{\xi'(s)}{\xi(s)} = \sum_{k=1}^{\infty} \sigma_k^K (1-s)^{k-1}. \quad (8)$$

The σ_k^K are given by:

$$\sigma_k^K = \sum \frac{1}{\rho^k}. \quad (9)$$

They are always real since every zero ρ can be paired with its conjugate, also a zero. Their modulus displays a simple exponential decrease, governed by

the modulus of the first zero (around 14.1436). However the signs of the real quantities σ_k vary in a complicated fashion when k becomes large, since the first and second terms in the expansion (9) may become at times of comparable magnitude.

The value of σ_1^K is analytic:

$$\sigma_1^K = 1 + \frac{\gamma}{2} - \frac{1}{2} \log(4\pi) \approx 0.023095709 \dots \quad (10)$$

Keiper [1] gives numerical values for certain low order σ_k^K , with a more extensive and more accurate tabulation having been constructed by Dr. Rick Kreminski [10]. For σ_2^K , we obtain

$$\sigma_2^K = 1 + \gamma^2 - \frac{\pi^2}{8} + 2\gamma_1 \approx -0.0461543172 \dots \quad (11)$$

Another useful value is that of

$$\sum_{\rho} \frac{1}{|\rho|^2} = 2\sigma_1^K, \quad (12)$$

if the Riemann hypothesis holds.

Interconnecting relationships among the σ_k provided by Keiper [1] include

$$\sum_{k=1}^{\infty} \frac{1}{k} \sigma_k = 0, \quad \sigma_1 = - \sum_{k=1}^{\infty} \sigma_k. \quad (13)$$

A more general result is

$$\sigma_{j+1} = (-1)^{j+1} \sum_{k=1}^{\infty} \binom{k-1}{j} \sigma_k. \quad (14)$$

We now turn to quantities λ , used by both Keiper [1] and Li [2] in discussions relating to the Riemann hypothesis. The definition of these linked quantities we now give comes from Li:

$$(n-1)! \lambda_n^L = \frac{d^n}{ds^n} [s^{n-1} \log(2\xi(s))]_{s=1} = n! \lambda_n^K. \quad (15)$$

The λ_k^K are related to the σ_j , as shown by Keiper:

$$\lambda_0 = 0, \quad \lambda_1 = \sigma_1, \quad \lambda_k^K = \sum_{j=1}^k \frac{(-1)^{j-1}}{j} \binom{k-1}{j-1} \sigma_j. \quad (16)$$

The connection of the λ_k^K with the Riemann hypothesis is discussed by Keiper in connection with the relation:

$$\lambda_m^L = m \lambda_m^K = \sum_{\rho} \left[1 - \left(\frac{\rho}{\rho-1} \right)^m \right]. \quad (17)$$

If the Riemann hypothesis holds, then all the zeros ρ lie on the critical line, with $|\rho| = |\rho - 1|$. The sum over zeros in (17) can not then be negative, so $\lambda_m > 0$ for all m is a necessary condition for the Riemann hypothesis, as stated by Keiper. He also provided the first two terms in a large m expansion of λ_m^K , based on assuming the Riemann hypothesis and "very evenly distributed" zeros:

$$\lambda_m^K \approx \frac{1}{2} \log m - \frac{1}{2}(\log(2\pi) + 1 - \gamma). \quad (18)$$

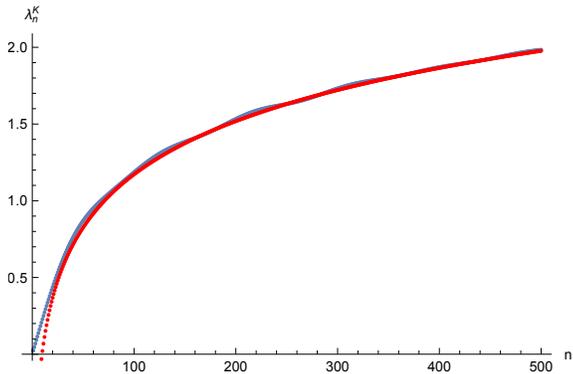


Figure 1: The values λ_m^K as a function of m determined numerically (blue) are compared with Keiper's formula (18) (red).

Figure 1 shows the behaviour of the λ_m^K up to $m = 500$. It consists of an obvious logarithmic smooth trend [11], plus superimposed oscillations. (Note that, as in all numerical cases studied in this paper, calculations were carried out on a laptop using Mathematica.) Maślanka [11] and others such as M. W. Coffey [12, 13] were inspired by a paper by Bombieri and Lagarias [14], which introduced a splitting of λ_n^L into trend and oscillation terms:

$$\lambda_n^L = \bar{\lambda}_n + \tilde{\lambda}_n, \quad (19)$$

where the trend is

$$\bar{\lambda}_n = 1 - (\log(4\pi) + \gamma) \frac{n}{2} + \sum_{j=2}^n (-1)^j \binom{n}{j} (1 - 2^{-j}) \zeta(j), \quad (20)$$

and the oscillation is

$$\tilde{\lambda}_n = - \sum_{j=1}^n \binom{n}{j} \eta(j-1). \quad (21)$$

Here the η_m can be defined [14] as the coefficients occurring in the expansion

$$\log(s\zeta(s+1)) = - \sum_{n=0}^{\infty} \eta_n \frac{s^n}{n+1}. \quad (22)$$

Coffey [12] gives the η_n in terms of the σ_k and $\zeta(k)$:

$$(-1)^n \eta_{n-1} = \sigma_n + (1 - 2^{-n})\zeta(k) - 1. \quad (23)$$

The trend contains a sum over the poles of on the real axis $\zeta(s)$, while the oscillation counteracts the poles with zeros on the real axis and adds in the sum over zeros off the real axis σ_j .

Coffey [12, 13] bounds the sum in equation (20) to give:

$$\frac{n}{2} \ln n + (\gamma - 1)\frac{n}{2} + \frac{1}{2} \leq S_1(n) \leq \frac{n}{2} \ln n + (\gamma + 1)\frac{n}{2} - \frac{1}{2}. \quad (24)$$

The leading term in (24) corresponds to the leading term in Keiper's representation (18), with the former not being associated with the assumptions said to lead to (18).

2 Keiper's sums τ and their generalisation

In recent years Keiper's paper [1] on the sums over zeros λ has begun to receive more attention. However, not as much attention has been paid to the second set of sums (τ) he studied in the same work. (Keiper died in 1995, and so was not able to continue his research on this topic). In order to introduce these sums, we define the central difference operator \mathcal{C}_m acting on a sequence $f(m)$:

$$\mathcal{C}_m f(m) = f(m+1) - 2f(m) + f(m-1). \quad (25)$$

We apply this to λ_m^L :

$$\tau_m = \mathcal{C}_m \sum_{\rho} \left[1 - \left(\frac{\rho}{\rho-1} \right)^m \right], \quad (26)$$

giving Keiper's result:

$$\tau_m = - \sum_{\rho} \left(\frac{\rho}{\rho-1} \right)^{m+1} \frac{1}{\rho^2}. \quad (27)$$

This can also be expressed in terms of the σ_j :

$$\tau_0 = \sigma_1, \quad \tau_k = \sum_{j=1}^k \binom{k-1}{j-1} (-1)^j \sigma_{j+1} \text{ for } k \geq 1. \quad (28)$$

Another expression for the τ_n comes from the application of the central difference operator to the defining relationship (15). This is

$$\tau_n = \frac{1}{(n-1)!} \frac{d^{n-2}}{ds^{n-2}} \left[s^{n-1} \frac{d^2}{ds^2} \ln(\xi(s)) \right]_{s=1}. \quad (29)$$

The τ_m have been expressed in terms of the central differences of the λ 's. We can go in the opposite direction using the fact that the central difference is the difference of the first differences, to obtain two new expressions:

$$\sum_{n=1}^m \tau_n = \lambda_{m+1}^L - \lambda_m^L - \lambda_1^L, \quad (30)$$

and

$$\sum_{n=1}^{m-1} n\tau_n = m\lambda_{m+1}^L - (m+1)\lambda_m^L. \quad (31)$$

These may be combined to give

$$\sum_{n=1}^{m-1} (m-n)\tau_n = \sum_{n=1}^m (m-n)\tau_n = \lambda_m^L - m\lambda_1^L. \quad (32)$$

Keiper [1] argues from (27) that the Riemann hypothesis implies that $|\rho/(\rho-1)| = 1$ for all ρ , and so the values of $|\tau_k|$ must be bounded by $2\sigma_1^K$ from (12). Keiper's expression analogous to (29) is used by him to argue the converse: that if the $|\tau_k|$ are bounded, the Riemann hypothesis must hold.

The central difference operator applied to the leading term (24) gives $1/(2k)$. Interestingly, terms linear in k or constant give zero for this operation. In Fig. 2 we compare this leading term estimate with numerical values of the τ_k . Unlike the situation with the λ 's, this smooth trend line is no longer dominant over the oscillations. However, numerical evidence is that the λ_k 's increase monotonically with k , and this is of course a sufficient condition for the Riemann hypothesis. It is also sufficient to show from (30) that $\lambda_1 + \sum_{n=1}^m \tau_n > 0$ for all m , presumably due to the influence of the trend term.

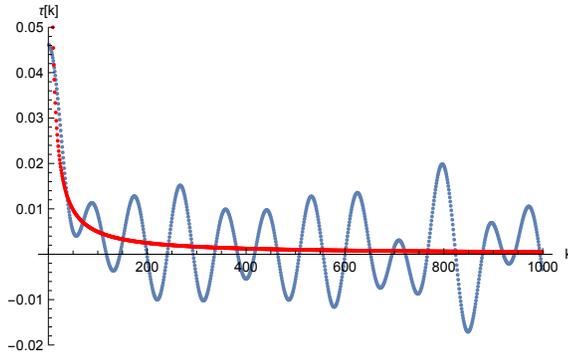


Figure 2: The values τ_k as a function of k determined numerically (blue) are compared with $1/(2k)$ (red).

