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AN ASYMPTOTIC REPRESENTATION FOR $\zeta(\frac{1}{2}+it)$

R. B. Paris and S. Cang

ABSTRACT. A representation for the Riemann zeta function $\zeta(s)$ is given as an absolutely convergent expansion involving incomplete gamma functions which is valid for all finite complex values of s ($\neq 1$). It is then shown how use of the uniform asymptotics of the incomplete gamma function leads to an asymptotic representation for $\zeta(s)$ on the critical line $s = \frac{1}{2} + it$ when $t \to \infty$. This result, which represents an improvement on an earlier treatment [10], involves an error function smoothing of the original Dirichlet series together with a correction term whose coefficients can be given explicitly to any desired order in terms of coefficients arising in the asymptotics of the incomplete gamma function. By examination of the higher-order coefficients in the correction term, it is shown that the expansion diverges like the familiar 'factorial divided by a power' dependence, decorated by a slowly varying multiplier function, as has recently been demonstrated by M. V. Berry for the Riemann-Siegel formula.

1. Introduction

The two well-established methods of computing $\zeta(s)$ on the critical line $s = \frac{1}{2} + it$ (t real) are the Gram and Riemann-Siegel formulas [6, 7]. The first of these formulas consists of a truncation after N terms (the finite main sum) of the original Dirichlet series representation of $\zeta(s)$ in $\mathrm{Re}(s) > 1$, together with a simple series of correction terms involving the Bernoulli numbers. For these correction terms to furnish an asymptotic expansion, it is necessary to select $N > t/2\pi$, with the result that the number of terms in the finite main sum (the computationally most expensive part of the formula) when t is large is $O(t/2\pi)$. The Riemann-Siegel formula, on the other hand, involves correction terms which are more complicated to evaluate, but the associated finite main sum consists of the Dirichlet series truncated after $O((t/2\pi)^{\frac{1}{2}})$ terms. This reduction of the number of terms in the finite main sum makes this formula the more powerful and standard means of computing $\zeta(\frac{1}{2}+it)$.

Alternative methods for calculating $\zeta(\frac{1}{2}+it)$ to high accuracy when t is large have recently been given in [2, 10]; see also [12]. These new expansions have been developed for the real function $Z(t) = \exp(i\vartheta)\zeta(\frac{1}{2}+it)$ where the phase-angle $\vartheta \equiv \vartheta(t)$ is given by

$$\vartheta(t) = \arg\Gamma(\tfrac{1}{4} + \tfrac{1}{2}it) - \tfrac{1}{2}t\log\pi. \tag{1.1}$$

The leading term of the asymptotic formula given by Berry and Keating [2] consists of a *convergent* expansion in which the terms of the original Dirichlet series are smoothed by a complementary error function. In [10], a different form of expansion of $Z(t)$,

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which also involves the complementary error function, was given using the normalized incomplete gamma function $Q(a,z) = \Gamma(a,z)/\Gamma(a)$ as the smoothing function. This procedure was based on the expansion of $\zeta(s)$ in the form

$$\zeta(s) = \sum_{n=1}^{N} n^{-s} + \chi(s)\sum_{n=1}^{\infty} n^{s-1}\Lambda_n(s) + \frac{(N+\frac{1}{2})^{1-s}}{s-1} \tag{1.2}$$

where N denotes an *arbitrary* positive integer,

$$\chi(s) = 2^s\pi^{s-1}\sin\frac{1}{2}\pi s\,\Gamma(1-s) = \pi^{s-\frac{1}{2}}\frac{\Gamma(\frac{1}{2}-\frac{1}{2}s)}{\Gamma(\frac{1}{2}s)}, \tag{1.3}$$

and the coefficients $\Lambda_n(s)$ involve the incomplete gamma functions

$$Q(1-s, \pm 2\pi i n(N+\frac{1}{2})).$$

Both of these new expansions, although involving a little extra computational effort, were found to be more accurate than the Riemann-Siegel formula for the same number of correction terms.

In this paper, we present an alternative, improved asymptotic representation for $Z(t)$ based on the absolutely convergent expansion for $\zeta(s)$ given by

$$\zeta(s) = \frac{(\pi\xi)^{\frac{1}{2}s}}{\Gamma(\frac{1}{2}s)}\left(\frac{\xi^{-\frac{1}{2}}}{s-1} - \frac{1}{s}\right) + \sum_{n=1}^{\infty} n^{-s}Q(\tfrac{1}{2}s, \pi n^2\xi)$$
$$+\,\chi(s)\sum_{n=1}^{\infty} n^{s-1}Q(\tfrac{1}{2}-\tfrac{1}{2}s, \pi n^2/\xi), \tag{1.4}$$

which holds for all values of s ($\neq 1$), where ξ is a complex parameter satisfying $|\arg\xi| \leq \frac{1}{2}\pi$. The result (1.4) is the expansion given by Lavrik [8] for the Dirichlet L-function specialized to $\zeta(s)$. We remark that the case $\xi = 1$ is effectively embodied in Riemann's 1859 paper, though he did not explicitly identify the incomplete gamma functions. As in [10], an asymptotic approximation for $Z(t)$ is then constructed from (1.4) by use of the uniform asymptotic expansion of the incomplete gamma function.

The form (1.4) differs significantly from that in (1.2) in that the n-dependence of the incomplete gamma functions is quadratic, rather than linear. This fact results in a final asymptotic formula which is easier to compute and analyse than the one developed in [10]. The coefficients in the correction terms of this new formula present two important features. First, they can be explicitly formulated to any desired order in terms of coefficients which appear in the asymptotics of the incomplete gamma function. Secondly, and most importantly, their structure becomes simpler for higher orders. This last fact means that it is then relatively straightforward to examine the nature of the divergence of the sum of correction terms by determining their late behavior. In this way, we establish that although the correction terms diverge in typical asymptotic fashion like a 'factorial divided by a power', they also contain a slowly varying multiplier function. An equivalent result for the higher-order correction terms in the Riemann-Siegel formula recently has been demonstrated by Berry [1].

2. The derivation of the expansion

We prove (1.4) by a slight modification of Riemann's original analysis; alternative methods of establishing this result are described in [8, 11, 12]. When $\mathrm{Re}(s) > 1$, Riemann obtained the representation

$$\pi^{-\frac{1}{2}s}\Gamma(\tfrac{1}{2}s)\zeta(s) = \int_0^\infty x^{\frac{1}{2}s-1}\psi(x)\,dx, \qquad \psi(x) = \sum_{n=1}^\infty e^{-\pi n^2 x} \tag{2.1}$$

where $\psi(x)$ satisfies the well-known Poisson summation formula,

$$2\psi(x) + 1 = x^{-\frac{1}{2}}\{2\psi(1/x) + 1\}, \tag{2.2}$$

valid when $|\arg x| < \frac{1}{2}\pi$.

Instead of dividing the path of integration in (2.1) into [0,1] and [1,∞), we divide the path into $[0,\xi]$ and $[\xi,\infty)$ where, for the moment, we restrict ξ to lie in $|\arg\xi| < \frac{1}{2}\pi$, cf. also [9]. Then, from (2.1) and (2.2), we find

$$\pi^{-\frac{1}{2}s}\Gamma(\tfrac{1}{2}s)\zeta(s) = \left\{\int_0^\xi + \int_\xi^\infty\right\} x^{\frac{1}{2}s-1}\psi(x)dx,$$

so that

$$\begin{aligned}\pi^{-\frac{1}{2}s}\Gamma(\tfrac{1}{2}s)\zeta(s) - \frac{\xi^{\frac{1}{2}s-\frac{1}{2}}}{s-1} + \frac{\xi^{\frac{1}{2}s}}{s} &= \int_0^\xi x^{\frac{1}{2}s-\frac{3}{2}}\psi(1/x)dx + \int_\xi^\infty x^{\frac{1}{2}s-1}\psi(x)dx \\ &= \int_{1/\xi}^\infty x^{-\frac{1}{2}s-\frac{1}{2}}\psi(x)dx + \int_\xi^\infty x^{\frac{1}{2}s-1}\psi(x)dx. \end{aligned} \tag{2.3}$$

Reversal of the order of summation and integration (which is justified by absolute convergence), followed by introduction of the new variable $u = \pi n^2 x$, enables the right-hand side of (2.3) to be written in the form

$$\pi^{\frac{1}{2}s-\frac{1}{2}}\sum_{n=1}^\infty n^{s-1}\int_{\pi n^2/\xi}^\infty u^{-\frac{1}{2}s-\frac{1}{2}}e^{-u}du + \pi^{-\frac{1}{2}s}\sum_{n=1}^\infty n^{-s}\int_{\pi n^2\xi}^\infty u^{\frac{1}{2}s-1}e^{-u}du.$$

The resulting integrals can be expressed in terms of the normalized incomplete gamma function

$$Q(a,z) = \frac{\Gamma(a,z)}{\Gamma(a)} = \frac{1}{\Gamma(a)}\int_z^\infty u^{a-1}e^{-u}du$$

to yield the expansion

$$\zeta(s) = \frac{(\pi\xi)^{\frac{1}{2}s}}{\Gamma(\frac{1}{2}s)}\left(\frac{\xi^{-\frac{1}{2}}}{s-1} - \frac{1}{s}\right) + \sum_{n=1}^\infty n^{-s}Q(\frac{1}{2}s, \pi n^2\xi) + \chi(s)\sum_{n=1}^\infty n^{s-1}Q(\tfrac{1}{2} - \tfrac{1}{2}s, \pi n^2/\xi) \tag{2.4}$$

where $\chi(s)$ is defined in (1.3). Since $\Gamma(a,z) \sim z^{a-1}e^{-z}$ as $|z| \to \infty$ in $|\arg z| < \frac{3}{2}\pi$, both sums in (2.4) converge absolutely for all values of s, with late terms behaving like $n^{-2}\exp(-\pi n^2\xi^{\pm1})$, respectively. Consequently, the result (2.4), which was derived for $\mathrm{Re}(s) > 1$ and $|\arg\xi| < \frac{1}{2}\pi$, holds for all values of s ($\neq 1$) and ξ satisfying $|\arg\xi| \le \frac{1}{2}\pi$ by analytic continuation.

