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An asymptotic expansion for the Stieltjes constants

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Abstract

The Stieltjes constants γ_n appear in the coefficients in the Laurent expansion of the Riemann zeta function $\zeta(s)$ about the simple pole $s = 1$. We present an asymptotic expansion for γ_n as $n \to \infty$ based on the approach described by Knessl and Coffey [Math. Comput. **80** (2011) 379–386]. A truncated form of this expansion with explicit coefficients is also given. Numerical results are presented that illustrate the accuracy achievable with our expansion.

Mathematics Subject Classification: 30E20, 34E05, 41A60, 11M06

Keywords: Stieltjes constants, Laurent expansion, asymptotic expansion

1. Introduction The Stieltjes constants γ_n appear in the coefficients in the Laurent expansion of the Riemann zeta function $\zeta(s)$ about the point $s = 1$ given by

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

where $\gamma_0 = 0.577216\ldots$ is the well-known Euler-Mascheroni constant. Some historical notes and numerical values of γ_n for $n \leq 20$ are given in [3]. Recent high-precision evaluations of γ_n based on numerical integration have been described in [5, 8]. In [5], Keiper lists various γ_n up to $n = 150$, whereas in [8], Kreminski has computed values to several thousand digits for $n \leq 10^4$ and for further selected values (accurate to 10^3 digits) up to $n = 5 \times 10^4$. All values up to $n = 10^5$ have been computed by Johansson in [4] to about 10^4 digits.

Upper bounds for $|\gamma_n|$ in the form

$$|\gamma_n| \leq \{3 + (-)^n\}\,\frac{\lambda_n\,\Gamma(n)}{\pi^n},$$

have been obtained by Berndt [1] with $\lambda_n = 1$, and by Zhang and Williams [13] with $\lambda_n = (2/n)^n \pi^{-\frac{1}{2}}\Gamma(n+\frac{1}{2}) \sim \surd 2(2/e)^n$ for $n \to \infty$. On the other hand, Matsuoka [9] has shown that

$$|\gamma_n| \leq 10^{-4} e^{n \log \log n} \qquad (n \geq 10).$$

However, all these bounds grossly overestimate the growth of $|\gamma_n|$ for large values of n. An asymptotic approximation for γ_n has recently been given by Knessl and Coffey [6] in the form

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \cos(na+b) \qquad (n \to +\infty), \tag{1.1}$$

where A, B, a and b are functions that depend weakly on n; see Section 2 for the definition of these quantities. Knessl and Coffey have verified numerically that for $n \leq 3.5 \times 10^4$ the above formula accounts for the asymptotic growth and oscillatory pattern of γ_n, with the exception of $n = 137$ where the cosine factor in (1.1) becomes very small.

The aim in this note is to extend the analysis in [6] to generate an asymptotic expansion for γ_n as $n \to +\infty$. The coefficients in this expansion are determined numerically by application of Wojdylo's formulation [14] for the coefficients in the expansion of a Laplace-type integral. An explicit evaluation of the coefficients is obtained in the case of the expansion truncated after three terms. This approximation is extended to the more general Stieltjes constants $\gamma_n(\alpha)$ appearing in the Laurent expansion of the Hurwitz zeta function $\zeta(s,\alpha)$. Numerical results are presented in Section 3 to demonstrate the accuracy of our expansion compared to that in (1.1).

2. Asymptotic expansion for γ_n We start with the integral representation for $n \geq 1$ given in [13]

$$\gamma_n = \int_1^\infty B_1(x-[x]) \frac{\log^{n-1} x}{x^2} (n - \log x)\, dx,$$

where $B_1(x-[x]) = -\sum_{j=1}^\infty \frac{\sin 2\pi jx}{\pi j}$ is the first periodic Bernoulli polynomial. With the change of variable $t = \log x$, we obtain [6, Eq. (2.3)]

$$\gamma_n = -\Im \biggl\{ \sum_{k=1}^\infty \frac{1}{\pi k} \int_0^\infty \exp[2\pi ike^t + n \log t - t] \left(\frac{n}{t} - 1\right) dt \biggr\}.$$