Motivated by these results, we define a general sum over the zeros ρ :

$$\mathcal{S}_{m,q} = - \sum_{\rho} \frac{1}{\rho^{2q}} \left(\frac{\rho}{\rho-1} \right)^{m+q} = - \sum_{\rho} \frac{\rho^{m-q}}{(\rho-1)^{m+q}}. \quad (33)$$

We note that

$$\tau_m = \mathcal{S}_{m,1} = \lambda_{m+1}^L - 2\lambda_m^L + \lambda_{m-1}^L. \quad (34)$$

The $\mathcal{S}_{m,q}$ obey a recurrence relation in q :

$$\mathcal{S}_{m,q+1} = \mathcal{S}_{m+1,q} - 2\mathcal{S}_{m,q} + \mathcal{S}_{m-1,q}. \quad (35)$$

Putting $q = 1$, this enables us to conclude the elegant continuation of (34) and (35):

$$\mathcal{S}_{m,2} = \tau_{m+1} - 2\tau_m + \tau_{m-1}. \quad (36)$$

Keiper [1] in his equations (25) and (28) gives expressions for his τ_m as sums over σ_m^K . The following expressions generalise these to the $\mathcal{S}_{m,q}$:

$$\mathcal{S}_{m,q} = - \sum_{j=2q}^{\infty} \binom{j+m-q-1}{m+q-1} \sigma_j \quad (37)$$

and, if $m > q$,

$$\mathcal{S}_{m,q} = - \sum_{j=2q-1}^{m+q-1} (-1)^j \binom{m-q}{j+1-2q} \sigma_j. \quad (38)$$

Particular cases of $\mathcal{S}_{m,q}$ are of interest. We note that the correspondence between zeros ρ and $1 - \rho$ of $\zeta(s)$ implies the following symmetry relationship:

$$\mathcal{S}_{-m,q} = \mathcal{S}_{m,q}. \quad (39)$$

Putting $m = 0$ in (33), we have

$$\mathcal{S}_{0,q} = - \sum_{\rho} \frac{1}{\rho^q(\rho-1)^q} = (-1)^{q+1} \sum_{\rho} \frac{1}{\rho^q(1-\rho)^q}. \quad (40)$$

If the Riemann hypothesis holds, the summand in (40) becomes $1/|\rho|^{2q}$, and thus $\mathcal{S}_{0,q}$ strictly alternates in sign as q increases. Of course $\mathcal{S}_{0,0}$ is undefined, while $\mathcal{S}_{0,1} = 2\sigma_1$.

Another interesting case is:

$$\mathcal{S}_{m,m} = - \sum_{\rho} \frac{1}{(1-\rho)^{2m}} = -\sigma_{2m}, \quad (41)$$

which is absolutely convergent for $m \geq 1$. We generalise this:

$$\mathcal{S}_{m,m+\delta q} = - \sum_{\rho} \frac{1}{\rho^{\delta q}(1-\rho)^{2m+\delta q}}, \quad (42)$$

absolutely convergent for $\delta q \geq 0$ if $m \geq 1$.

The equivalent of (30) for the \mathcal{S} 's is

$$\sum_{p=m-l}^m \mathcal{S}_{p,q} = \mathcal{S}_{m+1,q-1} - \mathcal{S}_{m,q-1} - \mathcal{S}_{m-l,q-1} + \mathcal{S}_{m-l-1,q-1}. \quad (43)$$

If $l = m - 1$ and $q \geq 2$, (43) is

$$\sum_{p=1}^m \mathcal{S}_{p,q} = \mathcal{S}_{m+1,q-1} - \mathcal{S}_{m,q-1} - \mathcal{S}_{1,q-1} + \mathcal{S}_{0,q-1}. \quad (44)$$

We show the behaviour of low order sums $\mathcal{S}_{m,q}$ as a function of m in Figs. 3-5. Rapid convergence is evident as q increases towards a single term driven by the first zero of $\zeta(s)$, $\rho_1 = 1/2 + it_1$. The complicated behaviour evident in Fig. 2 for $q = 1$ rapidly becomes more simple, with slight deviations from the ρ_1 term explicable by the inclusion of a ρ_2 term.

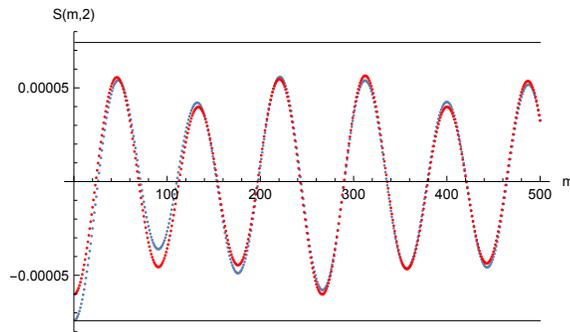


Figure 3: The values $\mathcal{S}_{m,2}$ (blue) as a function of m , determined by summation over the first 1000 zeros ρ are compared with the results of summation over the first two zeros (red). The two black lines correspond to $\pm\mathcal{S}_{0,2}$.

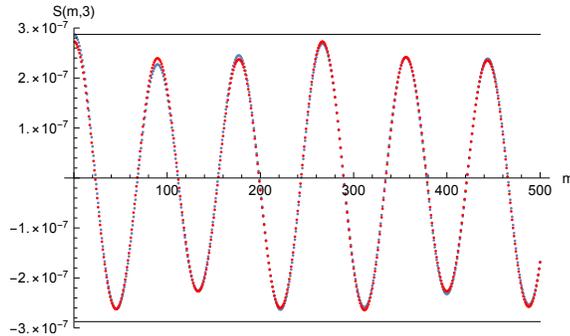


Figure 4: The values $\mathcal{S}_{m,3}$ (blue) as a function of m , determined by summation over the first 1000 zeros ρ are compared with the results of summation over the first two zeros (red). The two black lines correspond to $\pm\mathcal{S}_{0,3}$.

Note that Keiper's argument in relation to $\mathcal{S}_{m,1} = \tau_m$ and the Riemann hypothesis applies equally to the $\mathcal{S}_{m,q}$ for $q > 1$. In each case, the relevant bounds on the $\mathcal{S}_{m,q}$ are given by $\pm\mathcal{S}_{0,q}$.

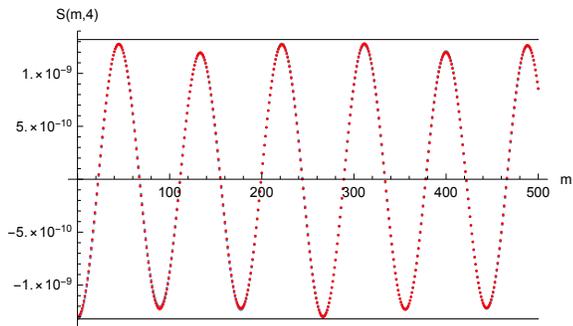


Figure 5: The values $\mathcal{S}_{m,4}$ (blue) as a function of m , determined by summation over the first 1000 zeros ρ are compared with the results of summation over the first two zeros (red). The two black lines correspond to $\pm\mathcal{S}_{0,4}$.

3 Li's necessary and sufficient condition for the Riemann hypothesis

Li's paper [2] was written after Keiper's [1] and does not cite it. It is written in the classical style of theorem and proof, while Keiper was providing an early example of what has come to be known as experimental mathematics. Here we will be interested in providing further details and understanding of the following theorem:

Theorem 1. (*Li*) *A necessary and sufficient condition for the nontrivial zeros of the Riemann zeta function to lie on the critical line is that λ_n^L is non-negative for every positive integer n .*

Here of course we have used the notation λ_n^L to avoid confusion with Keiper's use of the same Greek symbol. Li frames his proof of this theorem using the same mapping as Keiper from the complex s plane to the unit circle, and writing two key expansions:

$$\phi(z) = 2\xi\left(\frac{1}{1-z}\right) = 1 + \sum_{j=1}^{\infty} a_j z^j, \quad (45)$$

and

$$\frac{\phi'(z)}{\phi(z)} = \sum_{n=0}^{\infty} \lambda_{n+1}^L z^n. \quad (46)$$

These two equations are used by Li to connect the λ_n^L and the a_n in the following recurrence relation:

$$\lambda_n^L = na_n - \sum_{j=1}^{n-1} \lambda_j^L a_{n-j}. \quad (47)$$

Li does not give any representation for the quantities a_n , but provides a proof that they are positive. We can derive a convenient representation for them using the expansion (4), re-expanding about $s = 1$ using the Binomial Theorem, and then the following expansion in the variable $w = 1/(1 - s)$:

$$\left(\frac{1+w}{1-w}\right)^r = 1 + \sum_{n=1}^{\infty} a_r(n)w^n. \quad (48)$$

Here the coefficients $a_r(n)$ are explicit:

$$a_r(n) = \sum_{p=0}^n \binom{r+n-p-1}{r-1} \binom{r}{p}. \quad (49)$$

The $a_r(n)$ are polynomials in r of degree n . The result of this procedure is

$$a_n = 2 \sum_{r=1}^{\infty} \frac{\xi_r}{2^{2r}} a_{2r}(n), \text{ for } n = 1, 2, 3, \dots, \quad (50)$$

with $n = 0$ corresponding to the identity

$$2\xi_0 + 2 \sum_{r=1}^{\infty} \frac{\xi_r}{2^{2r}} = 1. \quad (51)$$

Now, all the coefficients ξ_r are positive, as proved by Pustyl'nikov [3], a fact known to Hurwitz and Jensen. (I am indebted to J. Gélinas for this comment.) Given the positivity of the $a_r(n)$ from (49), this provides an alternative proof to that of Li [2] that the a_n are all positive. It is also evident that they increase monotonically with n .