We now specialize (2.4) to the critical line $s = \frac{1}{2} + it$ where $\chi(\frac{1}{2} + it) = \exp(-2i\vartheta)$, and by the symmetry of the zeta function, it is sufficient to take $t \ge 0$. In this case it is more convenient to consider the *real* even function $Z(t)$ given by

$$Z(t) = e^{i\vartheta(t)}\zeta(\tfrac{1}{2} + it)$$

where $\vartheta(t)$ is defined in (1.1). In order to retain (2.4) in a symmetrical form, we put $|\xi| = 1$ and, accordingly, write $\xi = e^{i\phi}$ where ϕ is real. Then, since $Q(\overline{a}, \overline{z}) = \overline{Q(a,z)}$

(where the bar denotes the complex conjugate), we find the elegant result (where $s = \frac{1}{2} + it$)

$$Z(t) = 2\,\mathrm{Re}\, e^{i\vartheta} \left\{ \sum_{n=1}^{\infty} n^{-s} Q(\tfrac{1}{2}s, \pi n^2 e^{i\phi}) - \frac{\pi^{\frac{1}{2}s} e^{\frac{1}{2}i\phi s}}{s\Gamma(\frac{1}{2}s)} \right\}, \quad (|\phi| \le \tfrac{1}{2}\pi). \tag{2.5}$$

We observe that the factor $e^{\frac{1}{2}i\phi s}/\Gamma(\frac{1}{2}s)$ contains the exponential term $\exp\{(\frac{1}{4}\pi - \frac{1}{2}\phi)t\}$ for large t. (Such a compensating factor also appears in $Q(\frac{1}{2}s, \pi n^2 i)$; see §3.) When $\phi < \frac{1}{2}\pi$, this represents a numerically large factor which would require the evaluation of the terms to exponentially small accuracy. Thus, we are effectively forced to set $\phi = \frac{1}{2}\pi$ to avoid such undesirable terms in computations of $Z(t)$ high up on the critical line.

When $\phi = \frac{1}{2}\pi$, we remark that the sum in (2.5) then represents the original Dirichlet series "smoothed" by the incomplete gamma function $Q(\frac{1}{2}s, \pi n^2 i)$. To see this, we note that the behavior of this latter function for large t changes abruptly in the neighborhood of its transition point given by $\frac{1}{2}s = \pi n^2 i$; that is, when n attains roughly the Riemann-Siegel cut-off value N_t defined by

$$N_t = \mathrm{Int}(t/2\pi)^{\frac{1}{2}}, \qquad p(t) = (t/2\pi)^{\frac{1}{2}} - N_t \tag{2.6}$$

where Int denotes the integer part. Then for values of $n \simeq N_t$, the behavior of $Q(\frac{1}{2}s, \pi n^2 i)$ where $s = \frac{1}{2} + it$ with $t \gg 1$ is approximately described by (see §3)

$$\begin{aligned} Q(\frac{1}{2}s, \pi n^2 i) &\sim \frac{1}{2}\,\mathrm{erfc}\Big[\pi t^{-\frac{1}{2}}\Big(n^2 - \frac{t}{2\pi}\Big)e^{\frac{1}{4}\pi i}\Big] \\ &\simeq \frac{1}{2}\,\mathrm{erfc}\Big[\sqrt{2\pi i}(n - N_t - p(t))\Big], \qquad t \to +\infty. \end{aligned} \tag{2.7}$$

Thus, for large t, we have $Q(\frac{1}{2}s, \pi n^2 i) \sim 1$ when $n \lesssim N_t$, while $Q(\frac{1}{2}s, \pi n^2 i)$ decays (algebraically) to zero when $n \gtrsim N_t$. Loosely speaking, therefore, the terms in the smoothed Dirichlet series effectively "switch off" when $n \simeq N_t$. This behavior is illustrated in Figure 1 for the particular case $t = 800$.

3. An asymptotic approximation for $Z(t)$

To obtain an approximation for $Z(t)$ as $t \to +\infty$, we employ the uniform asymptotic expansion of the incomplete gamma function $Q(a, z)$ which holds for $a \to \infty$ when $|z| \in [0, \infty)$ in the domains $|\arg a| \le \pi - \epsilon_1$ and $|\arg(z/a)| \le 2\pi - \epsilon_2$ where ϵ_1, ϵ_2 are positive numbers satisfying $0 < \epsilon_1 < \pi$, $0 < \epsilon_2 < 2\pi$. This is given in terms of the complementary error function by [13]

$$Q(a,z) = \frac{1}{2}\,\mathrm{erfc}\,(\eta\sqrt{(a/2)}) + \frac{e^{-\frac{1}{2}a\eta^2}}{\sqrt{2\pi a}} \left\{ \sum_{r=0}^{m-1} a^{-r} c_r(\eta) + a^{-m} G_m(a,\eta) \right\}, \; m = 1, 2, \ldots, \tag{3.1}$$

where

$$c_r(\eta) = (-)^r \frac{Q_r(\mu)}{\mu^{2r+1}} - \frac{D_r}{\eta^{2r+1}}, \quad D_r = (-2)^r \frac{\Gamma(r+\frac{1}{2})}{\Gamma(\frac{1}{2})}, \tag{3.2}$$

$$\frac{1}{2}\eta^2 = \lambda - 1 - \log\lambda, \qquad \lambda = z/a, \qquad \mu = \lambda - 1, \tag{3.3}$$

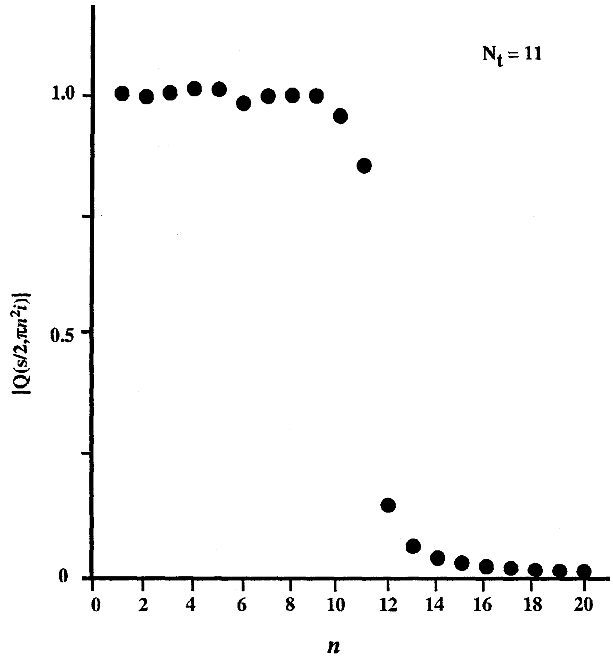

FIGURE 1. The behavior of $|Q(\frac{1}{2}s, \pi n^2 i)|$ as a function of n for the case $s = \frac{1}{2} + 800i$.

and $G_m(a, \eta)$ is the remainder in the expansion truncated after m terms. The coefficients $c_r(\eta)$ are specified in terms of the polynomial

$$Q_r(\mu) = \sum_{k=0}^{2r} \alpha_k^{(r)} \mu^k \tag{3.4}$$

of degree $2r$ and are analytic at $\eta = 0$. Recurrence relations for the coefficients $\alpha_k^{(r)}$ are given in Appendix A; values of these coefficients for $0 \leq k \leq 12$ are presented in Table 6. The choice of the square-root branch for $\eta(\lambda)$ is made such that $\eta(\lambda)$ and $\lambda - 1$ have the same sign when $\lambda > 0$. We note that $\eta \simeq \lambda - 1$ when $\lambda \simeq 1$.