Following the approach used in [6], we define

$$\psi_k(t) \equiv \psi_k(t;n) = -\frac{2\pi ik}{n} e^t - \log t, \qquad f(t) \equiv f(t;n) = \frac{e^{-t}}{t}\left(1 - \frac{t}{n}\right) \tag{2.1}$$

and write

$$\gamma_n = -\Im \sum_{k=1}^\infty J_k, \qquad J_k := \frac{n}{\pi k} \int_0^\infty e^{-n\psi_k(t)} f(t)\, dt. \tag{2.2}$$

We employ the method of steepest descents to estimate the integrals J_k for large values of n. Saddle points of the exponential factor occur at the zeros of $\psi_k'(t)=0$; that is, they satisfy

$$te^t = \frac{ni}{2\pi k}. \tag{2.3}$$

There is an infinite string of saddle points, which is approximately parallel to the imaginary t-axis, given by [6]

$$t_m = \log\frac{n}{2\pi k} - \log\log n + (2m+\tfrac{1}{2})\pi i + O\Big(\frac{\log\log n}{\log n}\Big)$$

for $m = 0, \pm 1, \pm 2, \ldots$ and large n. For fixed k and m, the value of $\Re\,\psi_k(t_m)$ is then

$$-\Re\,\psi_k(t_m) = \log\log n - \frac{1}{\log n}(1+\log(2\pi k\log n)) + O((\log n)^{-2})$$

as $n\to\infty$, where the dependence on m is contained in the order term. This shows that the heights of the saddles corresponding to $k \geq 2$ are exponentially smaller as $n\to\infty$ than the saddle with $k=1$, so that to within exponentially small correction terms we may neglect the contribution in (2.2) arising from k values corresponding to $k\geq 2$; but see the discussion in Section 3. From hereon, we shall drop the subscript k and write $\psi_1(t)\equiv\psi(t)$.

Typical paths of steepest descent and ascent through the saddles t_0 and t_1 are shown in Fig. 1. Steepest descent and ascent paths terminate at infinity in the right-half plane in the directions $\Im(t) = (2j+\frac{1}{2})\pi$ and $\Im(t) = (2j+\frac{3}{2})\pi$ ($j = 0, \pm 1, \pm 2, \ldots$), respectively. The steepest descent paths through t_0 and t_1 emanate from the origin and pass to infinity in the directions $\Im(t) = \frac{1}{2}\pi$ and $\frac{5}{2}\pi$, respectively. Similarly, the steepest descent path through t_{-1} (not shown) emanates from the origin and passes to infinity in the direction $\Im(t) = -\frac{3}{2}\pi$. The integration path in (2.2) can then be deformed to pass through the saddle t_0 as shown in Fig. 1.

Application of the method of steepest descents (see, for example, [10, p. 127] and [11, p. 14]) then yields

$$J_1 \sim \frac{n}{\pi}\,\frac{\sqrt{2\pi}\,e^{-n\psi(t_0)-t_0}}{t_0(-\psi''(t_0))^{1/2}}\Big(1-\frac{t_0}{n}\Big)\sum_{s=0}^\infty \frac{\hat{c}_{2s}(\frac{1}{2})_s}{n^{s+1/2}}, \tag{2.4}$$

where $(a)_s = \Gamma(a+s)/\Gamma(a)$ is the Pochhammer symbol and $\hat{c}_0 = 1$. The normalised coefficients $\hat{c}_{2s}$ can be obtained by an inversion process and are listed for $s\leq 4$ in [2, p. 119] and for $s\leq 2$ in [11, p. 13]; see below. Alternatively, they can be obtained by an expansion process to yield Wojdylo's formula [14] given by

$$\hat{c}_s = \alpha_0^{-s/2}\sum_{k=0}^{s}\frac{\beta_{s-k}}{\beta_0}\sum_{j=0}^{k}\frac{(-)^j(\frac{1}{2}s+\frac{1}{2})_j}{j!\,\alpha_0^j}\,\mathcal{B}_{kj}\,; \tag{2.5}$$