The relationship (49) can be written in terms of the Pochhammer symbol $(x)_n$:

$$a_r(n) = \sum_{p=0}^n \frac{1}{(n-p)!p!} r(r-p+1)_{n-1}, \quad (52)$$

where

$$(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)} = x(x+1)(x+2)\dots(x+n-1). \quad (53)$$

The series expansion of the Pochhammer symbol is given in terms of Stirling numbers of the first kind [15]. We will use the following result:

$$r(r-x)_n = \begin{cases} r & n = 0 \\ r^2 - xr & n = 1 \\ \sum_{k=0}^n S_1(n, k)(-1)^{n-k} r^{k+1} & n > 1, x = 0 \\ \sum_{k=1}^n S_1(n, k)(-1)^{n-k} \sum_{l=0}^k \binom{k}{l} r^{l+1} (-1)^{k-l} x^{k-l} & n > 1, x \neq 0 \end{cases} \quad (54)$$

Here the combination $S_1(n, k)(-1)^{n-k}$ renders the Stirling number of the first kind always positive. Using the relationship $S_1(n, 0) = \delta_{n,0}$ in (52) and (54), we

obtain two particular cases of $a_r(n)$: $a_r(1) = 2r$ and $a_r(2) = 2r^2$. The general expression is:

$$a_r(n) = \sum_{p=0}^n \frac{1}{(n-p)!p!} \sum_{k=1}^{n-1} (-1)^{n-1-k} S_1(n-1, k) [\delta_{p,1} r^{k+1} + (1 - \delta_{p,1}) \sum_{l=0}^k \binom{k}{l} r^{l+1} (-1)^{k-l} (p-1)^{k-l}]. \quad (55)$$

Some properties of the $a_r(n)$ follow easily from the definition (48). Let

$$F_r(w) = \left(\frac{1+w}{1-w} \right)^r = \frac{1}{F_r(-w)} = \frac{1}{F_{-r}(w)} = F_{-r}(-w). \quad (56)$$

It follows from this that $a_{-r}(n) = (-1)^n a_r(n)$, so that $a_r(n)$ is an even function of r if n is even, and an odd function if n is odd. Another interesting result comes from expansion of the relationship $F_r(w)F_{-r}(w) = 1$:

$$a_r(n)(1 + (-1)^n) + \sum_{p=1}^{n-1} (-1)^{n-p} a_r(p) a_r(n-p) = 0. \quad (57)$$

This yields $0 = 0$ for n odd, but for n even expresses $2a_r(2n)$ in terms of products of two lower-index $a_r(n)$'s.

We next rewrite equation (47) as:

$$\frac{\lambda_n^L}{a_n} = n - \sum_{j=1}^{n-1} \lambda_j^L \frac{a_{n-j}}{a_n}. \quad (58)$$

The left-hand side of this equation is plotted as a function of n in Fig. 6. It can be seen from this figure that Li's condition will become ever more ill-conditioned as n increases. A reasonably accurate fit to the data in Fig. 6 is provided by the following function:

$$\left[\frac{\lambda_n^L}{a_n} \right]_{app} = 1.86537n \exp(-0.06607n). \quad (59)$$

This has the exponential factor optimized to fit the tail of the data in Fig. 6, and the multiplying constant from a best fit to all the data. The exponential decay towards zero in the graph and the fit function show that the sum on the right-hand side is very close to n for large n . Li's criterion requires us to prove that the sum tends up to n from below, and the data here shows the sum will be exponentially close to n , evincing the difficulty in providing a proof based on the criterion.

To go further into the details of the equation (47), we consider additional properties of the $a_{2r}(n)$. These satisfy the following recurrence relation for n varying:

$$a_{2r}(n) = \frac{4r}{n} a_{2r}(n-1) + \frac{(n-2)}{n} a_{2r}(n-2). \quad (60)$$

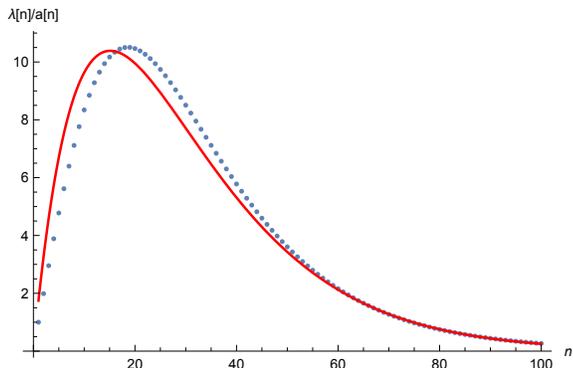


Figure 6: The first 100 values of λ_n/a_n (blue) as a function of n , compared with the fit function (59) .

Considering the ratio of successive terms in (60):

$$\rho_n = \frac{a_{2r}(n)}{a_{2r}(n-1)} \quad (61)$$

the large n analysis of equation (60) leads to the asymptotic estimate

$$\rho_n = 1 + \frac{(2r-1)}{n} + \frac{(2r-1)}{n^2} + \dots \quad (62)$$

For $r = 1$, equation (62) is exact.

The recurrence relation (60) can be used to calculate easily these polynomials, starting from $a_{2r}(1) = 4r$ and $a_{2r}(2) = 8r^2$. The next two polynomials are $a_{2r}(3) = 4r/3 + 32r^3/3$ and $a_{2r}(4) = 16r^2/3 + 32r^4/3$, as seen in the expansion:

$$\left(\frac{1+w}{1-w}\right)^{2r} = 1 + 4rw + 8r^2w^2 + \frac{4}{3}(8r^3 + r)w^3 + \frac{16}{3}(2r^4 + r^2)w^4 + O(w^5). \quad (63)$$

The remaining polynomials up to order $n = 20$ are specified in Table 3 by giving the coefficients $C_{n,p}$ of r^p for p ranging up to $p = n$:

$$a_{2r}(n) = \sum_{p=1}^n C_{n,p} r^p. \quad (64)$$

It will be noted that the polynomials are of order n and comprise even order terms if n is even, and odd order terms if n is odd. One further property of interest is that the sum of all the coefficients in each polynomial is just $4n$. Given each coefficient is positive, this bounds the coefficients, or gives their mean as 4.

From (60), the coefficients $C_{n,p}$ satisfy the general recurrence relation:

$$C_{n,p} = \frac{4}{n}C_{n-1,p-1} + \frac{(n-2)}{n}C_{n-2,p}, \text{ for } 1 \leq p \leq (n-2), \quad (65)$$

with the special cases

$$\mathcal{C}_{2n+1,1} = \frac{(2n-1)}{2n+1} \mathcal{C}_{2n-1,1}, \text{ and } \mathcal{C}_{n,n} = \frac{4}{n} \mathcal{C}_{n-1,n-1}. \quad (66)$$

The first of these gives for all positive integers n :

$$\mathcal{C}_{2n-1,1} = \frac{4}{2n-1}, \quad (67)$$

while the second gives:

$$\mathcal{C}_{n,n} = \frac{4^n}{n!}. \quad (68)$$

In this second case, the coefficient has its maximum value at $n = 3, 4$ and then falls away rapidly with increasing n . It falls below the mean coefficient (four) for n between 6 and 7.

The first non-zero entry for n even satisfies the recurrence relation:

$$\mathcal{C}_{2n,2} = \frac{8}{n(2n-1)} + \frac{(n-1)}{n} \mathcal{C}_{2n-2,2}, \quad (69)$$

and commences with $\mathcal{C}_{2,2} = 8$. The solution of this recurrence relation is

$$\mathcal{C}_{2n,2} = \frac{8}{n} \sum_{p=1}^n \frac{1}{(2n-(2p-1))} = \frac{8}{n} \left[\frac{1}{2} \psi \left(n + \frac{1}{2} \right) + \frac{1}{2} \gamma + \ln 2 \right], \quad (70)$$

where the ψ function is the zeroth order polygamma function [15].

Another way of expressing the $\mathcal{C}_{2n,2}$ is in terms of harmonic numbers, where the n th harmonic number H_n is defined by [16]:

$$H_n = \sum_{k=1}^n \frac{1}{k}. \quad (71)$$

We then have:

$$\mathcal{C}_{2n,2} = \frac{8}{n} \left[H_{2n} - \frac{1}{2} H_n \right]. \quad (72)$$

The asymptotic expansion of the harmonic numbers is given in an expression involving the Bernoulli numbers B_{2k} :

$$H_n \sim \log(n) + \gamma + \frac{1}{2n} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2kn^{2k}}, \quad (73)$$

leading to the asymptotic series for $\mathcal{C}_{2n,2}$:

$$\mathcal{C}_{2n,2} \sim \frac{8}{n} \left[\frac{1}{2} \log(n) + \log(2) + \frac{1}{2} \gamma + \sum_{k=1}^{\infty} \frac{B_{2k}}{4kn^{2k}} \left(1 - \frac{1}{2^{(2k-1)}} \right) \right]. \quad (74)$$

The asymptotic formula (74) has good accuracy for n as low as two. We also have:

$$\frac{\mathcal{C}_{2n+2,2}}{\mathcal{C}_{2n,2}} \sim 1 - \frac{1}{n} \left(1 - \frac{1}{\gamma + \log(4n)} \right) + \frac{-3 + 2\gamma + 2 \log(4n)}{2(\gamma + \log(4n))n^2} + O\left(\frac{1}{n^3}\right). \quad (75)$$

The ratio of successive values of $\mathcal{C}_{2n,2}$ starts at $2/3$ and, in keeping (75), increases monotonically towards unity. $\mathcal{C}_{2n,2}$ itself decreases monotonically as n increases, in keeping with (74).

Consider next $\mathcal{C}_{2n-1,3}$. The formula for this is

$$\mathcal{C}_{2n-1,3} = \frac{4}{2n-1} \sum_{p=1}^{n-1} \mathcal{C}_{2n-2p,2} = \frac{4}{2n-1} \sum_{p=1}^{n-1} \mathcal{C}_{2p,2}. \quad (76)$$

Note that $\mathcal{C}_{3,3} = \mathcal{C}_{5,3} = 32/3$: thereafter, $\mathcal{C}_{2n-1,3}$ decreases as n increases. For $\mathcal{C}_{2n,4}$ a similar relation applies:

$$\mathcal{C}_{2n,4} = \frac{4}{2n} \sum_{p=2}^n \mathcal{C}_{2p-1,3}. \quad (77)$$

This quantity increases with n up until $n = 4$, and thereafter decreases monotonically.