As in [10], we now define the *modified* complementary error function by

$$\operatorname{erfc}(z; m) = \operatorname{erfc} z - \frac{e^{-z^2}}{z\sqrt{\pi}} \sum_{r=0}^{m-1} D_r (2z^2)^{-r}, \qquad m = 1, 2, \ldots \quad (z \neq 0), \tag{3.5}$$

which corresponds to the removal from the complementary error function erfc z of the first m terms of its asymptotic expansion for $|z| \to \infty$ in $|\arg z| < \frac{3}{4}\pi$. The expansion in (3.1) then can be written in the modified form more suitable for the present application as

$$Q(a,z)=\frac{1}{2}\operatorname{erfc}(\eta\sqrt{(a/2)};m)+\frac{e^{-\frac{1}{2}a\eta^2}}{\sqrt{2\pi a}}\left\{\sum_{r=0}^{m-1}(-)^r a^{-r}\frac{Q_r(\mu)}{\mu^{2r+1}}+a^{-m}G_m(a,\eta)\right\},\tag{3.6}$$

from which it is possible to represent $Q(\frac{1}{2}s,\pi n^2e^{i\phi})$ appearing in (2.5) uniformly as $t\to\infty$ for $n\geq 1$ when we identify a and λ with

$$a\equiv\frac{1}{2}s=\frac{1}{4}+\frac{1}{2}it,\quad \lambda=2\pi n^2e^{i\phi}/s.$$

It then follows from (3.3) that $\eta\equiv\eta_n(t)$ and $\mu\equiv\mu_n(t)$; for simplicity in presentation, we shall omit the dependence on t, except where it is essential. Then, since $\exp(-\frac{1}{2}a\eta_n^2)=\exp(-\pi n^2e^{i\phi})n^s e^{\frac{1}{2}i\phi s}(2\pi e/s)^{\frac{1}{2}s}$, we can express $Z(t)$ in the form

$$Z(t)=\operatorname{Re}e^{i\vartheta}\left\{\sum_{n=1}^{\infty}n^{-s}\operatorname{erfc}(\tfrac{1}{2}\eta_n\sqrt{s};m)\right.$$
$$\left.+\frac{e^{\frac{1}{2}i\phi s}}{\sqrt{\pi s}}\left(\frac{2\pi e}{s}\right)^{\frac{1}{2}s}\left(\sum_{r=0}^{m-1}(-)^{r-1}(\tfrac{1}{2}s)^{-r}A_r(s)+(\tfrac{1}{2}s)^{-m}\hat{R}_m\right)\right\}\tag{3.7}$$

where the remainder $\hat{R}_m$ and the coefficients $A_r(s)$ are defined by

$$\hat{R}_m=2\sum_{n=1}^{\infty}\exp(-\pi n^2e^{i\phi})G_m(\tfrac{1}{2}s,\eta_n)-H_m(\tfrac{1}{2}s)\tag{3.8}$$

and

$$A_r(s)=(-)^r\gamma_r-2\sum_{n=1}^{\infty}\exp(-\pi n^2e^{i\phi})\frac{Q_r(\mu_n)}{\mu_n^{2r+1}}$$
$$=\sum_{n=-\infty}^{\infty}\exp(-\pi n^2e^{i\phi})\frac{Q_r(\mu_n)}{(-\mu_n)^{2r+1}},\tag{3.9}$$

in which $\mu_n=2\pi n^2e^{i\phi}/s-1$ (with $s=\frac{1}{2}+it$), and we have used the result $Q_r(-1)=(-)^r\gamma_r$ from (A.1). In (3.7), we have employed the well-known expansion of the gamma function for large z given by

$$\frac{1}{\Gamma(z)}=(2\pi)^{-\frac{1}{2}}z^{\frac{1}{2}-z}e^z\left\{\sum_{r=0}^{m-1}\gamma_r z^{-r}+z^{-m}H_m(z)\right\},\qquad m=1,2,\ldots,\tag{3.10}$$

where $H_m(z)$ is a remainder and the first few Stirling coefficients γ_r are

$$\gamma_0=1,\quad\gamma_1=-\frac{1}{12},\quad\gamma_2=\frac{1}{288},\quad\gamma_3=\frac{139}{51840},$$
$$\gamma_4=-\frac{571}{2488320},\quad\gamma_5=-\frac{163879}{209018880}.$$

4. Numerical illustrations and discussion

Following the remark at the end of §2, we set $\phi=\frac{1}{2}\pi$ throughout the remainder of this paper and define the variable ω by

$$\omega^2\equiv-\frac{1}{2}\pi is=\frac{1}{2}\pi(t-\tfrac{1}{2}i).\tag{4.1}$$

From (3.9), the coefficients $A_r(s)$ are then given by

$$A_r(s) = \sum_{n=-\infty}^{\infty} (-)^n \frac{Q_r(\mu_n)}{(-\mu_n)^{2r+1}} \qquad (\mu_n = (\pi n/\omega)^2 - 1)$$
$$= \sum_{k=0}^{2r} (-)^k \alpha_k^{(r)} \sum_{n=-\infty}^{\infty} (-)^n \left(\frac{\omega^2}{\omega^2 - (\pi n)^2}\right)^{2r+1-k} \tag{4.2}$$

where the coefficients $\alpha_k^{(r)}$ are specified in (3.4) (see also Table 6). The inner sum in (4.2) may be expressed in terms of the functions $S_k(\omega)$ defined by

$$S_k(\omega) = 2^{k-1} \sum_{n=-\infty}^{\infty} (-)^n \frac{\omega^k}{(\omega^2 - (\pi n)^2)^k}, \qquad k = 1, 2, \ldots, \tag{4.3}$$

so that

$$A_r(s) = 2^{-2r} \omega^{2r+1} B_r(\omega), \quad B_r(\omega) = \sum_{k=0}^{2r} (-)^k \alpha_k^{(r)} (\tfrac{1}{2}\omega)^{-k} S_{2r+1-k}(\omega). \tag{4.4}$$

The functions $S_k(\omega)$ can be written in terms of cosec ω and its derivatives from the recursion

$$S_1(\omega) = \operatorname{cosec} \omega, \qquad S_{k+1}(\omega) = \frac{1}{\omega} S_k(\omega) - \frac{1}{k} \frac{dS_k(\omega)}{d\omega}, \qquad k \geq 1. \tag{4.5}$$

The expansion for $Z(t)$ in (3.8) on the critical line $s = \frac{1}{2} + it$ then becomes

$$Z(t) = \operatorname{Re} e^{i\vartheta} \left\{ \sum_{n=1}^{\infty} n^{-s} \operatorname{erfc}(\tfrac{1}{2}\eta_n \sqrt{s}; m) + R^{(m)}(t) \right\} \tag{4.6}$$

where, for $m = 1, 2, \ldots$, the correction term $R^{(m)}(t)$ is given by

$$R^{(m)}(t) = 2^{-\frac{1}{2}} e^{\frac{3}{4}\pi i} (\pi e^{\frac{1}{2}}/\omega)^s \left(\sum_{r=0}^{m-1} (\pi i/4)^r B_r(\omega) + \omega^{-2m+1} R_m \right), \tag{4.7}$$

$R_m = (-)^{m+1} (\pi i)^m \hat{R}_m / \omega^2$ and η_n is defined in (3.3) with $\lambda_n = (\pi n/\omega)^2$.

An alternative form for the correction term $R^{(m)}(t)$, which exhibits the associated asymptotic scale, can be found by a straightforward regrouping of the terms in the finite sum in (4.7). Thus, we define the coefficients $C_k^{(m)}(\omega)$ by

$$\sum_{r=0}^{m} (\pi i/4)^r B_r(\omega) = \sum_{k=0}^{2m} (-\omega)^{-k} C_k^{(m)}(\omega)$$

where

$$C_k^{(m)}(\omega) = 2^k \sum_{j=0}^{2m-k} (\pi i/4)^{(k+j)/2} \alpha_k^{(\frac{1}{2}k + \frac{1}{2}j)} S_{j+1}(\omega), \qquad 0 \leq k \leq 2m, \tag{4.8}$$

and $\alpha_k^{(r)}$ are to be interpreted as zero for half-integer values of r. The expression in (4.7) then takes the alternative form[1]

$$R^{(m)}(t) = 2^{-\frac{1}{2}} e^{\frac{3}{4}\pi i} (\pi e^{\frac{1}{2}}/\omega)^s \bigg(\sum_{r=0}^{2m-2} (-\omega)^{-r} C_r^{(m-1)}(\omega) + \omega^{-2m+1} R_m \bigg). \qquad (4.9)$$

We remark that the correction terms in (4.9) involve an expansion in descending powers of $\omega \simeq \pi(t/2\pi)^{\frac{1}{2}}$, with the factor $(\pi e^{\frac{1}{2}}/\omega)^s$ multiplying this sum being $O(t^{-\frac{1}{4}})$ for large t; cf. the Riemann-Siegel formula.

The formula (4.6) consists of the (absolutely convergent) sum resulting from the original Dirichlet series smoothed by a (modified) complementary error function together with the correction term $R^{(m)}(t)$. If we use the reflection formula for the modified complementary error function given by [10], $\operatorname{erfc}(-z;m) = 2 - \operatorname{erfc}(z;m)$, then we can separate out from the sum of error functions in (4.6) the finite main sum $2\sum_{n=1}^{N} n^{-\frac{1}{2}} \cos(\vartheta - t\log n)$. Thus, when $s = \frac{1}{2} + it$,

$$\operatorname{Re} e^{i\vartheta} \sum_{n=1}^{\infty} n^{-s} \operatorname{erfc}(\tfrac{1}{2}\eta_n\sqrt{s}; m) = 2\sum_{n=1}^{N} n^{-\frac{1}{2}} \cos(\vartheta - t\log n) + \operatorname{Re}\{e^{i\vartheta} E_m(t;N)\} \qquad (4.10)$$

where we have defined

$$E_m(t;N) = \sum_{n=1}^{\infty} \epsilon_N n^{-s} \operatorname{erfc}(\tfrac{1}{2}\epsilon_N\eta_n\sqrt{s}; m), \qquad \epsilon_N = \begin{cases} +1 & n > N, \\ -1 & n \le N. \end{cases} \qquad (4.11)$$

Then (4.6) takes the final form

$$Z(t) = 2\sum_{n=1}^{N} n^{-\frac{1}{2}} \cos(\vartheta - t\log\, n) + \operatorname{Re} e^{i\vartheta}\{E_m(t;N) + R^{(m)}(t)\} \qquad (4.12)$$

where $R^{(m)}(t)$ is defined in (4.7) or (4.9), and N is an *arbitrary* positive integer.