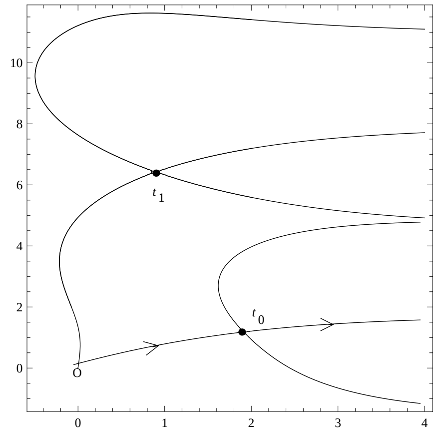

Figure 1: Paths of steepest descent and ascent through the saddles t_0 and t_1 when $n = 100$ and $k = 1$. The steepest paths through the saddle t_{-1} (not shown) in the lower half-plane are similar to those through t_1. The arrows indicate the direction of integration.

see also [12, p. 25]. Here $\mathcal{B}_{kj} \equiv \mathcal{B}_{kj}(\alpha_1, \alpha_2, \ldots, \alpha_{k-j+1})$ are the partial ordinary Bell polynomials generated by the recursion[1]

$$\mathcal{B}_{kj} = \sum_{r=1}^{k-j+1} \alpha_r \mathcal{B}_{k-r,j-1}, \qquad \mathcal{B}_{k0} = \delta_{k0},$$

where δ_{mn} is the Kronecker symbol, and the coefficients α_r and β_r appear in the expansions

$$\psi(t) - \psi(t_0) = \sum_{r=0}^{\infty} \alpha_r (t-t_0)^{r+2}, \qquad f(t) = \sum_{r=0}^{\infty} \beta_r (t-t_0)^r \tag{2.6}$$

valid in a neighbourhood of the saddle $t = t_0$.

Following [6], we put $t_0 = u + iv$, where u, v are real, and write $-\psi(t_0) = A + ia$, where

$$\left.\begin{array}{ll} A: & = \Re(\log t_0 - 1/t_0) = \frac{1}{2}\log(u^2+v^2) - \dfrac{u}{u^2+v^2}, \\ a: & = \Im(\log t_0 - 1/t_0) = \arctan\Big(\dfrac{v}{u}\Big) + \dfrac{v}{u^2+v^2}. \end{array}\right\} \tag{2.7}$$

We have $\psi''(t_0) = (1+t_0)/t_0^2$ and accordingly define[2]

$$B := 2\sqrt{2\pi}\left|\frac{t_0}{\sqrt{1+t_0}}\right|, \qquad b := \tfrac{1}{2}\pi - v - \arctan\Big(\frac{v}{1+u}\Big). \tag{2.8}$$

[1]For example, this generates the values $\mathcal{B}_{41} = \alpha_4$, $\mathcal{B}_{42} = \alpha_3^2 + 2\alpha_1\alpha_3$, $\mathcal{B}_{43} = 3\alpha_1^2\alpha_2$ and $\mathcal{B}_{44} = \alpha_1^4$.

[2]In [6], the quantity $\frac{1}{2}\pi - v$ appearing in the definition of b is written as $\arctan(v/u)$ by virtue of the first relation in (2.9).

A simple calculation using (2.3) with $k = 1$ shows that

$$\tan v = \frac{u}{v}, \qquad e^{-u} = \frac{2\pi|t_0|}{n}. \tag{2.9}$$

Then, from (2.2) with $k = 1$, (2.4) and the second relation in (2.9), we find upon incorporating the factor $1 - t_0/n$ into the asymptotic series that

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \Re\biggl\{e^{i(na+b)} \sum_{s=0}^{\infty} \frac{c'_{2s}(\frac{1}{2})_s}{n^s}\biggr\},$$

where

$$c'_{2s} = \hat{c}_{2s} - \frac{2t_0}{2s-1}\,\hat{c}_{2s-2} \qquad (s \geq 1). \tag{2.10}$$

If we now introduce the real and imaginary parts of the coefficients $\hat{c}_{2s}$ by

$$c'_{2s} := C_s + iD_s \qquad (s \geq 1), \qquad C_0 = 1, \quad D_0 = 0, \tag{2.11}$$

where we recall that C_s and D_s contain an n-dependence, then we have the expansion of γ_n given by the following theorem.