The pattern in the expressions for these sums is that even order terms are expressed as a sum of odd order terms, with the second index lowered by one. The sum over the first index runs from the term given in (68) to one less than the first index on the left-hand side. A similar description applies to odd order terms. The derivations rely on the following equations:

$$n\mathcal{C}_{2n,2} - (n-1)\mathcal{C}_{2n-2,2} = \frac{8}{(2n-1)}, \quad (2n-1)\mathcal{C}_{2n-1,3} - (2n-3)\mathcal{C}_{2n-3,3} = 4\mathcal{C}_{2n-2,2}. \quad (78)$$

Here first differences generate elements with an intervening first index and the second index lowered by one. These properties are generic, as the recurrence relations (65), (66) show.

The general expression for the \mathcal{C} can be derived from equation (48). It is, for $n \geq 3$:

$$\begin{aligned} \mathcal{C}_{n,q} &= \frac{2^q}{(n-1)!} (-1)^{n-q} S_1(n-1, q-1) + \\ &\sum_{p=0}^n \frac{2^q}{(n-p)! p!} \sum_{k=q-1}^{n-1} (-1)^{n-1-k} S_1(n-1, k) \binom{k}{q-1} (1 - \delta_{p,1}) (-1)^{k-q+1} (p-1)^{k-q+1}. \end{aligned} \quad (79)$$

We can rewrite the equation (47) as

$$\lambda_k^L = 2 \left\{ \sum_{r=1}^{\infty} \frac{\xi_r}{2^{2r}} \left[k a_{2r}(k) - \sum_{j=1}^{k-1} \lambda_j^L a_{2r}(k-j) \right] \right\}. \quad (80)$$

To sum over the polynomials in r quoted above and in Table 3, we define the following sums over a single term:

$$\Sigma_p^\xi = \sum_{r=1}^{\infty} \frac{\xi_r}{2^{2r}} r^p. \quad (81)$$

Then we find

$$a_n = 2 \sum_{p=1}^n C_{n,p} \Sigma_p^\xi \quad (82)$$

and

$$\lambda_m^L = 2m \sum_{p=1}^m C_{m,p} \Sigma_p^\xi - 2 \sum_{n=1}^{m-1} \lambda_n^L \sum_{p=1}^{m-n} C_{m-n,p} \Sigma_p^\xi. \quad (83)$$

We can compare (83) with equation (16):

$$\lambda_m^L = \sum_{n=1}^m (-1)^{n-1} \binom{m}{n} \sigma_n, \quad (84)$$

and establish a connection between the σ_n and the Σ_p^ξ , or (indirectly) the ξ_p .

The result of this procedure is analytic equations which increase rapidly in complexity with increasing order, as seen below:.

$$\sigma_1 = 8\Sigma_1^\xi, \quad \sigma_2 = 16(\Sigma_1^\xi + 4(\Sigma_1^\xi)^2 - 2\Sigma_2^\xi), \quad (85)$$

$$\sigma_3 = 32[\Sigma_1^\xi + 6(\Sigma_1^\xi)^2 + 16(\Sigma_1^\xi)^3 - 3\Sigma_2^\xi - 12\Sigma_1^\xi \Sigma_2^\xi + 2\Sigma_3^\xi], \quad (86)$$

$$\begin{aligned} \sigma_4 = & \frac{64}{3}[3\Sigma_1^\xi + 22(\Sigma_1^\xi)^2 + 96(\Sigma_1^\xi)^3 + 192(\Sigma_1^\xi)^4 - 11\Sigma_2^\xi - 72\Sigma_1^\xi \Sigma_2^\xi \\ & - 192(\Sigma_1^\xi)^2 \Sigma_2^\xi + 24(\Sigma_2^\xi)^2 + 12\Sigma_3^\xi + 12\Sigma_3^\xi + 32(\Sigma_1^\xi)^2 \Sigma_3^\xi - 4\Sigma_4^\xi], \quad (87) \end{aligned}$$

and

$$\begin{aligned} \sigma_5 = & \frac{64}{3}[6\Sigma_1^\xi + 50(\Sigma_1^\xi)^2 + 280(\Sigma_1^\xi)^3 + 960(\Sigma_1^\xi)^4 + 1536(\Sigma_1^\xi)^5 \\ & - 25\Sigma_2^\xi - 210\Sigma_1^\xi \Sigma_2^\xi - 960(\Sigma_1^\xi)^2 \Sigma_2^\xi - 1920(\Sigma_1^\xi)^3 \Sigma_2^\xi + 120(\Sigma_2^\xi)^2 + 480\Sigma_1^\xi (\Sigma_2^\xi)^2 \\ & + 35\Sigma_3^\xi + 160\Sigma_1^\xi \Sigma_3^\xi + 320(\Sigma_1^\xi)^2 \Sigma_3^\xi - 80\Sigma_2^\xi \Sigma_3^\xi - 20\Sigma_4^\xi - 40\Sigma_1^\xi \Sigma_4^\xi + 4\Sigma_5^\xi]. \quad (88) \end{aligned}$$

Of course, the same procedure may be used to construct more compact equations with purely numeric coefficients, or to find particular terms in exact form for equations of higher order.

The final three figures relate to the numerical evaluation of the Σ_n^ξ . The number of terms needed in the summand for accurate evaluation (Fig. 7) is governed by the value of r , r_{max} , for which the summand is maximised. This value increases roughly as $n/8$, and the summand falls away rapidly as r moves away from r_{max} . The values of $\Sigma_{n+1}^\xi/\Sigma_n^\xi$ in Fig. 8 increase in a similar fashion as n increases, again roughly as $n/8$. The data in Fig. 9 shows that the maximum values in the summands for the Σ_n^ξ are relatively slowly varying for n small, but then increase at a faster than exponential rate.

n	$C_{n,p}, p = 1, 2, 3, \dots$
5	$4/5, 0, 32/3, 0, 128/15$
6	$0, 184/45, 0, 128/9, 0, 256/45$
7	$4/7, 0, 448/45, 0, 128/9, 0, 1024/315$
8	$0, 352/105, 0, 704/45, 0, 512/45, 0, 512/315$
9	$4/9, 0, 26176/2835, 0, 2432/135, 0, 1024/135, 0, 2048/2835$
10	$0, 4504/1575, 0, 45952/2835, 0, 11008/675, 0, 4096/945, 0, 4096/14175$
11	$4/11, 0, 1504/175, 0, 58496/2835, 0, 8192/675, 0, 2048/945, 0, 16384/155925$
12	$\{0, \frac{26032}{10395}, 0, \frac{696224}{42525}, 0, \frac{34816}{1701}, 0, \frac{108544}{14175}, 0, \frac{8192}{8505}, 0, \frac{16384}{467775}\}$
13	$\{\frac{4}{13}, 0, \frac{418016}{51975}, 0, \frac{956672}{42525}, 0, \frac{704512}{42525}, 0, \frac{59392}{14175}, 0, \frac{16384}{42525}, 0, \frac{65536}{6081075}\}$
14	$\{0, \frac{704552}{315315}, 0, \frac{363776}{22275}, 0, \frac{1019392}{42525}, 0, \frac{3362816}{297675}, 0, \frac{4096}{2025}, 0, \frac{65536}{467775}, 0, \frac{131072}{42567525}\}$
15	$\{\frac{4}{15}, 0, \frac{536786048}{70945875}, 0, \frac{33472256}{1403325}, 0, \frac{13236224}{637875}, 0, \frac{5933056}{893025}, 0, \frac{557056}{637875}, 0, \frac{65536}{1403325}, 0, \frac{524288}{638512875}\}$
16	$\{0, \frac{91072}{45045}, 0, \frac{1147994752}{70945875}, 0, \frac{37803008}{1403325}, 0, \frac{9614336}{637875}, 0, \frac{3063808}{893025}, 0, \frac{2392064}{7016625}, 0, \frac{262144}{18243225}, 0, \frac{131072}{638512875}\}$
17	$\{\frac{4}{17}, 0, \frac{33825664}{4729725}, 0, \frac{5289724672}{212837625}, 0, \frac{34588672}{1403325}, 0, \frac{42010624}{4465125}, 0, \frac{1409024}{893025}, 0, \frac{851968}{7016625}, 0, \frac{524288}{127702575}, 0, \frac{524288}{10854718875}, 0, 0, 0\}$
18	$\{0, \frac{12746152}{6891885}, 0, \frac{10198727936}{638512875}, 0, \frac{169341297152}{5746615875}, 0, \frac{397316096}{21049875}, 0, \frac{68857856}{13395375}, 0, \frac{288948224}{442047375}, 0, \frac{10878976}{273648375}, 0, \frac{2097152}{1915538625}, 0, \frac{1048576}{97692469875}, 0, 0\}$
19	$\{\frac{4}{19}, 0, \frac{148857952}{21928725}, 0, \frac{1485985024}{58046625}, 0, \frac{162381873152}{5746615875}, 0, \frac{1825937408}{147349125}, 0, \frac{33406976}{13395375}, 0, \frac{9895936}{40186125}, 0, \frac{2097152}{174139875}, 0, \frac{524288}{1915538625}, 0, \frac{4194304}{1856156927625}, 0\}$
20	$\{0, \frac{124151504}{72747675}, 0, \frac{3513939808}{223348125}, 0, \frac{2244810752}{70945875}, 0, \frac{650484697088}{28733079375}, 0, \frac{1046880256}{147349125}, 0, \frac{800899072}{736745625}, 0, \frac{488636416}{5746615875}, 0, \frac{32505856}{9577693125}, 0, \frac{2097152}{32564156625}, 0, \frac{4194304}{9280784638125}\}$

Table 1: The polynomial coefficients $C_{n,p}$ in the expansion (82), for n in the range 5 – 20.