The rate of convergence of the sum $E_m(t;N)$ is a crucial factor in the applicability of (4.12) as a means of computing $Z(t)$ for $t \gg 1$. From the asymptotic behavior

$$\operatorname{erfc}(z;m) \sim \sqrt{(2/\pi)} D_m (2z^2)^{-m-\frac{1}{2}} e^{-z^2} \quad \text{as} \quad z \to \infty \quad \text{in } |\arg z| < \frac{3}{4}\pi$$

(see [10, Appendix A]), together with the result, from (3.3), $\eta_n^2 \sim 2\lambda_n = 4\pi n^2 i/s$ as $n \to \infty$, we find that the terms in $E_m(t;N)$ ultimately lose their n^{-s} dependence to behave like

$$\begin{aligned} \big|n^{-s} \operatorname{erfc}(\tfrac{1}{2}\eta_n\sqrt{s}; m)\big| &\sim (2/\pi)^{\frac{1}{2}} |D_m| \big|(\tfrac{1}{2}\eta_n^2 s)^{-m-\frac{1}{2}}\big| (t/2\pi)^{-\frac{1}{4}} \\ &= (2\pi n^2)^{-m-\frac{1}{2}} O\big((t/2\pi)^{-\frac{1}{4}}\big). \end{aligned}$$

Thus, although the decay of the terms is algebraic rather than exponential (since the phase of the modified complementary error functions in (4.11) is $\simeq \pi/4$ for large t), this algebraic decay is controlled by n^{-2m-1} together with a scaling factor depending weakly on t like $t^{-\frac{1}{4}}$. This nonetheless represents a considerable improvement of the convergence of $E_m(t;N)$ for moderate values of m.

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[1]Preliminary estimates have shown that $R_m = O(\omega)$ as $t \to \infty$, rather than the sharper result $R_m = o(\omega)$ required to establish the asymptotic nature of the expansion (4.9).

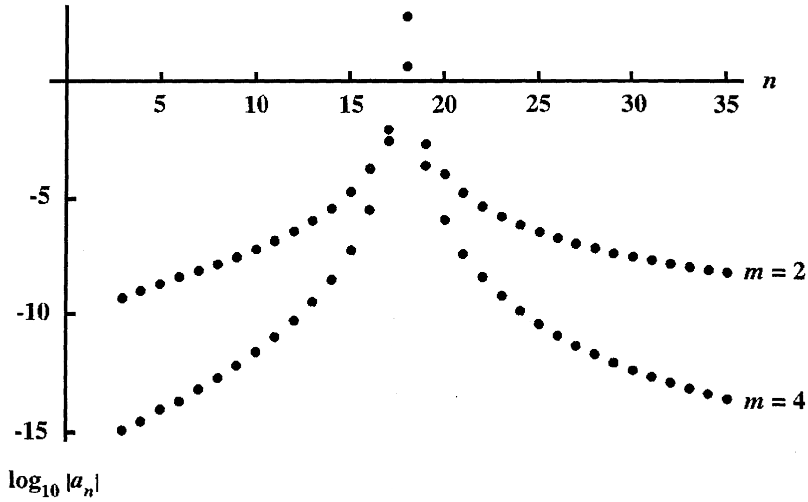

FIGURE 2. The behavior of $E_m(t;N)$ for different m when $t = 2000$ and $N = N_t = 17$.

We now choose the number of terms N in the finite main sum in (4.12) equal to the Riemann-Siegel cut-off value N_t given in (2.6). As discussed in [10], this choice has the consequence of making the terms in the sum $E_m(t;N)$ decay rapidly on either side of $n = N_t$. In Figure 2, we illustrate this decay for different values of m in the particular case $t = 2000$ when $N = N_t = 17$.

An important feature in the calculations is that this rapid fall-off of the terms in $E_m(t;N_t)$ away from $n = N_t$ is essentially independent of t. This can be seen from (2.7) which shows that (up to a sign) the argument of the modified complementary error functions in $E_m(t;N_t)$ has the same form when $n \simeq N_t$, thus revealing that (apart from the presence of the term $p(t)$) the decay on both sides is controlled only by the difference $|n - N_t|$.

We truncate the sum $E_m(t;N_t)$ at n_1 and n_2 (where $n_1 < N_t < n_2$) determined by when the modulus of the argument of the modified complementary error function attains a prescribed value, i.e., when $|\frac{1}{2}\eta_n\sqrt{s}| \simeq K\sqrt{2\pi}$, say, where K is an integer. From (2.7), this occurs roughly when $|n - N_t| = K$; that is, we take

$$n_{1,2} = N_t \pm K. \tag{4.13}$$

The magnitude of the terms in $E_m(t;N_t)$ at these truncation values is then given approximately (when $N_t \gg K$) by

$$(2/\pi)^{\frac{1}{2}}|D_m|(t/2\pi)^{-\frac{1}{4}}(4\pi K^2)^{-m-\frac{1}{2}}.$$

Thus, for example, the choice $K = 10$ corresponds to neglecting terms in $E_m(t;N_t)$ for $t \gg 1$ of magnitude smaller than roughly $2.63 \times 10^{-10}t^{-\frac{1}{4}}$ when $m = 3$, and $1.07 \times 10^{-14}t^{-\frac{1}{4}}$ when $m = 5$.

	$t = 18$ $Z(t) = 2.3367996899$ $N_t = 1$			
	$p(t) = 0.693$ $\vartheta(t) = 0.0809107577$			
	RS value: $Z_{approx} = 2.33679617$		$\lvert Z - Z_{approx}\rvert = 3.5 \times 10^{-6}$	
	$m = 2$		$m = 3$	
n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
2	2.33612 94955	6.7×10^{-4}	2.33652 96514	2.7×10^{-4}
3	2.33682 83433	2.8×10^{-5}	2.33680 73737	7.7×10^{-6}
4	2.33678 65806	1.3×10^{-5}	2.33679 91542	5.4×10^{-7}
5	2.33679 40559	5.6×10^{-6}	2.33679 99857	3.0×10^{-7}
	$m = 4$		$m = 5$	
n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
2	2.33688 18864	8.2×10^{-5}	2.33684 54911	4.6×10^{-5}
3	2.33679 91036	5.9×10^{-7}	2.33679 95068	1.8×10^{-7}
4	2.33679 96930	3.1×10^{-9}	2.33679 96947	4.8×10^{-9}
5	2.33679 96660	2.4×10^{-8}	2.33679 96896	3.7×10^{-10}

TABLE 1. Computations of $Z(t)$ for $t = 18$.

To proceed further with the analysis of (4.6) or (4.12) would require a bound on the remainder term R_m. This will be considered elsewhere; accordingly, we formally disregard this term here and employ the expansion truncated after m terms. To illustrate the accuracy of (4.12), we present the results for the three cases

$$t = 18, \qquad t = 7005.08186, \qquad t = 250000,$$

which are the three values considered in [10] and, apart from the last value, in [2]. The first value of t is very low and is situated approximately midway between the first two non-trivial zeros of $\zeta(s)$. In this case $N_t = 1$, so that summation in $E_m(t; N_t)$ is carried out over $1 \leq n \leq n_2$. The second value corresponds to the first pair of close zeros in between which $Z(t)$ is very small. The third value chosen corresponds to a point high up on the critical line in the asymptotic range.

The results are presented in Tables 1–3 for different values of m and different truncation indices n_1, n_2. In the computations, we found it more convenient to use the correction term in (4.7) given in terms of the coefficients $B_r(\omega)$. For the lowest value of t, we computed $\vartheta(t)$ by means of (1.1), whereas for large values of t, it was sufficient to use the well-known asymptotic expansion for $\vartheta(t)$. For comparison, we give the value of $Z(t)$ computed using *Mathematica* and the value of $Z(t)$ computed using the Riemann-Siegel (RS) formula with five correction terms. Comparison with the corresponding results in [10] shows that the truncated expansion (4.12) yields a similar accuracy, which can exceed that achievable by the Riemann-Siegel formula for *the same number of correction terms.* As with the Berry-Keating formula [2], this increased accuracy comes at the cost of extra computational effort in the evaluation of the error functions in the sum $E_m(t; N_t)$ (although this can be reduced by use of an asymptotic algorithm for the error functions in the tails of this sum). The actual number of error functions required to obtain a high degree of accuracy, however, is