Theorem 1. *Let the quantities A, B, a and b, and the coefficients C_s, D_s, be as defined in (2.7), (2.8) and (2.11). Then, neglecting exponentially smaller terms, we have*

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \biggl\{\cos{(na+b)} \sum_{s=0}^{\infty} \frac{C_s(\frac{1}{2})_s}{n^s} - \sin{(na+b)} \sum_{s=1}^{\infty} \frac{D_s(\frac{1}{2})_s}{n^s}\biggr\} \tag{2.12}$$

as $n \to \infty$.

We note that to leading order $A \sim \log\log n$ and $B \sim (8\pi \log n)^{1/2}$ for large n.

A simpler form of the expansion (2.12) can be given by truncating the above series at $s = 2$ and use of the form of the normalised coefficients $\hat{c}_{2s}$ in (2.4) expressed in the form

$$\hat{c}_2 = \frac{1}{2\psi''(t_0)}\{2F_2 - 2\Psi_3 F_1 + \tfrac{5}{6}\Psi_3^2 - \tfrac{1}{2}\Psi_4\},$$

$$\hat{c}_4 = \frac{1}{(2\psi''(t_0))^2}\{\tfrac{2}{3}F_4 - \tfrac{20}{9}\Psi_3 F_3 + \tfrac{5}{3}(\tfrac{7}{3}\Psi_3^2 - \Psi_4)F_2 - \tfrac{35}{9}(\Psi_3^3 - \Psi_3\Psi_4 + \tfrac{6}{35}\Psi_5)F_1$$
$$+\tfrac{35}{9}(\tfrac{11}{24}\Psi_3^4 - \tfrac{3}{4}(\Psi_3^2 - \tfrac{1}{6}\Psi_4)\Psi_4 + \tfrac{1}{5}\Psi_3\Psi_5 - \tfrac{1}{35}\Psi_6)\}$$

where, for brevity, we have defined

$$\Psi_m := \frac{\psi^{(m)}(t_0)}{\psi''(t_0)} \quad (m \geq 3), \qquad F_m := \frac{f^{(m)}(t_0)}{f(t_0)} \quad (m \geq 1);$$

see [2, p. 119], [11, pp. 13–14].

From (2.1) and (2.10), use of *Mathematica* shows that

$$c_2' = \frac{\wp_2(t_0)}{12(1+t_0)^3} + \frac{(4+3t_0)t_0^2}{n(1+t_0)^2} + O(n^{-2}), \qquad c_4' = \frac{\wp_4(t_0)}{864(1+t_0)^6} + O(n^{-1}),$$

where

$$\wp_2(t_0) = 2 - 18t_0 - 20t_0^2 - 3t_0^3 + 2t_0^4,$$

$$\wp_4(t_0) = 4 - 72t_0 - 332t_0^2 - 8028t_0^3 - 19644t_0^4 - 20280t_0^5 - 9911t_0^6 - 1884t_0^7 + 4t_0^8.$$

Then we obtain the following result.

Theorem 2. *Let the quantities A, B, a and b be as defined in (2.7) and (2.8). Then, with*

$$c_1 + id_1 = \frac{\wp_2(t_0)}{24(1+t_0)^3}, \qquad c_2 + id_2 = \frac{\wp_4(t_0)}{1152(1+t_0)^6} + \frac{(4+3t_0)t_0^2}{2(1+t_0)^2},$$

where c_s, d_s $(s = 1, 2)$ are real (and independent of n) and t_0 is the saddle point given by the principal solution of (2.3) with $k = 1$, we have the asymptotic approximation

$$\gamma_n \sim \frac{Be^{nA}}{\sqrt{n}} \left\{\cos(na+b)\left(1 + \frac{c_1}{n} + \frac{c_2}{n^2}\right) - \sin(na+b)\left(\frac{d_1}{n} + \frac{d_2}{n^2}\right)\right\} \tag{2.13}$$

as $n \to \infty$.

We remark that the expansion of the integrals J_k for fixed $k \geq 2$ follows the same procedure. If we still refer to the real and imaginary parts of the contributory saddle t_0 (when $k \geq 2$) as u and v, the second relation in (2.9) is now replaced by $e^{-u} = 2\pi k|t_0|/n$. It then follows that the form of the expansion for $-\Im J_k$ is given by (2.12), provided the quantities A, B, a and b, and the coefficients C_s, D_s, are interpreted as corresponding to the saddle t_0 with the k-value under consideration.