n	a_n
1	$8\Sigma_1^\xi$
2	$16\Sigma_2^\xi$
3	$\frac{8}{3}\Sigma_1^\xi + \frac{64}{3}\Sigma_3^\xi$
4	$\frac{32}{3}\Sigma_2^\xi + \frac{64}{3}\Sigma_4^\xi$
5	$\frac{8}{5}\Sigma_1^\xi + \frac{64}{3}\Sigma_3^\xi + \frac{256}{15}\Sigma_5^\xi$
6	$\frac{368}{45}\Sigma_2^\xi + \frac{256}{9}\Sigma_4^\xi + \frac{512}{45}\Sigma_6^\xi$
7	$\frac{8}{7}\Sigma_1^\xi + \frac{896}{45}\Sigma_3^\xi + \frac{256}{9}\Sigma_5^\xi + \frac{2048}{315}\Sigma_7^\xi$
8	$\frac{704}{105}\Sigma_2^\xi + \frac{1408}{45}\Sigma_4^\xi + \frac{1024}{45}\Sigma_6^\xi + \frac{1024}{315}\Sigma_8^\xi$
9	$\frac{8}{9}\Sigma_1^\xi + \frac{52352}{2835}\Sigma_3^\xi + \frac{4864}{135}\Sigma_5^\xi + \frac{2048}{135}\Sigma_7^\xi + \frac{4096}{2835}\Sigma_9^\xi$
10	$\frac{9008}{1575}\Sigma_2^\xi + \frac{91904}{2835}\Sigma_4^\xi + \frac{22016}{675}\Sigma_6^\xi + \frac{8192}{945}\Sigma_8^\xi + \frac{8192}{14175}\Sigma_{10}^\xi$
11	$\frac{8}{11}\Sigma_1^\xi + \frac{3008}{175}\Sigma_3^\xi + \frac{116992}{2835}\Sigma_5^\xi + \frac{16384}{675}\Sigma_7^\xi + \frac{4096}{945}\Sigma_9^\xi + \frac{32768}{155925}\Sigma_{11}^\xi$
12	$\frac{52064}{10395}\Sigma_2^\xi + \frac{1392448}{42525}\Sigma_4^\xi + \frac{69632}{1701}\Sigma_6^\xi + \frac{217088}{14175}\Sigma_8^\xi + \frac{16384}{8505}\Sigma_{10}^\xi + \frac{32768}{467775}\Sigma_{12}^\xi$
13	$\frac{8}{13}\Sigma_1^\xi + \frac{836032}{51975}\Sigma_3^\xi + \frac{1913344}{42525}\Sigma_5^\xi + \frac{1409024}{42525}\Sigma_7^\xi + \frac{118784}{14175}\Sigma_9^\xi + \frac{32768}{42525}\Sigma_{11}^\xi + \frac{131072}{6081075}\Sigma_{13}^\xi$
14	$\frac{1409104}{315315}\Sigma_2^\xi + \frac{727552}{22275}\Sigma_4^\xi + \frac{2038784}{42525}\Sigma_6^\xi + \frac{6725632}{297675}\Sigma_8^\xi + \frac{8192}{2025}\Sigma_{10}^\xi + \frac{131072}{467775}\Sigma_{12}^\xi + \frac{262144}{42567525}\Sigma_{14}^\xi$
15	$\frac{8}{15}\Sigma_1^\xi + \frac{1073572096}{70945875}\Sigma_3^\xi + \frac{66944512}{1403325}\Sigma_5^\xi + \frac{26472448}{637875}\Sigma_7^\xi + \frac{11866112}{893025}\Sigma_9^\xi + \frac{1114112}{637875}\Sigma_{11}^\xi + \frac{131072}{6081075}\Sigma_{13}^\xi$
16	$+\frac{1048576}{638512875}\Sigma_{15}^\xi$ $\frac{182144}{45045}\Sigma_2^\xi + \frac{2295989504}{70945875}\Sigma_4^\xi + \frac{75606016}{1403325}\Sigma_6^\xi + \frac{19228672}{637875}\Sigma_8^\xi + \frac{6127616}{893025}\Sigma_{10}^\xi + \frac{4784128}{7016625}\Sigma_{12}^\xi + \frac{524288}{18243225}\Sigma_{14}^\xi$ $+\frac{262144}{638512875}\Sigma_{16}^\xi$
17	$\frac{8}{17}\Sigma_1^\xi + \frac{67651328}{4729725}\Sigma_3^\xi + \frac{10579449344}{212837625}\Sigma_5^\xi + \frac{69177344}{1403325}\Sigma_7^\xi + \frac{84021248}{4465125}\Sigma_9^\xi + \frac{2818048}{893025}\Sigma_{11}^\xi + \frac{1703936}{7016625}\Sigma_{13}^\xi$ $+\frac{1048576}{127702575}\Sigma_{15}^\xi + \frac{1048576}{10854718875}\Sigma_{17}^\xi$
18	$\frac{25492304}{6891885}\Sigma_2^\xi + \frac{20397455872}{638512875}\Sigma_4^\xi + \frac{338682594304}{5746615875}\Sigma_6^\xi + \frac{794632192}{21049875}\Sigma_8^\xi + \frac{137715712}{13395375}\Sigma_{10}^\xi + \frac{577896448}{442047375}\Sigma_{12}^\xi$ $+\frac{21757952}{273648375}\Sigma_{14}^\xi + \frac{4194304}{1915538625}\Sigma_{16}^\xi + \frac{2097152}{97692469875}\Sigma_{18}^\xi$
19	$\frac{4}{19}\Sigma_1^\xi + \frac{148857952}{21928725}\Sigma_3^\xi + \frac{1485985024}{58046625}\Sigma_5^\xi + \frac{162381873152}{5746615875}\Sigma_7^\xi + \frac{1825937408}{147349125}\Sigma_9^\xi + \frac{33406976}{13395375}\Sigma_{11}^\xi$ $+\frac{9895936}{40186125}\Sigma_{13}^\xi + \frac{2097152}{174139875}\Sigma_{15}^\xi + \frac{524288}{1915538625}\Sigma_{17}^\xi + \frac{4194304}{1856156927625}\Sigma_{19}^\xi$
20	$\frac{124151504}{72747675}\Sigma_2^\xi + \frac{3513939808}{223348125}\Sigma_4^\xi + \frac{2244810752}{70945875}\Sigma_6^\xi + \frac{650484697088}{28733079375}\Sigma_8^\xi + \frac{1046880256}{147349125}\Sigma_{10}^\xi + \frac{800899072}{736745625}\Sigma_{12}^\xi$ $+\frac{488636416}{5746615875}\Sigma_{14}^\xi + \frac{32505856}{9577693125}\Sigma_{16}^\xi + \frac{2097152}{32564156625}\Sigma_{18}^\xi + \frac{4194304}{9280784638125}\Sigma_{20}^\xi$

Table 2: The coefficients a_n of Li expressed in terms of ξ sums for n in the range 1 – 20.

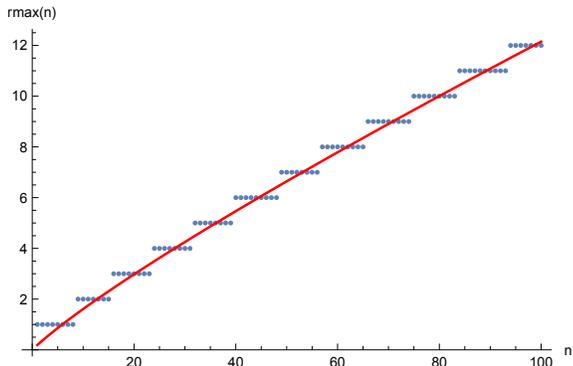


Figure 7: The values of r , r_{max} , which maximise the summand in the evaluation of Σ_n^ξ (blue) as a function of n , showing an underlying linear relationship of r_{max} with n when it is moderately large. The red line gives the asymptotic result (112).

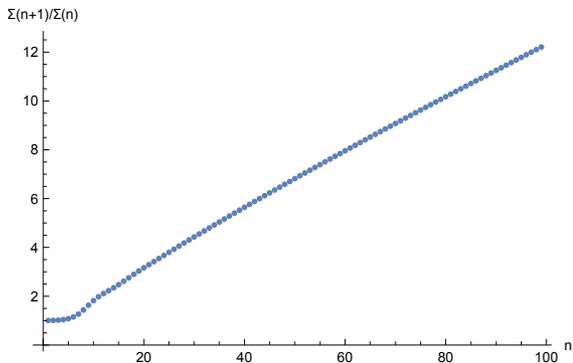


Figure 8: The values $\Sigma_{n+1}^\xi / \Sigma_n^\xi$ (blue) as a function of n , showing an approximately linear relationship for n large.

4 Asymptotics of the Griffin, Ono, Rolen, Zagier Formula

We now consider the Griffin, Ono, Rolen and Zagier (GORZ) formula [8] for the even-order derivatives of the ξ function at $s = 1/2$. The expansion is written in terms of a parameter L , solution of the equation [7]

$$Le^L = \frac{n}{\pi} - \frac{3L}{4\pi}. \quad (89)$$

We wish to obtain analogous results to those of Romik [17] for the leading order terms of the GORZ formula for n very large, and so we first establish the leading order terms of the expansion of L . The leading term arises from the neglect of the second term on the right-hand side, and is just the principal branch of

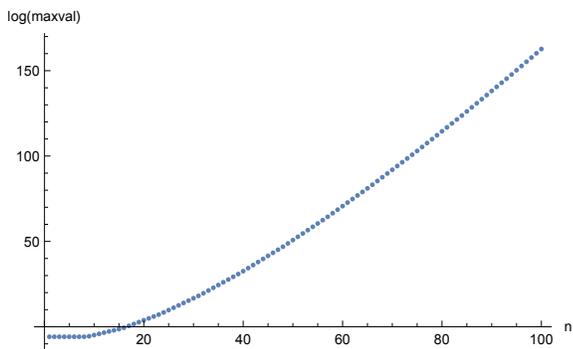


Figure 9: The maximum values of the summand in the evaluation of Σ_n^ξ (blue) as a function of n , showing a stronger than exponential dependence.