$t = 7005.08186$	$Z(t) = 0.00396\ 73572\ 77190\ 50701\ 38402$	$N_t = 33$
$p(t) = 0.390$	$\vartheta(t) = 21072.69411\ 88214\ 748710$	
RS value: $Z_{approx} = 0.00396\ 73572\ 77296$	$\lvert Z - Z_{approx}\rvert = 1.2 \times 10^{-13}$	
	$m = 2$	
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
25, 40	0.00396 73466 99530	1.1×10^{-8}
20, 45	0.00396 73581 32790	8.6×10^{-10}
15, 50	0.00396 73571 15795	1.6×10^{-10}
10, 55	0.00396 73573 23010	4.6×10^{-11}
5, 60	0.00396 73572 60638	1.7×10^{-11}
1, 80	0.00396 73572 75878	1.3×10^{-12}
	$m = 3$	
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
25, 40	0.00396 73570 94439	1.8×10^{-10}
20, 45	0.00396 73572 82710	5.5×10^{-12}
15, 50	0.00396 73752 76642	5.5×10^{-13}
10, 55	0.00396 73572 77288	9.8×10^{-14}
5, 60	0.00396 73572 77166	2.4×10^{-14}
1, 80	0.00396 73572 77190	6.9×10^{-16}
	$m = 4$	
n_1, n_2	$Z_{approx} - 0.00396\ 73572 \times 10^{10}$	$\lvert Z - Z_{approx}\rvert$
25, 40	0.78008 75339 81159	2.9×10^{-12}
20, 45	0.77181 53319 69707	9.0×10^{-15}
15, 50	0.77190 97396 11027	4.7×10^{-16}
10, 55	0.77190 45497 58332	5.2×10^{-17}
5, 60	0.77190 51617 73206	9.2×10^{-18}
1, 80	0.77190 50710 54550	9.2×10^{-20}
	$m = 5$	
n_1, n_2	$Z_{approx} - 0.00396\ 73572 \times 10^{10}$	$\lvert Z - Z_{approx}\rvert$
25, 40	0.77216 38928 99974	2.6×10^{-14}
20, 45	0.77190 39853 44752	1.1×10^{-16}
15, 50	0.77190 51001 29593	3.0×10^{-18}
10, 55	0.77190 50680 40141	2.1×10^{-19}
5, 60	0.77190 50703 94288	2.6×10^{-20}
1, 80	0.77190 50701 39322	9.2×10^{-23}

TABLE 2. Computations of $Z(t)$ for $t = 7005.08186$.

$t = 250000$	$Z(t) = -0.78556\ 62503\ 91741\ 40098$	$N_t = 199$
$p(t) = 0.471$	$\vartheta(t) = 1198916.99860\ 53813\ 84823\ 28173$	
RS value:	$Z_{approx} = -0.78556\ 62503\ 91741\ 39954$	$\lvert Z - Z_{approx}\rvert = 1.4 \times 10^{-18}$
	$m = 2$	
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
195, 205	−0.78556 62603 41323 49713	9.9×10^{-9}
185, 215	−0.78556 62504 05226 17559	1.3×10^{-11}
175, 225	−0.78556 62503 91703 94678	3.7×10^{-14}
160, 240	−0.78556 62503 91852 44540	1.1×10^{-13}
150, 250	−0.78556 62503 91797 57472	5.6×10^{-14}
100, 300	−0.78556 62503 91745 87341	4.5×10^{-15}
50, 350	−0.78556 62503 91742 32636	9.2×10^{-16}
1, 400	−0.78556 62503 91741 70624	3.1×10^{-16}
	$m = 3$	
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
195, 205	−0.78556 62507 86823 34227	4.0×10^{-10}
185, 215	−0.78556 62503 91815 13885	7.4×10^{-14}
175, 225	−0.78566 62503 91741 31837	8.3×10^{-17}
160, 240	−0.78566 62503 91741 49139	9.0×10^{-17}
150, 250	−0.78566 62503 91741 43034	2.9×10^{-17}
100, 300	−0.78566 62503 91741 40156	5.8×10^{-19}
50, 350	−0.78566 62503 91741 40103	5.0×10^{-20}
1, 400	−0.78566 62503 91741 40098	8.9×10^{-21}
	$m = 4$	
n_1, n_2	$(Z_{approx} + 0.78556\ 62503)\times10^{10}$	$\lvert Z - Z_{approx}\rvert$
195, 205	−0.87855 03469 95247 02768	3.9×10^{-12}
185, 215	−0.91741 31051 37297 02262	9.0×10^{-17}
175, 225	−0.91741 40101 32104 92281	3.8×10^{-20}
160, 240	−0.91741 40095 89730 77506	1.6×10^{-20}
150, 250	−0.91741 40097 18392 52601	3.4×10^{-21}
100, 300	−0.91741 40097 52146 40716	1.7×10^{-23}
50, 350	−0.91741 40097 52307 72376	6.6×10^{-25}
1, 400	−0.91741 40097 52313 70093	6.3×10^{-26}
	$m = 5$	
n_1, n_2	$(Z_{approx} + 0.78556\ 62503)\times10^{10}$	$\lvert Z - Z_{approx}\rvert$
195, 205	−0.91508 46382 69843 63431	2.3×10^{-13}
185, 215	−0.91741 40020 54094 38755	7.7×10^{-19}
175, 225	−0.91741 40097 53615 52319	1.3×10^{-22}
160, 240	−0.91741 40097 52106 42307	2.1×10^{-23}
150, 250	−0.91741 40097 52286 42267	2.8×10^{-24}
100, 300	−0.91741 40097 52314 29814	2.8×10^{-24}
50, 350	−0.91741 40097 52314 33242	6.1×10^{-29}
1, 400	−0.91741 40097 52314 33300	3.0×10^{-30}

TABLE 3. Computations of $Z(t)$ for $t = 250000$.

not very great. For example, when $t = 250000$, it is found that, for $m = 5$, a value of K in (4.13) as small as only about 12 yields an accuracy comparable with the Riemann-Siegel formula with five correction terms.

5. Modification of (4.12) in the neighborhood of a discontinuity in N_t

The formula (4.12) is an attractive alternative to the Riemann-Siegel formula since its coefficients $B_r(\omega)$ can be calculated to as high an order as required by simple recursive relations. Although the expansion is found to yield very accurate results, an inconvenience appears when we attempt to compute $Z(t)$ for values of t which make ω lie close to an integer multiple of π (this corresponds to the transition point of the incomplete gamma function $Q(\frac{1}{2}s, \pi n^2 i)$). From (2.6) and (4.1) when t is large, this arises when $p(t) \simeq 0$ or 1, i.e., at a discontinuity in N_t. Although the coefficients $B_r(\omega)$, or $C_r^{(m-1)}(\omega)$ (and the sum $E_m(t;N)$), are not singular for such critical t values (because ω always has a small imaginary part) there will be loss of accuracy due to round-off error when computing with fixed-decimal arithmetic. In [10], where the critical t values occurred when $p(t) \simeq \frac{1}{4}$ and $\frac{3}{4}$, it was possible to circumvent this difficulty by suitable fine-tuning of the index N appearing in the finite main sum. This was possible because N also appeared in the analogue of the coefficients $B_r(\omega)$. However, with (4.12), this is not the case, so that similar fine-tuning is no longer possible.

In order to deal with this difficulty, we modify the asymptotic formula for $Z(t)$ by separating off from $E_m(t;N)$ the terms responsible for this behavior and combining them with corresponding terms in the coefficients $B_r(\omega)$, or equivalently in $C_r^{(m-1)}(\omega)$. In Figure 3, we show an example of the behavior of the real part of $\eta_n \equiv \eta_n(t)$ (the imaginary part is very small of $O(t^{-1})$ and slowly varying) for different n as a function of t in the neighborhood containing the discontinuous change from $N_t = 17$ to $N_t = 18$, that is, in the neighborhood of $t = 2\pi \times 18^2 = 2035.75\ldots$. It is seen that when $n = 18$, $\mathrm{Re}\,\eta_n(t)$ becomes very small near this change and inclusion of these terms in the modified complementary error functions in (4.11) will result in $E_m(t;N)$ (and correspondingly the coefficients $B_r(\omega)$) becoming large.

We modify $E_m(t;N)$ by deleting from the sum in (4.11) the term involving D_r in the modified complementary error function (see (3.4)) which corresponds to $n = n_*$. Thus, we write

$$E_m(t;N) = E_m^*(t;N) + (-)^{n_*} 2^{-\frac{1}{2}} e^{\frac{3}{4}\pi i} (\pi e^{\frac{1}{2}}/\omega)^s \sum_{r=0}^{m-1} \frac{(-)^r (\pi i/4)^r D_r}{(\frac{1}{2}\omega\eta_*)^{2r+1}} \tag{5.1}$$

where

$$E_m^*(t;N) = {\sum_{n=0}^{\infty}}' \epsilon_N n^{-s} \operatorname{erfc}(\tfrac{1}{2}\epsilon_N \eta_n \sqrt{s}; m) + \epsilon_N n_*^{-s} \operatorname{erfc}(\tfrac{1}{2}\epsilon_N \eta_* \sqrt{s}). \tag{5.2}$$

The prime on the summation sign denotes the deletion of the term corresponding to $n = n_*$, and, for simplicity in presentation, we write η_* and μ_* as the values of η_n and μ_n when $n = n_*$. The second term on the right-hand side of (5.1) is then combined with the sum involving $B_r(\omega)$ in (4.7) to yield the coefficients

$$B_r^*(\omega) = B_r(\omega) + (-)^{n_*+r} \frac{D_r}{(\frac{1}{2}\omega\eta_*)^{2r+1}}.$$

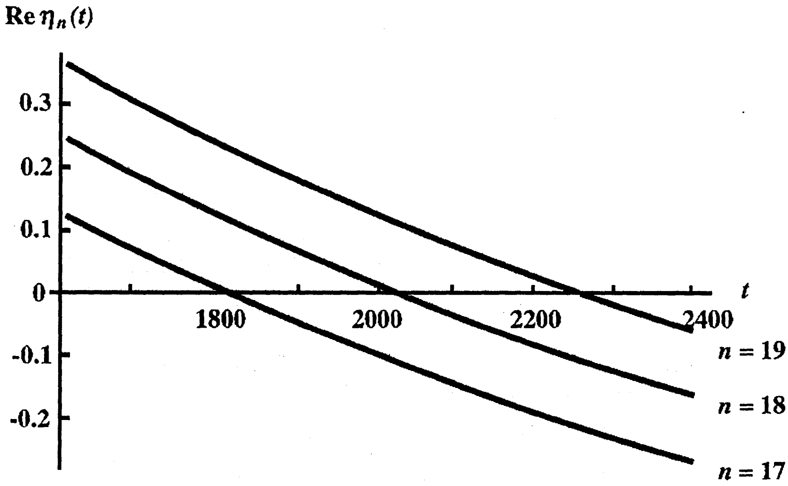

FIGURE 3. The behavior of the real part of $\eta_n(t)$ for $n = 17$, 18, and 19.