3. Numerical results and concluding remarks We discuss numerical computations carried out using the expansions given in Theorems 1 and 2. For a given value of n the saddle t_0 is computed from (2.3) with $k = 1$ to the desired accuracy. *Mathematica* is used to determine the coefficients α_r and β_r in (2.6) for $0 \leq r \leq 2s_0$, where in the present computations $s_0 = 6$. The coefficients C_s and D_s can then be calculated for $0 \leq s \leq s_0$ from (2.5), (2.10) and (2.11).

We display the computed values of C_s and D_s for two values of n in Table 1. We repeat that these coefficients contain an n-dependence and so have to be computed for each value of n chosen. In Table 2, the values of the absolute

Table 1: Values of the coefficients C_s and D_s (to 10 dp) for $1 \le s \le 6$ for two values of n.

s	$n = 100$		$n = 1000$	
	C_s	D_s	C_s	D_s
1	-0.3158578918	$+0.1626819326$	-0.0885061806	$+0.1958085240$
2	-2.9096870797	-2.1947177121	-6.5840165991	-2.6459812815
3	-0.3804847598	-3.3953890569	-9.4682639154	-10.09635962642
4	$+1.4820479884$	-0.1130053628	-1.3074432243	-11.31040992292
5	-0.2630549338	$+0.9253656779$	$+4.9469591967$	-1.67819725309
6	-0.3783700609	-0.3119889058	$+0.8180579543$	$+3.98701271605$

Table 2: Values of the absolute relative error in the computation of γ_n from (2.12) as a function of the truncation index s for different n.

s	$n = 75$	$n = 100$	$n = 137$	$n = 1000$
0	1.759×10^{-3}	1.412×10^{-3}	—	1.597×10^{-4}
1	6.503×10^{-4}	3.226×10^{-4}	2.701×10^{-1}	2.649×10^{-6}
2	1.244×10^{-5}	4.472×10^{-6}	8.775×10^{-2}	4.125×10^{-9}
3	3.063×10^{-7}	9.370×10^{-8}	3.811×10^{-5}	7.711×10^{-11}
4	2.535×10^{-9}	7.850×10^{-10}	2.183×10^{-6}	2.026×10^{-13}
5	5.101×10^{-10}	9.022×10^{-11}	1.248×10^{-8}	6.157×10^{-16}
6	1.850×10^{-11}	1.982×10^{-12}	9.415×10^{-10}	2.743×10^{-18}

relative error in the computation of γ_n from the expansion (2.12) are presented as a function of the truncation index s for several values of n.

The case $n = 137$ has been included in Table 2 since this corresponds to the factor $\cos(na+b)$ possessing the very small value $\simeq 1.69881 \times 10^{-4}$. The leading term approximation in (1.1), and (2.12) (with $s = 0$), yields an incorrect sign, namely $+3.89874 \times 10^{27}$ when $\gamma_{137} = -7.99522199\ldots \times 10^{27}$. According to [4], this is the only instance for $n \le 10^5$ when the leading approximation produces the wrong sign. It is seen that inclusion of the higher order correction terms with $s \le 6$ yields a relative error of order 10^{-10} in this case. When $n = 10^5$, [4] gives the value

$$\gamma_{100000} = 1.991927306312541095658227243 15\ldots \times 10^{83432}.$$

The expansion (2.12) for this value of n with truncation index $s = 6$ is found to yield a relative error of order 10^{-30}; that is, the expansion correctly reproduces all the digits displayed above.

Table 3: Values of the absolute relative error in the computation of γ_n from (2.12) with $k = 1$ and $k \leq 2$ as a function of the truncation index s for $n = 25$.

s	$k = 1$	$k \leq 2$
0	1.051×10^{-2}	1.052×10^{-2}
1	2.909×10^{-3}	2.894×10^{-3}
2	2.608×10^{-4}	2.460×10^{-4}
3	2.390×10^{-6}	1.723×10^{-5}
4	1.518×10^{-5}	3.412×10^{-7}
5	1.495×10^{-5}	1.160×10^{-7}
6	1.482×10^{-5}	1.189×10^{-8}

For the smallest value $n = 75$ presented in Table 2, it is found numerically that the contribution to (2.2) corresponding to $k = 2$ is about 11 orders of magnitude smaller than the dominant term with $k = 1$. For the larger n values, this contribution is even smaller and the terms with $k \geq 2$ can be safely neglected. However, for smaller n this is no longer the case and a meaningful approximation has to take into account the contribution from other $k \geq 2$ values.