Lambert's W function, which satisfies [18]:

$$W(z)e^{W(z)} = z. \quad (90)$$

We write

$$L(n) = L_0(n) + \frac{L_1(n)}{n} + \frac{L_2(n)}{n^2} + \dots, \quad (91)$$

and substitute into (89), solving in a self-consistent fashion. We find

$$L_0(n) = W\left(\frac{n}{\pi}\right), \quad (92)$$

$$L_1(n) = \left(\frac{-3}{4}\right) \frac{L_0(n)^2}{1 + L_0(n)}, \quad (93)$$

and

$$L_2(n) = -\frac{9}{32} \left(\frac{-2L_0(n)^3 + L_0(n)^5}{(1 + L_0(n))^3} \right). \quad (94)$$

In what follows, we will use only the expressions for $L_0(n)$ and $L_1(n)$ and will use chiefly the inverse powers of n to choose which terms may be discarded.

The GORZ formula [8, 7] is written in terms of a function $F(n)$, where

$$F(n) \approx \sqrt{2\pi} \frac{L^{n+1}}{\sqrt{(1+L)n - 3L^2/4}} e^{L/4 - n/L + 3/4} \left(1 + \frac{b_1(L)}{n} + \frac{b_2(L)}{n^2} + \dots \right). \quad (95)$$

As we are interested in the leading terms in (95) which do not tend to zero as $n \rightarrow \infty$, we will not use the correction terms involving $b_1(L)$, $b_2(L)$. Using (91-93) in (95) we obtain:

$$F(n) \approx F_{lo}(n)F_{zo}(n), \quad (96)$$

n	$F(95)$	$F(95)/F_{lo}(n)$	$F(95)/(F_{lo}(n) * F_{zo}(n))$
10	0.000158915	0.766616	1.00369
30	0.203491	0.727793	0.998342
50	67530.7	0.692067	0.997971
100	9.70356×10^{22}	0.634681	0.99819
1000	$3.571049805 \times 10^{532}$	0.4343107094	0.999500421
100000	$2.825033093 \times 10^{86422}$	0.1695059281	0.999987430
1000000	$1.101679602 \times 10^{972298}$	0.1019359097	0.999998337

Table 3: The values of the GORZ function (95) are compared with their leading order approximations and their leading plus zeroth order approximations (using ratios).

where $F_{lo}(n)$ contains simple leading order terms which contribute most strongly to the result, and $F_{zo}(n)$ contains the remaining terms which do not tend to zero as $n \rightarrow \infty$. Here

$$F_{lo}(n) = \exp \left[n \left(\log \left(W \left(\frac{n}{\pi} \right) \right) - \frac{1}{W(n/\pi)} \right) \right] \quad (97)$$

and

$$F_{zo}(n) = \exp \left[\frac{1}{2} \log(n) + \frac{1}{2} \log \left(\frac{2}{\pi} \right) - \frac{1}{2} \log \left(1 + W \left(\frac{n}{\pi} \right) \right) - \frac{3}{4} \left(1 - \frac{1}{4n} \right) W \left(\frac{n}{\pi} \right) - \frac{9}{16n} + \frac{3}{8n(1 + W(n/\pi))^2} + \frac{3}{16n(1 + W(n/\pi))} \right]. \quad (98)$$

In Table 4 we compare the values of the function $F(n)$ of (95) with the leading order term of (97) and the combined leading and zero order terms of (97) and (98). The leading order term by itself is an overestimate, and drifts slowly away from the correct value, while the combined terms are quite accurate for n larger than 50 or 100, while also approaching the correct values from above.

Using the logarithm of (90), we can rewrite the leading order term as

$$F_{lo}(n) = \exp \left[n \left(\log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right) - \frac{1}{W(n/\pi)} \right) \right]. \quad (99)$$

We now evaluate some derivatives of this function, using the following results for its component parts:

$$\frac{d}{dn} W \left(\frac{n}{\pi} \right) = \frac{W(n/\pi)}{n(1 + W(n/\pi))}, \quad \frac{d^2}{dn^2} W \left(\frac{n}{\pi} \right) = \frac{-W(n/\pi)^2 (W(n/\pi) + 2)}{n^2(1 + W(n/\pi))^3} \quad (100)$$

and

$$\frac{d}{dn} \left(\frac{1}{W(n/\pi)} \right) = \frac{1}{nW(n/\pi)(1 + W(n/\pi))}. \quad (101)$$

Then

$$\frac{d}{dn} \left[n \left(\log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right) - \frac{1}{W(n/\pi)} \right) \right] = \log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right), \quad (102)$$

and

$$\frac{d^2}{dn^2} \left[n \left(\log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right) - \frac{1}{W(n/\pi)} \right) \right] = \frac{1}{n(1 + W(n/\pi))}. \quad (103)$$

Combining these derivative values, we find

$$\frac{d}{dn} \log F_{lo}(n) = \log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right), \quad (104)$$

and

$$\frac{d^2}{dn^2} \log F_{lo}(n) = \frac{1}{n(1 + W(n/\pi))}. \quad (105)$$

Hence the Taylor series for the logarithm of the leading order term $F_{lo}(n)$ is

$$\begin{aligned} \log F_{lo}(n+x) &= \left[n \left(\log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right) - \frac{1}{W(n/\pi)} \right) \right] + x \left(\log \left(\frac{n}{\pi} \right) - W \left(\frac{n}{\pi} \right) \right) \\ &\quad + \frac{x^2}{2n(1 + W(n/\pi))} + \dots \end{aligned} \quad (106)$$

The result (106) is important in that it shows that $\log F_{lo}(n-2)$ and $\log F_{lo}(n)$ have the same leading term, and their difference is of order $\log \log(n/\pi)$.

These asymptotic results for the function $F(n)$ can now be used in the expression [8] for the $2n$ -th derivative of the xi function:

$$\xi^{(2n)} \left(\frac{1}{2} \right) = \frac{1}{2^{2n+2}} [16(2n)(2n-1)F(2n-2) - F(2n)]. \quad (107)$$

We wish to find the leading two orders in the expression for these derivatives, which, as we have just commented, in fact are contributed entirely by the first term in square brackets in (107):

$$\xi^{(2n)} \left(\frac{1}{2} \right) \approx \frac{1}{2^{2n-2}} (2n)(2n-1)F(2n-2). \quad (108)$$

We can re-express (108) to deliver a leading-order approximation for the ξ_r of Pustil'nikov:

$$\xi_r = \frac{\xi^{(2r)} \left(\frac{1}{2} \right)}{(2r)!} \approx \frac{1}{2^{2r-2}} \frac{(2r)(2r-1)F(2r-2)}{(2r)!} = \frac{F(2r-2)}{2^{2r-2}(2r-2)!}. \quad (109)$$

Another leading order approximation for the ξ_r is available in the literature, due to D. Romik [17]:

$$\xi_n \approx 2 \frac{\pi^{1/4}}{2^{2n-5/2}(2n)!} \left(\frac{2n}{\log 2n} \right)^{7/4} \exp [2n (\log(2n/\pi) - W(2n/\pi) - 1/W(2n/\pi))]. \quad (110)$$

n	$\log \xi_r$ (107)	$\log \xi_r$ (109)	$\log \xi_r$ (110)
10^1	-55.8378	-55.83721474	-56.12211477
10^2	-835.9650723	-835.9637026	-836.0992830
10^3	-11823.58874	-11823.58844	-11823.58015
10^4	-156402.6563	-156402.6562	-156402.5434
10^5	-1.965649078 10^6	-1.965649078 10^6	-1.965648889 10^6
10^6	-2.379580712 10^7	-2.379580712 10^7	-2.379580688 10^7

Table 4: The values of ξ_r calculated from two terms of the GORZ equation are compared with those from the first terms only, and with those from the asymptotic formula of Romik.

Here the first factor of 2 is a correction due to J. G elinas [7].

The best way to compare such leading-order approximations is through their logarithms, as in Table 4. The Table shows that the neglect of the second F term in the GORZ formula becomes increasingly accurate as r increases, while the asymptotic formula of Romik delivers good accuracy for r beyond 10^4 .

We can use either of the asymptotic expressions (109) or (110) to determine the value of r , r_m , for which the summand in the expression (81) for Σ_p is maximal. We then require the derivative of

$$\log \xi_r + p \log(r) - 2r \log(2) \quad (111)$$

to be zero at $r = r_m$. The leading term equation resulting from this procedure is

$$\frac{p}{2r_m} - \log(4\pi) = W\left(\frac{2r_m}{\pi}\right), \quad (112)$$

where W denotes the W function of Lambert, which is positive for $r > 0$. Hence, p/r_m must be larger than $2 \log(4\pi) \approx 5.06204$. The equation (112) may be solved numerically to give r_m as a function of p . As Fig. 7 shows, this works well even for p only moderately large.

In order to provide asymptotic estimates for the sums Σ_p^ξ in equation 81, we need to be able to invert the expression 112 in order to obtain r_m as a function of p . This highly nontrivial task can be carried out using generalised Lambert functions [19], [20], in a way discussed in the Appendix, kindly provided by T. C. Scott and A. Maignan. The results presented in Table 6 show all the formulae presented give highly accurate values for r_m , which grow more accurate as p increases. They all are utilisable without difficulty, even for p very large.

Let us take the logarithm of Romik’s asymptotic expression (110) and combine it with the logarithm of the factor $n^p/2^{2n}$ in (81), denoting the result by $\mathcal{S}(n, p)$. Then we can break $\mathcal{S}(n, p)$ up into its terms of differing order:

$$\mathcal{S}(n, p) = \mathcal{S}_1(n, p) + \mathcal{S}_2(n, p) + \mathcal{S}_3(n, p) + \mathcal{S}_4(n, p) - \frac{1}{24n} + O\left(\frac{1}{n^2}\right). \quad (113)$$

The last element and order estimate on the right-hand side in (113) arise from

the asymptotic expansion of the logarithm of the denominator term $(2n)!$, and will be neglected in what follows.