Using the definition of $c_r(\eta)$ in (3.2), we can rewrite the above relation as

$$B_r^*(\omega) = \hat{B}_r^*(\omega) + (-)^{n_*+r-1}(\tfrac{1}{2}\omega)^{-2r-1}c_r(\eta_*) \tag{5.3}$$

where

$$\hat{B}_r^*(\omega) = B_r(\omega) + (-)^{n_*}\frac{Q_r(\mu_*)}{(\frac{1}{2}\omega\mu_*)^{2r+1}} = \sum_{k=0}^{2r}(-)^k\alpha_k^{(r)}(\tfrac{1}{2}\omega)^{-k}S_{2r+1-k}^*(\omega). \tag{5.4}$$

The functions $S_k^*(\omega)$ are given by (4.3) with the deletion of the terms corresponding to $n = \pm n_*$ from the sum. Thus the coefficients $\hat{B}_r^*(\omega)$ are obtained from the same expression for $B_r(\omega)$ in (4.4), but with the sums $S_k(\omega)$ replaced by the deleted sums $S_k^*(\omega)$.

The expression for $Z(t)$ is then associated with the modified correction term

$$\operatorname{Re} e^{i\vartheta}\left\{E_m^*(t;N) + 2^{-\frac{1}{2}}e^{\frac{3}{4}\pi i}(\pi e^{\frac{1}{2}}/\omega)^s\left(\sum_{r=0}^{m-1}(\pi i/4)^r B_r^*(\omega) + \omega^{-2m+1}R_m\right)\right\}, \tag{5.5}$$

which replaces (4.12) and (4.7) for t values in the neighborhood of a discontinuity in N_t. An expression analogous to (4.9) with the modified coefficients $C_k^{*(m-1)}(\omega)$, where $C_k^{*(m-1)}(\omega)$ are given by (4.8) with $S_k(\omega)$ replaced by $S_k^*(\omega)$, can similarly be obtained. The calculation of the sums $S_k^*(\omega)$ can be achieved either by using higher-precision arithmetic or by writing $\omega = \pi n_* + \epsilon$ where $\epsilon = \epsilon(t)$ is a small (complex) variable in the neighborhood of the transition and employing a straightforward expansion in powers of ϵ. The coefficients $c_r(\eta_*)$ in (5.3) may be computed from the Maclaurin series $c_r(\eta) = \sum_{k=0}^{\infty}\beta_{rk}\eta^k$ for $|\eta| < 2\sqrt{\pi}$, where values of the coefficients β_{rk} are given in [13].

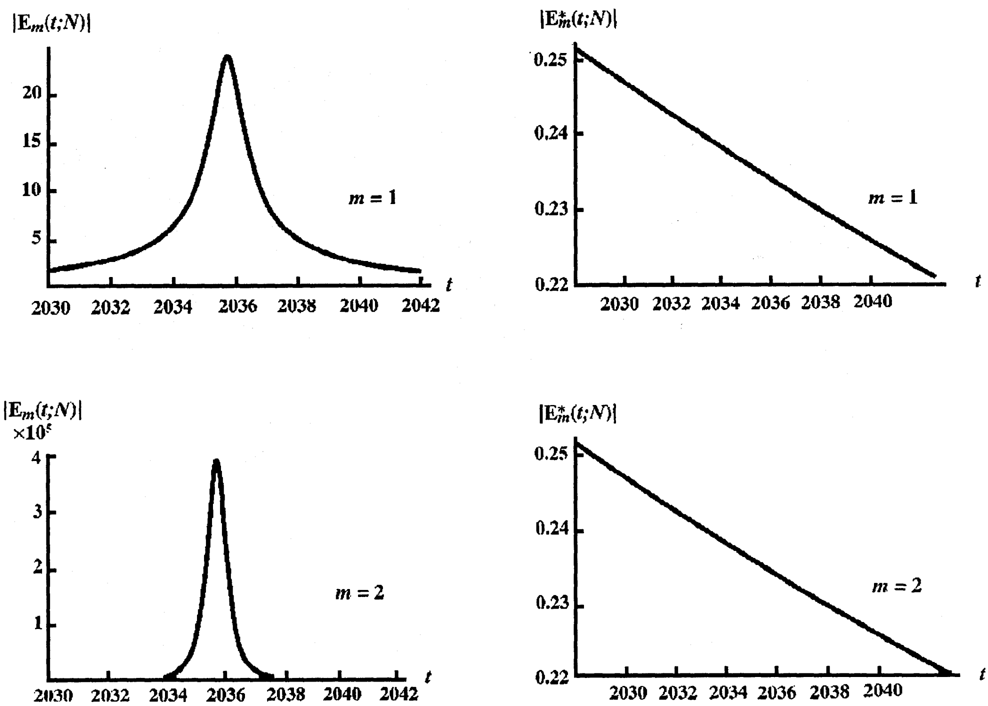

FIGURE 4. The behavior of $|E_m(t;N)|$ and $|E^*_m(t;N)|$ corresponding to $m = 1, 2$ when $n^* = N = 18$ for values of t near the critical value $t = 2\pi \times 18^2 \simeq 2035.75$.

Thus, if we wish to compute $Z(t)$ through a critical value, we set $n_* = N_t$, where N_t corresponds to the value of $\mathrm{Int}(t/2\pi)^{\frac{1}{2}}$ on the *right*-hand side of the discontinuity. Because N can be chosen arbitrarily in (4.12) and (5.5), we can fix N to be the value of N_t on either side: *it is not necessary to change N discontinuously as we pass through a critical t value.* To illustrate the formula (5.5), we first show in Figure 4 the behavior of the magnitudes of $E_m(t;N)$ and $E^*_m(t;N)$ when $m = 1, 2$ for values of t in the range containing the critical value $t = 2\pi \times 18^2 = 2035.75\ldots$ and $n_* = N = 18$. It is seen that without the deletion of the terms corresponding to $n_* = 18$, the sum $E_m(t;N)$ increases dramatically in the neighborhood of the critical value when $m = 2$ (a compensatory increase also occurs for the coefficients $B_r(\omega)$), while the modified sum $E^*_m(t;N)$ (and $B^*_r(\omega)$) remains $O(1)$ throughout this range. From numerical computations, it is found that it is better to employ (5.5) once $p(t)$ differs from 0 or 1 by about 0.05 (for $m \leq 5$). Table 4 illustrates the results of computing $Z(t)$ from (5.5) when $t = 2036$, which is very close to a critical value and corresponds to $p(t) \simeq 0.001$.

6. The late terms in the expansion (4.9)

Since $E_m(t;N)$ is an absolutely convergent sum, the divergence of the correction term in (4.9) as $m \to \infty$ must result from the divergence of the finite sum involving the

$t = 2036$ $Z(t) = -2.17639\ 46337\ 82407$ $N_t = 18$		
$p(t) = 0.00110$ $\vartheta = 4866.52819\ 80145\ 50511$		
$m = 1$		
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
15, 20	−2.17624 88970 97689	1.5×10^{-4}
10, 25	−2.17640 21868 15247	7.6×10^{-6}
5, 30	−2.17639 29879 43421	1.6×10^{-6}
1, 35	−2.17639 50679 45421	4.3×10^{-7}
$m = 2$		
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
15, 20	−2.17639 65132 11745	1.9×10^{-6}
10, 25	−2.17639 46210 91239	1.3×10^{-8}
5, 30	−2.17639 46348 48888	1.1×10^{-9}
1, 35	−2.17639 46335 90736	1.9×10^{-10}
$m = 3$		
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
15, 20	−2.17639 48212 47665	1.9×10^{-7}
10, 25	−2.17639 46335 74247	2.1×10^{-10}
5, 30	−2.17639 46337 89532	7.1×10^{-12}
1, 35	−2.17639 46337 81708	7.0×10^{-13}
$m = 4$		
n_1, n_2	Z_{approx}	$\lvert Z - Z_{approx}\rvert$
15, 20	−2.17639 46275 48719	6.2×10^{-9}
10, 25	−2.17639 46337 83343	9.4×10^{-13}
5, 30	−2.17639 46337 82449	4.2×10^{-14}
1, 35	−2.17639 46337 82404	3.1×10^{-15}

TABLE 4. Computation of $Z(t)$ near a critical value using (5.5).

coefficients $C_k^{(m-1)}(\omega)$. In this section, we shall examine the large-m behavior of these coefficients to determine the nature of this divergence. For convenience in presentation, we shall replace m by $m+1$, so that the sum we shall consider is

$$\sum_{k=0}^{2m}(-\omega)^{-k}C_k^{(m)}(\omega) \tag{6.1}$$

where $C_k^{(m)}(\omega)$ are defined in (4.8).