In Table 3, we illustrate this situation by taking $n = 25$. The second column shows the absolute relative error in the computation of γ_n with $k = 1$ for different truncation index s; that is, with the approximation $\gamma_n \simeq -\Im J_1$. For $4 \leq s \leq 6$, this error is seen to remain essentially constant at $O(10^{-5})$. The contribution with $k = 2$ is about 5 orders of magnitude smaller than the $k = 1$ contribution, so that this additional contribution needs to be included for larger index s. The absolute relative error including the contribution with $k = 2$ is shown in the third column; that is, with the approximation $\gamma_n \simeq -\Im(J_1 + J_2)$. The expansion with $k = 3$ is about 8 orders of magnitude smaller than the $k = 1$ contribution, so this would only begin to make a significant contribution for $s \geq 6$. This problem becomes even more acute for smaller n values, say $n = 10$, where higher k values need to be retained. However, the chief interest in the asymptotic expansion in (2.12) is for large n, where this problem is of no real concern.

In Table 4 we show some examples of the asymptotic approximation given in (2.13). We compare these with the values produced by the leading approximation (1.1) and the exact value of γ_n obtained from *Mathematica* using the command `StieltjesGamma[n]`. It will be observed that for $n = 500$ the approximation (2.13) yields nine significant figures.

Table 4: Values for γ_n obtained from (1.1) and (2.13) compared with the exact value.

n	Eq. (1.1)	Eq. (2.13)	Exact γ_n
10	$+2.105395 \times 10^{-4}$	$+2.04713213 \times 10^{-4}$	$+2.05332814\ldots \times 10^{-4}$
50	$+1.275493 \times 10^{2}$	$+1.26823798 \times 10^{2}$	$+1.26823602\ldots \times 10^{2}$
80	$+2.514857 \times 10^{10}$	$+2.51633995 \times 10^{10}$	$+2.51634410\ldots \times 10^{10}$
100	-4.259408×10^{17}	$-4.25340036 \times 10^{17}$	$-4.25340157\ldots \times 10^{17}$
137	$+3.898740 \times 10^{27}$	$-7.99377883 \times 10^{27}$	$-7.99522199\ldots \times 10^{27}$
200	-7.060244×10^{55}	$-6.97465335 \times 10^{55}$	$-6.97464971\ldots \times 10^{55}$
500	$-1.165662 \times 10^{204}$	$-1.16550527 \times 10^{204}$	$-1.16550527\ldots \times 10^{204}$

Finally, we remark that the analysis in Section 2 is immediately applicable to the more general Stieltjes constants $\gamma_n(\alpha)$ appearing in the Laurent expansion for the Hurwitz zeta function $\zeta(s,\alpha)$ about the point $s=1$. These constants are defined by

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

where $\gamma_0(\alpha) = -\Gamma'(\alpha)/\Gamma(\alpha)$ and $\gamma_n(1) = \gamma_n$. It is shown in [7, Eq. (2.9)] that

$$C_n(\alpha) := \gamma_n(\alpha) - \frac{1}{\alpha}\,e^{n \log\log \alpha} = -\Im \sum_{k=1}^{\infty} e^{-2\pi i k\alpha} J_k.$$

Then it follows that the expansions in Theorems 1 and 2 are modified only in the argument of the trigonometric functions appearing therein, which become $na + b - 2\pi\alpha$. Thus, for example, from (2.13) we have

$$C_n(\alpha) \sim \frac{Be^{nA}}{\sqrt{n}} \left\{ \cos(na+b-2\pi\alpha)\left(1 + \frac{c_1}{n} + \frac{c_2}{n^2}\right) - \sin(na+b-2\pi\alpha)\left(\frac{d_1}{n} + \frac{d_2}{n^2}\right)\right\}$$

as $n \to \infty$, where the quantities A, B, a, b and the coefficients c_s, d_s $(s = 1, 2)$ are as specified in Theorem 2. The leading approximation agrees with that obtained in [7, Eq. (2.4)].

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