The leading term is

$$\mathcal{S}_1(n, p) = p \log(n) - 2n \left[\log(4\pi) - 1 + W\left(\frac{2n}{\pi}\right) \right], \quad (114)$$

and mixes terms of order $p \log(n)$, $n \log(n)$ and n . The term $n \log(n)$ comes from the Lambert W term. The equation (112) arises from the leading terms of the derivative of $\mathcal{S}_1(n, p)$. The second term is of order $n/\log(n)$, and has a single element:

$$\mathcal{S}_2(n, p) = -2n \left[\frac{1}{W(2n/\pi)} \right]. \quad (115)$$

The third term combines elements of order $\log(n)$ and $\log(\log(2n))$:

$$\mathcal{S}_3(n, p) = \frac{5}{4} \log(n) - \frac{7}{4} \log(\log(2n)). \quad (116)$$

The fourth term is order unity:

$$\mathcal{S}_4(n, p) = \frac{-1}{4} \log(\pi) + \frac{7}{4} \log(2). \quad (117)$$

4.1 Evaluation of the sums Σ_p^ξ for p large

The elements have now been assembled which are necessary for the evaluation of the sums Σ_p^ξ defined in equation (81). We wish to consider formulae appropriate for these sums when p is very large, a case relevant to their use in the investigation of the Li-Keiper criterion for the Riemann hypothesis. The key element is the knowledge of the range of the summand n which contributes most heavily to the sum- see equation (128) for the exact result relating to this. As shown in Table 6 of the Appendix, the formulae exhibited for determining this range work well even for p extremely large ($O(10^{40})$).

Here we will consider two related methods for evaluating the sums. The first of these is based on the expansion of the logarithm of the summand $\mathcal{S}(n, p)$ around $n = n_m$:

$$\mathcal{S}(n, p) = \mathcal{S}(n_m, p) + \frac{1}{2} \mathcal{S}''(n_m, p) (n - n_m)^2 + \dots \quad (118)$$

where

$$\mathcal{S}''(n_m, p) = -\frac{p}{n_m^2} - \frac{2W(2n_m/\pi)}{n_m(1+W(2n_m/\pi))} + \frac{7+7\log(2n_m)-5\log(2n_m)^2}{4n_m^2 \log(2n_m)^2}, \quad (119)$$

manifestly negative. So, if we approximate the sum by an integral, this is an integral of (to leading order) Gaussian form. Thus the result of this simple treatment is analytic:

$$\Sigma_p^\xi \approx \exp(\mathcal{S}(n_m, p)) \sqrt{\frac{2\pi}{\mathcal{S}''(n_m, p)}}. \quad (120)$$

To apply this numerically, the results given here have used the rapidly convergent, iterative method of the Appendix to find n_m from p . This is used to evaluate $\mathcal{S}(n_m, p)$ and the Gaussian integral. Another useful quantity is the standard deviation corresponding to the Gaussian:

$$\sigma(p) = \sqrt{\frac{-1}{\mathcal{S}''(n_m, p)}}. \quad (121)$$

Note that it is convenient in avoiding exponential overflows numerically to keep the $\mathcal{S}(n_m, p)$ as is, and if desired to add the logarithm of the integral to it, or to hold the exponent value at n_m and the integral as separate values. As we will see, the exponent value greatly exceeds in magnitude the integral value.

The values of $\mathcal{S}(n_m, p)$ are dominated by those of $\mathcal{S}_1(n, p)$ for p very large: $\log p \gg 1$. We use the approximations

$$\frac{p}{n_m} = 2[\log p - 2 \log(\log(p)) + \log(4)] \quad (122)$$

and

$$W\left(\frac{2n_m}{\pi}\right) = \log p - 2 \log(\log(p)) - \log(\pi). \quad (123)$$

These are respectively accurate to 3.1% and 3.5% at $p = 10^{10}$, 0.86% and 0.91% at $p = 10^{20}$, and (both) 0.04% at $p = 10^{100}$. Using them we find

$$\mathcal{S}_1(n_m, p) \approx p \left[\log p - \log(\log(p)) - 2 + \frac{2 \log(\log(p))}{\log p} - \frac{\log(4\pi^2)}{\log p} \right]. \quad (124)$$

The value of $\mathcal{S}_2(n_m, p)$ is smaller than this by a factor of order $1/\log(p)^3$. The value for $\mathcal{S}_1(n, p)$ given by the approximation (124) is accurate to 2.5% at $p = 10^{10}$, 0.9% at $p = 10^{20}$ and 0.1% at $p = 10^{100}$.

From (121), we find the leading terms in the expansion of $\sigma(p)$ are:

$$\sigma(p) \approx \frac{\sqrt{p}}{2 \log p} \left(1 + \frac{\log(4) - 2 \log(\log(p))}{\log p} \right)^{-1}. \quad (125)$$

Hence the ratio $\sigma(p)/\mathcal{S}_1(n_m, p)$ goes to zero as $1/(2\sqrt{p}\log(p)^2)$ as p goes to infinity.

The expressions (122-125) are useful for analytic purposes, but previous expressions not relying on slowly converging logarithmic expansions are more useful for accurate numerics. However, an approach using direct summation based on the knowledge of an almost Gaussian summand can yield accurate numeric estimates. This approach uses direct summation of the summand divided by its value at n_m , so keeping function values bounded by unity. The summation is carried out over a region symmetric about n_m , of width five to seven times $\sigma(p)$, to ensure good accuracy. The results shown in Table 4.1 show that the Gaussian approximation and the direct sum method agree very well, and increasingly well as p increases. Note that the direct sum method slowly

p	$\mathcal{S}(n_m, p)$	$\sqrt{(2\pi)/(\mathcal{S}''(n_m, p))}$	Direct Sum
10^5	773216.454845247262645	42.6542750759677	42.6549100287186
10^6	$9.83159041621098805554 \cdot 10^6$	112.279823862816957037	112.280001637404
10^7	$1.195836652616223797330 \cdot 10^8$	302.564643162281697308	302.56469321694
10^8	$1.410711383470056930638 \cdot 10^9$	830.810395365553885241	830.810409565
10^9	$1.627353529697758035010 \cdot 10^{10}$	2316.34932127632390101	2316.34799775
10^{10}	$1.845432238547395356783 \cdot 10^{11}$	6539.40520716042875530	6539.4014688
10^{11}	$2.064693729563438373551 \cdot 10^{12}$	18654.74614331614399149	18654.74614
10^{12}	$2.2849417700654827485508 \cdot 10^{13}$	53683.7690078777092085	53683.7690
10^{13}	$2.5060227704112369541113 \cdot 10^{14}$	155644.686125848856880	155644.69

Table 5: The values of p , of $\mathcal{S}(n_m, p)$, and those given by the two methods (integral and direct sum, seven standard deviations) for the contribution to Σ_p^ξ from summing over n .

loses digits of accuracy as p increases, since it involves summing over the difference between $\mathcal{S}(n, p)$ and $\mathcal{S}(n_m, p)$, and the magnitude of both of these strongly increases with p , while their difference does not increase as rapidly. Note also that, in order to assess the relative significance of the prefactor term $\mathcal{S}(n_m, p)$ and the sum/integral terms, the logarithm of the latter needs to be taken. Thus, for $p = 10^{13}$, the sum/integral contribute 11.96, compared with 2.50610^{14} from the prefactor. The integral expression is easily and quickly evaluated, while the sum expression becomes increasingly difficult and slow as p increases. Hence, for most purposes, the integral expression will provide sufficient asymptotic accuracy if it is necessary to go beyond $\mathcal{S}(n_m, p)$.

5 Appendix: Comments on the solution of Equation (112)

Eq. (112) can be rewritten as:

$$p = 2r_m \left(\ln(4\pi) + W \left(\frac{2r_m}{\pi} \right) \right),$$

where W is the standard Lambert W function[21, 18]. We want to invert this to get r_m in terms of p . The solver of the Maple Symbolic Computation System[22, 23] tells us that:

$$r_m = \frac{p}{2(\ln(4\pi) + \text{RootOf}(\pi z \exp(z) (\ln(4\pi) + z) - p))}, \quad (126)$$

where Maple's *RootOf* facility is a means of telling us that this part of the denominator is z such that:

$$\pi z \exp(z) (\ln(4\pi) + z) - p = 0,$$

which is exactly equal to:

$$e^{-z} = \frac{\pi z (\ln(4\pi) + z)}{p}. \quad (127)$$

This is an implicit equation in z governed by an exponential polynomial. If the RHS of Eq. (127) had been a polynomial in z of first order, the solution would be a standard Lambert W function. However, since the RHS is instead a quadratic in z , the solution of Eq. (127) is a *generalized* Lambert W function [20, 24, 25, 26]. The roots of this quadratic in z are $\{0, -\ln(4\pi)\}$ and thus the asymptotic series for when the quadratic in z has near equal roots[24] is not applicable here. Denoting the generalized Lambert W function according to [20, eq.28] as $\Omega_2(0, -\ln(4\pi))$ which is understood as the solution for z in Eq. (??), the solution of r_m of Eq. (??) is exactly:

$$r_m = \frac{p}{2(\ln(4\pi) + \Omega_2(0, -\ln(4\pi)))}. \quad (128)$$

Dividing both sides of Eq. (127) by πz and treating the z inside the brackets as a constant, we find that (127) is equivalent to:

$$z = W\left(\frac{p}{\pi(\ln(4\pi) + z)}\right). \quad (129)$$

Eq. (129) can provide numerical solutions for z by repeated iterations starting with a guess value for z , in a process known as *tetration*[27]. It also gives a hint of the lead asymptotic term. As p gets larger, so does z and it dominates the $\ln(4\pi)$ in Eq. (??). Solving $z/p = \exp(-z)/(z\pi)$ yields

$$2 W\left(\pm \frac{\sqrt{p}}{2\sqrt{\pi}}\right)$$

Since $z > 0$, we retain the solution with positive argument. Thus,

$$z \approx 2 W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right) + u \quad (130)$$

where u denotes the remaining terms in the asymptotic expansion. By plugging Eq. (130) into Eq. (129) (after dividing both sides by πz) and neglecting the terms in u and u^2 , we obtain for u :

$$u \approx \ln\left[\frac{2W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right)}{2W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right) + \ln(4\pi)}\right]. \quad (131)$$

Thus after simplifications (and resulting cancellations), the lead asymptotic terms for z are:

$$\Omega_2(0, -\ln(4\pi)) = z \approx W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right) + \ln\left[\frac{\sqrt{p}}{2\sqrt{\pi}(\ln(2\sqrt{\pi}) + W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right))}\right] \quad (132)$$

The reader might think the coefficient of 2 in the lead term of Eq. (130) is missing in Eq. (132). This is *not* the case: as a consequence of the identity: $\ln(W(x)) = \ln(x) - W(x)$, Eq. (132) is exactly equal to Eqs. (130) and (131) together.