The determination of the leading behavior of the late terms ($m \gg 1$) in (6.1) is greatly facilitated by a remarkable property of the coefficients $C_k^{(m)}(\omega)$: namely, *their structure becomes simpler as the index k increases.* For example, the last two coefficients with $k = 2m$ and $k = 2m-1$ both consist of only a single term given by

$$C_{2m}^{(m)}(\omega) = (-)^m\gamma_m(\pi i)^m S_1(\omega), \qquad C_{2m-1}^{(m)}(\omega) = (-)^{m-1}\gamma_{m-1}(\pi i)^m S_2(\omega)/2$$

where we have employed the identities $\alpha_{2m}^{(m)} = (-)^m\gamma_m$, $\alpha_{2m-1}^{(m)} = (-)^{m-1}\gamma_{m-1}$; see (A.2). From the asymptotic behavior of the Stirling coefficients γ_r for large r in (A.4), it then immediately follows that, as $m \to \infty$,

$$\omega^{-2m} C_{2m}^{(m)}(\omega) \sim \begin{cases} i\dfrac{\Gamma(m)}{(\pi t)^m} \mathcal{A}_0 S_1(\omega) & (m \text{ odd}) \\ \dfrac{\Gamma(m-1)}{(\pi t)^m} \mathcal{B}_0 S_1(\omega) & (m \text{ even}) \end{cases} \tag{6.2}$$

$$\omega^{-2m+1} C_{2m-1}^{(m)}(\omega) \sim \begin{cases} -\dfrac{\pi i}{\sqrt{2}} \dfrac{\Gamma(m-2)}{(\pi t)^{m-1/2}} \mathcal{B}_1 S_2(\omega) & (m \text{ odd}) \\ \dfrac{\pi}{\sqrt{2}} \dfrac{\Gamma(m-1)}{(\pi t)^{m-1/2}} \mathcal{A}_1 S_2(\omega) & (m \text{ even}) \end{cases} \tag{6.3}$$

where the constants $\mathcal{A}_p$, $\mathcal{B}_p$ are defined in (A.7), with $\mathcal{A}_0 = -\mathcal{A}_1 = 1/\pi$ and $\mathcal{B}_0 = -\mathcal{B}_1 = -1/6$.

The remaining higher-order terms can be similarly estimated by employing in (4.8) the asymptotic behavior of the coefficients $\alpha_{2r-p}^{(r)}$ for $r \gg 1$ with $p = 0, 1, 2, \ldots$, given in (A.6). If we define the functions

$$F_{1,2}^{(e)}(k,\omega) = \sum_{j=0}^{k} (-\pi i/4)^j \begin{Bmatrix} i\mathcal{A}_{2j} \\ \mathcal{B}_{2j} \end{Bmatrix} S_{2j+1}(\omega), \tag{6.4}$$

$$F_{1,2}^{(o)}(k,\omega) = \frac{\pi}{\sqrt{2}} \sum_{j=0}^{k} (-\pi i/4)^j \begin{Bmatrix} \mathcal{A}_{2j+1} \\ -i\mathcal{B}_{2j+1} \end{Bmatrix} S_{2j+2}(\omega) \tag{6.5}$$

where the subscripts 1 or 2 correspond to the sum involving the coefficients $\mathcal{A}_p$ or $\mathcal{B}_p$ respectively, the leading behavior of the coefficients $\omega^{-2m+M} C_{2m-M}^{(m)}(\omega)$ for $M = 0, 1, 2, \ldots$ when $m \to \infty$ is summarised in Table 5. It is seen that the form of the leading approximation to these coefficients depends not only on the parity of m but also on the value of M (modulo 4).

	$M = 4p$	$M = 4p+1$
m odd	$\dfrac{\Gamma(m-2p)}{(\pi t)^{m-2p}} F_1^{(e)}(2p,\omega)$	$\dfrac{\Gamma(m-2p-2)}{(\pi t)^{m-2p-1/2}} F_2^{(o)}(2p,\omega)$
m even	$\dfrac{\Gamma(2m-2p-1)}{(\pi t)^{m-2p}} F_2^{(e)}(2p,\omega)$	$\dfrac{\Gamma(m-2p-1)}{(\pi t)^{m-2p-1/2}} F_1^{(o)}(2p,\omega)$
	$M = 4p+2$	$M = 4p+3$
m odd	$\dfrac{\Gamma(m-2p-2)}{(\pi t)^{m-2p-1}} F_2^{(e)}(2p+1,\omega)$	$\dfrac{\Gamma(m-2p-2)}{(\pi t)^{m-2p-3/2}} F_1^{(o)}(2p+1,\omega)$
m even	$\dfrac{\Gamma(m-2p-1)}{(\pi t)^{m-2p-1}} F_1^{(e)}(2p+1,\omega)$	$\dfrac{\Gamma(m-2p-3)}{(\pi t)^{m-2p-3/2}} F_2^{(o)}(2p+1,\omega)$

TABLE 5. The leading behavior of the coefficients $\omega^{-k} C_k^{(m)}(\omega)$ for $m \to \infty$ where $k = 2m - M$, $M = 4p + j$ $(j = 0, 1, 2, 3)$ and $p = 0, 1, 2, \ldots$.

Thus the expansion (6.1) is divergent and possesses the "factorial divided by a power" dependence characteristic of an asymptotic series. Optimal truncation near the smallest term of this expansion is then seen to correspond to approximately $m = \mathrm{Int}(\pi t)$. The leading behavior of these coefficients is multiplied by the factors $F_{1,2}^{(e,o)}$, which consist of slowly oscillatory functions involving cosec ω and its derivatives. A similar result recently has been derived for the Riemann-Siegel expansion by Berry [1] using formal arguments.

In the neighborhood of a discontinuity in N_t, we saw in §5 that it was preferable to employ a different regrouping of the terms to yield the expansion (5.5). This expansion involves the coefficients $B_r^*(\omega)$, which are given in terms of $\hat{B}_r^*(\omega)$ and $c_r(\eta_*)$. The divergence of this form of the expansion likewise is found to be of a similar character. This follows by first observing that, from (5.4), the late terms in the series in (5.5) resulting from $\hat{B}_r^*(\omega)$ will evidently possess the same behavior as that given in Table 5, except that $S_k(\omega)$ is replaced by the deleted sums $S_k^*(\omega)$. And secondly, the higher-order behavior of the contribution to (5.5) from the coefficients $c_r(\eta_*)$ is proportional to $\{\Gamma(r+\frac{1}{2})/(\pi t)^{r+1/2}\}f_r(\eta_*)$ $(r \gg 1)$ since the coefficients $c_r(\eta)$ in the expansion of the incomplete gamma function behave like

$$c_r(\eta) \sim \frac{\Gamma(r+\frac{1}{2})}{(2\pi)^{r+1}} f_r(\eta)$$

for $r \to \infty$, where $f_r(\eta)$ (which we do not specify here) is a slowly varying function of η close to the real η-axis [5].

7. Concluding remarks

The principal result of this paper is the representation of $Z(t)$ for large t in (4.6), or equivalently, in (4.12). This asymptotic approximation, which is derived from the expansion of $\zeta(s)$ in terms of incomplete gamma functions in (2.5), consists of the original Dirichlet series defining $\zeta(s)$ in $\mathrm{Re}(s) > 1$ smoothed by a (modified) complementary error function together with a correction term. The correction term involves an expansion in descending powers of $\omega \simeq \pi(t/2\pi)^{\frac{1}{2}}$ multiplied by a factor of $O(t^{-\frac{1}{4}})$. The coefficients in this expansion can be given explicitly to any order in terms of cosec ω and its derivatives and are easier to compute than those given in [10]. In addition, it is found that there is an intimate connection between these coefficients and certain coefficients appearing in the uniform asymptotics of the incomplete gamma function. The numerical results in §4 reveal that, with a little additional computational effort, the expansion (4.6) is more accurate than the Riemann-Siegel formula and yields an accuracy comparable to other recent expansions given in [2, 10].

The expansion for $\zeta(s)$ in (2.4) in terms of the normalized incomplete gamma function $Q(a,z)$ has been generalized in two ways. First, an expansion in which a is a free real parameter is considered in [12]. Suitable choice of a then produces an expansion for $\zeta(s)$ in which the main sum consists of the original Dirichlet series smoothed either by the simple Gaussian exponential factor $\exp(-n^2/N^2)$ or a complementary error function of real argument $\mathrm{erfc}(n/N)$ where N is a positive number. For the correction term in these expansions to possess an asymptotic character, however, the "cut-off" in the main sum has to occur after $O(t/2\pi)$ terms, so that this simple smoothing of the Dirichlet sum results in formulas of the computationally less powerful Gram-type.