5.1 Asymptotic expansion of B. Salvy and J. Shackell

The approach used here is very similar to the steps in the algorithms developed by B. Salvy and J. Shackell[28, 29]. Eq. (132) has been vindicated numerically. To get the asymptotic expansion in terms of *elementary* functions, one could use the asymptotic expansion for W itself[18], namely

$$W(x) \approx \ln(x) - \ln(\ln(x)) + \dots$$

However this creates unwieldy arguments within logarithms. It is best to use Eq. (129) directly with B. Salvy's methods to approximate the Generalized Lambert W function. The first few terms of $\Omega_2(0, -\ln(4\pi)) = z$ are given by:

$$\begin{aligned} z &= \ln(p/\pi) - 2\ln(\ln(p)) + \frac{(4\ln(\ln(p)) + \ln(\pi/4))}{\ln(p)} & (133) \\ &+ \frac{(\ln(\pi)^2 - 8\ln(\ln(p))(\ln(2/\sqrt{\pi}) + 2) + 4\ln(2)^2 + 8\ln(\ln(p))^2 + \ln(256/\pi^4))}{2\ln(p)^2} \\ &+ O\left(\frac{1}{\ln(p)^3}\right) \end{aligned}$$

Higher-order terms in $1/\ln(p)^k$ where $k = 3, 4, 5 \dots$ can be readily generated with a computer algebra system like Maple[23]. However, for larger p , new techniques can improve the formal approximation of $\Omega_2(0, -\ln(4\pi))$.

5.2 Mean approximation

For $z > 0$, $z^2 < (\ln(4\pi) + z)z < (\ln(4\pi) + z)^2$ and the solution of Eq. (129) is included in the interval $]z_1, z_2[$ where z_1 is the positive solution of $e^z(\ln(4\pi) + z)^2 = \frac{p}{\pi}$ and z_2 is the positive solution of $e^z(\ln(4\pi) + z^2) = \frac{p}{\pi}$. We obtain

$$z_1 = 2W(\sqrt{p}) - \ln(4\pi), \quad z_2 = 2W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right).$$

A first approximation of $\Omega_2(0, -\ln(4\pi))$ can be

$$\frac{z_1 + z_2}{2} = W(\sqrt{p}) + W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right) - \frac{\ln(4\pi)}{2}$$

Now let set $z = \frac{z_1 + z_2}{2} + u$, after inserting this equation in Eq. (129) and neglected the u and u^2 value we obtain:

$$u = \ln\left(\frac{16W(\sqrt{p})W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right)}{4\left(W(\sqrt{p}) + W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right)\right)^2 - \ln(4\pi)^2}\right) \quad (134)$$

Finally,

$$z \approx \ln \left(\frac{p}{\pi \left(\left(W(\sqrt{p}) + W\left(\frac{\sqrt{p}}{2\sqrt{\pi}}\right) \right)^2 - \ln(2\sqrt{\pi})^2 \right)} \right) \quad (135)$$

5.3 Iterative approximation of $\Omega_2(0, -\ln(4\pi))$

A first approximation of $\Omega_2(0, -\ln(4\pi))$ can be obtained by approximating the polynomial $(\ln(4\pi) + z)z$ by its closest square polynomial $(z + \frac{\ln(4\pi)}{2})^2$. Indeed, Eq. (129) is equivalent to

$$e^z \left(\left(z + \frac{\ln(4\pi)}{2} \right)^2 - \left(\frac{\ln(4\pi)}{2} \right)^2 \right) = \frac{p}{\pi}$$

and, after neglecting the constant $(\frac{\ln(4\pi)}{2})^2$, we obtain as first approximation

$$2W \left(\frac{\sqrt{p}}{\pi^{1/4}\sqrt{2}} \right) - \frac{\ln(4\pi)}{2}$$

Now for all $z > 0$, there exists a positive value a such that $(z + \frac{1}{a} \ln(4\pi))^2 = z(z + \ln(4\pi))$. Eq. (129) is then equivalent to

$$\begin{cases} e^z (z + \frac{1}{a} \ln(4\pi))^2 = \frac{p}{\pi} \\ (z + \frac{1}{a} \ln(4\pi))^2 = z(z + \ln(4\pi)) \end{cases}$$

$$\text{which is equivalent to } \begin{cases} z = 2W \left(\frac{2^{1/a} \pi^{1/2a} \sqrt{p}}{2\sqrt{\pi}} \right) - \frac{1}{a} \ln(4\pi) \\ a = 1 + \frac{\sqrt{\ln(4\pi)z + z^2}}{z} \end{cases}$$

Starting from $a = 2$, we can iteratively compute the values of z and a . After two steps of iteration, we obtain:

$$z \approx 2W \left(\frac{2^{1/a} \pi^{1/2a} \sqrt{p}}{2\sqrt{\pi}} \right) - \frac{1}{a} \ln(4\pi) \text{ where } a = 1 + \sqrt{1 + \frac{\ln(4\pi)}{2W \left(\frac{\sqrt{p}}{\pi^{1/4}\sqrt{2}} \right) - \frac{\ln(4\pi)}{2}}} \quad (136)$$

5.4 Comparison

The Table 6 gives for various values of p the quality of the approximation of $\Omega_2(0, -\ln(4\pi))$ by computing $|\Omega_2(0, -\ln(4\pi)) - z|$ where z is the approximation following respectively the formula (133) (including the $1/\ln(p)^3$ term), (132), (135) and (136).

p	Solution (133)	Solution (132)	Solution (135)	Solution (136)
10 ²	0.0295201968	0.3552749979	0.0772180220	0.0068826104
10 ³	0.0057831067	0.1859192761	0.0181580288	0.0010208989
10 ⁴	0.0001735300	0.1078609703	0.0057913129	0.0002264369
10 ⁵	0.0008878914	0.0682012259	0.0022678410	0.0000663985
10 ⁶	0.0009195722	0.0461466918	0.0010300563	0.0000238040
10 ⁷	0.0007505178	0.0329200004	0.0005228858	0.0000099079
10 ⁸	0.0005758608	0.0244840646	0.0002892049	0.0000046227
10 ⁹	0.0004347967	0.0188273390	0.0001711726	0.0000023588
10 ¹⁰	0.0003282835	0.0148751824	0.0001070032	0.0000012931
10 ¹¹	0.0002494168	0.0120183075	0.0000699590	0.0000007517
10 ¹²	0.0001911372	0.0098933524	0.0000474827	0.0000004588
10 ¹⁵	0.0000908777	0.0060163620	0.0000176361	0.0000001303
10 ²⁰	0.0000306477	0.0031858748	0.0000049720	0.0000000262
10 ²⁵	0.0000116710	0.0019559139	0.0000018809	0.0000000077
10 ³⁰	0.0000046713	0.0013176093	0.0000008558	0.0000000029
10 ³⁵	0.0000018059	0.0009458036	0.0000004418	0.0000000012
10 ⁴⁰	0.0000005554	0.0007109412	0.0000002500	0.0000000006

Table 6: Comparison of several asymptotic values for z against the exact values.

5.5 Eq. (89) and the r-Lambert function

Equation (89) is rewritten here as:

$$Le^L + \frac{3}{4\pi}L = \frac{n}{\pi}, \quad (137)$$

which can be solved thanks to a specific generalization of the Lambert-W function named the r-Lambert function. In [30], Mezo et al. define the r-Lambert function as the inverse of the function $xe^x + rx$. It is denoted by W_r .

In ([30], Theorem 4), a classification of W_r is given. In the case of the GORZ formula, $r = \frac{3}{4\pi}$ satisfies $r > \frac{1}{e^2}$ and Theorem [4, [30]] stipulates that $W_r(y) : \mathbb{R} \rightarrow \mathbb{R}$ is a strictly increasing, everywhere differentiable function such that $\text{sgn}(W_r(y)) = \text{sgn}(y)$. In other words, $L = W_{\frac{3}{4\pi}}(\frac{n}{\pi})$ is the unique real solution of Eq. (137) (See Figure 10 for the graphical representation of $W_{\frac{3}{4\pi}}(\frac{n}{\pi})$ for n from 0 to 1000).

The numerical calculation of the real r-Lambert function is given in [31].

The first and second derivatives of the r-Lambert function are

$$W_r'(y) = \frac{1}{e^{W_r(y)}(1 + W_r(y)) + r}$$

and

$$\frac{d^2W_r(y)}{d^2y} = W_r''(y) = -\frac{e^{W_r(y)}(2 + W_r(y))}{(e^{W_r(y)}(1 + W_r(y)) + r)^3}$$

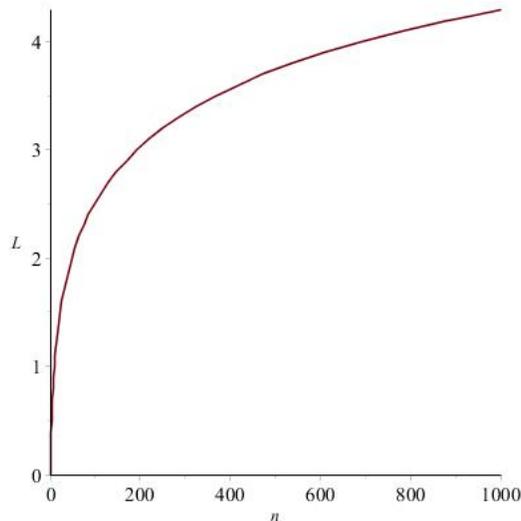


Figure 10: The r-Lambert function $W_{\frac{3}{4\pi}}\left(\frac{n}{\pi}\right)$

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