The second generalization of (2.4) allows for a dependence of the argument z on n which is stronger than the quadratic scaling in (2.4), i.e., we take z to scale like n^{2p}, with $p \geq 1$. This is carried out in [11] in an attempt to reduce the number of terms in the associated computationally-expensive main sum. It is shown that, provided $s \neq 1$,

$$\zeta(s) = \frac{\pi^{\frac{1}{2}s}}{\Gamma(\frac{s}{2p})}\xi^{s/2p}\Big(\frac{\Gamma(\frac{1}{2p})\xi^{-1/2p}}{\pi^{\frac{1}{2}}(s-1)} - \frac{p}{s}\Big) + \sum_{n=1}^{\infty} n^{-s} \mathcal{Q}\Big(\frac{s}{2p}, \pi^p n^{2p}\xi\Big)$$
$$+ \chi(s)\sum_{n=1}^{\infty} n^{s-1}\mathcal{Q}_p\Big(\frac{1-s}{2p}, \frac{\pi^p n^{2p}}{\xi}\Big) \tag{7.1}$$

where $p = 1, 2, \ldots$, $|\arg\xi| \leq \frac{1}{2}\pi$, and $\mathcal{Q}_p(a,z)$ is a generalized incomplete gamma function defined by

$$\mathcal{Q}_p(a,z) = \frac{\Gamma(\frac{1}{2} - ap)}{p\Gamma(ap)\Gamma(\frac{1}{2p} - a)}\int_z^{\infty} u^{a-1}F_p(u)\,du$$

with $F_p(u)$ denoting the generalized hypergeometric function

$$F_p(u) = \sum_{k=0}^{\infty}(-)^k \frac{\Gamma(\frac{k}{p} + \frac{1}{2p})}{k!\,\Gamma(k+\frac{1}{2})}u^{k/p}, \qquad |u| < \infty.$$

When $p = 1$, we have $F_1(u) = e^{-u}$ and $\mathcal{Q}_1(a,z) \equiv Q(a,z)$, so that (7.1) reduces to (2.4). When $\arg\xi = \frac{1}{2}\pi$, the "cut-offs" in the two sums in (7.1) on the critical line $s = \frac{1}{2} + it$ are found to occur approximately when n equals

$$n_1^* \simeq (p\pi^{p-1}/|\xi|)^{-1/2p}(|\xi|t/2\pi)^{1/2p}, \quad n_2^* \simeq (p\pi^{p-1}/|\xi|)^{1/2p}(t/2\pi)^{1-1/2p},$$

respectively. For $p > 1$, we consequently find $n_1^* \ll N_t$ while $n_2^* \gg N_t$ for fixed $|\xi|$ as $t \to \infty$. This imbalance in the values of n_1^* and n_2^* can be restored by allowing ξ to scale like a positive power of t. Then the optimal situation, corresponding to the cut-offs occurring for the same value of n, yields $n_1^* \simeq n_2^* \simeq (t/2\pi)^{\frac{1}{2}}$. Thus, it does not appear possible to simultaneously reduce *both* n_1^* and n_2^* below the value N_t, thereby thwarting any hope of reducing the number of terms in the main sum associated with the generalized expansion (7.1).

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Appendix A. The asymptotic behavior of the coefficients $\alpha_{2r-p}^{(r)}$ for $p = 0, 1, 2, \ldots$ and $r \gg 1$.

In this appendix, we examine the large-r behavior of the coefficients $\alpha_k^{(r)}$ appearing in the polynomial $Q_r(\mu)$ in (3.4) when $k = 2r - p$, $p = 0, 1, 2, \ldots$. Substitution of (3.2) into the relation [13] satisfied by the $c_r(\eta)$

$$c_0(\eta) = \frac{1}{\mu} - \frac{1}{\eta}, \qquad c_r(\eta) = \frac{1}{\eta}\frac{d}{d\eta}c_{r-1}(\eta) + \frac{\gamma_r}{\mu}, \quad r \geq 1,$$

where the Stirling coefficients γ_r are defined in (3.7), shows that $Q_r(\mu)$ satisfies the recursion

$$Q_r(\mu) = (1+\mu)\left\{(2r-1)Q_{r-1}(\mu) - \mu\frac{dQ_{r-1}(\mu)}{d\mu}\right\} + (-)^r\gamma_r\mu^{2r}, \quad r \geq 1 \tag{A.1}$$

with $Q_0(\mu) = 1$. It then follows that the coefficients $\alpha_k^{(r)}$, $k = 2r - p$ are defined by the recurrence relation

$$\begin{aligned} \alpha_{2r-p}^{(r)} &= (p-1)\alpha_{2r-p}^{(r-1)} + p\alpha_{2r-p-1}^{(r-1)}, \qquad 1 \leq p \leq 2r, \\ \alpha_{2r}^{(r)} &= (-)^r\gamma_r \end{aligned} \tag{A.2}$$

where $\alpha_{-1}^{(r)}$ is to be interpreted as zero. The coefficients $\alpha_k^{(r)}$ are presented in Table 6 for $0 \leq k \leq 12$; recurrence relations equivalent to (A.2) for these coefficients can be found in [13].

$r=0$	$k=0$ 1						
$r=1$	$k=0$ 1	$k=1$ 1	$k=2$ $\frac{1}{12}$				
$r=2$	$k=0$ 3	$k=1$ 5	$k=2$ $\frac{25}{12}$	$k=3$ $\frac{1}{12}$	$k=4$ $\frac{1}{288}$		
$r=3$	$k=0$ 15	$k=1$ 35	$k=2$ $\frac{105}{4}$	$k=3$ $\frac{77}{12}$	$k=4$ $\frac{49}{288}$	$k=5$ $\frac{1}{288}$	$k=6$ $\frac{-139}{51840}$
$r=4$	$k=0$ 105	$k=1$ 315	$k=2$ $\frac{1365}{4}$	$k=3$ $\frac{1883}{12}$	$k=4$ $\frac{2513}{96}$	$k=5$ $\frac{149}{288}$	$k=6$ $\frac{221}{51840}$
	$k=7$ $\frac{-139}{51840}$	$k=8$ $\frac{-571}{2488320}$					
$r=5$	$k=0$ 945	$k=1$ 3465	$k=2$ $\frac{19635}{4}$	$k=3$ $\frac{13321}{4}$	$k=4$ $\frac{102949}{96}$	$k=5$ $\frac{38291}{288}$	$k=6$ $\frac{35981}{17280}$
	$k=7$ $\frac{77}{10368}$	$k=8$ $\frac{-2783}{497664}$	$k=9$ $\frac{-571}{2488320}$	$k=10$ $\frac{163879}{209018880}$			
$r=6$	$k=0$ 10395	$k=1$ 45045	$k=2$ $\frac{315315}{4}$	$k=3$ $\frac{283283}{4}$	$k=4$ $\frac{3278275}{96}$	$k=5$ $\frac{797225}{96}$	$k=6$ $\frac{2792933}{3456}$
	$k=7$ $\frac{108251}{10368}$	$k=8$ $\frac{715}{55296}$	$k=9$ $\frac{-42887}{2488320}$	$k=10$ $\frac{67951}{209018880}$	$k=11$ $\frac{163879}{209018880}$	$k=12$ $\frac{5246819}{75246796800}$	

TABLE 6. The coefficients $\alpha_k^{(r)}$ $(0 \leq k \leq 2r)$ for $0 \leq k \leq 12$.

An examination of the recurrence relation (A.2) reveals that $\alpha_{2r-p}^{(r)}$ $(0 \leq p \leq 2r)$ can be expressed as a linear combination of the Stirling coefficients $\gamma_\kappa, \gamma_{\kappa-1}, \ldots, \gamma_{r-p}$ where κ denotes the integer

$$\kappa = r - \operatorname{Int}\left(\frac{p+1}{2}\right), \tag{A.3}$$

and γ_j is to be interpreted as zero for $j < 0$. From the well-known asymptotics of γ_r for $r \to \infty$ (see [3] and [4, p.159])

$$\gamma_r \sim \begin{cases} \dfrac{1}{\pi}(-)^{(r+1)/2}\dfrac{\Gamma(r)}{(2\pi)^r} & (r \text{ odd}), \\ -\dfrac{1}{6}(-)^{r/2}\dfrac{\Gamma(r-1)}{(2\pi)^r}, & (r \text{ even}), \end{cases} \tag{A.4}$$

it then follows that the large-r behavior of $\alpha_{2r-p}^{(r)}$ is determined by the Stirling coefficients with the largest indices. Thus we can express $\alpha_{2r-p}^{(r)}$ in the form

$$\alpha_{2r-p}^{(r)} \sim (-)^r(a_p\gamma_\kappa + b_p\gamma_{\kappa-1} + \cdots), \qquad r \to \infty, \quad p = 0, 1, 2, \ldots \tag{A.5}$$

where the constants a_p, b_p are independent of r; see Table 7.

p	0	1	2	3	4	5	6	7	8	9	10
a_p	1	−1	−1	5	3	−35	−15	315	105	−3465	−945
b_p	0	0	2	−6	−26	154	340	−3304	−4900	70532	78750

TABLE 7. Values of the constants a_p and b_p for $0 \le p \le 10$.

Use of (A.4) in (A.5) then shows that

$$(-)^r\alpha_{2r-p}^{(r)} \sim \begin{cases} \mathcal{A}_p(-)^{(\kappa+1)/2}\dfrac{\Gamma(\kappa)}{(2\pi)^\kappa} & (\kappa \text{ odd}) \\ \mathcal{B}_p(-)^{\kappa/2}\dfrac{\Gamma(\kappa-1)}{(2\pi)^\kappa} & (\kappa \text{ even}) \end{cases} \tag{A.6}$$

as $r \to \infty$ with $p = 0, 1, 2, \ldots$, where

$$\mathcal{A}_p = \frac{a_p}{\pi}, \qquad \mathcal{B}_p = 2b_p - \frac{a_p}{6}. \tag{A.7}$$

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Division of Mathematical Sciences, University of Abertay Dundee, Dundee DD1 1HG, UK
E-mail: R.Paris@TAY.AC.UK