

The Riemann–Siegel expansion for the zeta function: high orders and remainders

BY M. V. BERRY

H. H. Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

On the critical line $s = \frac{1}{2} + it$ (t real), Riemann's zeta function can be calculated with high accuracy by the Riemann–Siegel expansion. This is derived here by elementary formal manipulations of the Dirichlet series. It is shown that the expansion is divergent, with the high orders r having the familiar 'factorial divided by power' dependence, decorated with an unfamiliar slowly varying multiplier function which is calculated explicitly. Terms of the series decrease until $r = r^* \approx 2\pi t$ and then increase. The form of the remainder when the expansion is truncated near r^* is determined; it is of order $\exp(-\pi t)$, indicating that the critical line is a Stokes line for the Riemann–Siegel expansion. These conclusions are supported by computations of the first 50 coefficients in the expansion, and of the remainders as a function of truncation for several values of t .

1. Introduction

The Riemann–Siegel series, deciphered by Siegel in the 1920s from Riemann's manuscripts of the 1850s, is a very accurate and widely used method of calculating Riemann's function $\zeta(s)$ on the critical line (Edwards 1974). My aim here is to understand the structure of the series. By 'understanding' I mean three things; first, devising a transparent formalism for obtaining the terms in the expansion, enabling high orders to be calculated; second, establishing the dominant behaviour of the high orders; and third, estimating the dependence of the truncation error on the order of truncation when this is large, and thence the ultimate accuracy that can be obtained with the method. The latter is particularly interesting in view of the recent development of alternative methods for calculating ζ to high accuracy (Berry & Keating 1992; Paris 1994).

On the critical line $s = \frac{1}{2} + it$ (t real), $\zeta(s)$ is complex. However, it follows from the functional equation for $\zeta(s)$ that the function

$$Z(t) = \exp(i\theta(t))\zeta(\tfrac{1}{2} + it), \quad (1)$$

where

$$\theta(t) = \arg \Gamma(\tfrac{1}{4} + \tfrac{1}{2}it) - \tfrac{1}{2}t \log \pi \quad (2)$$

is real for real t (and also even). The Riemann–Siegel series is an expansion of $Z(t)$ for large t , whose starting-point is the separation of this function into a 'main sum' plus a remainder. It is convenient first to define

$$a \equiv \sqrt{(t/2\pi)}, \quad N \equiv \text{Int}(a), \quad a - N \equiv \tfrac{1}{2}(1 - z). \quad (3)$$

Then the separation is

$$Z(t) = 2 \sum_{n=1}^N \frac{\cos(\theta(t) - t \log n)}{n^{1/2}} + R(t). \quad (4)$$

The remainder $R(t)$ can be written as a formal power series in $1/a$, namely

$$R(t) = \frac{(-1)^{N+1}}{a^{1/2}} \sum_{r=0}^{\infty} \frac{C_r(z)}{a^r}. \quad (5)$$

This is the Riemann–Siegel expansion, whose coefficients $C_r(z)$ will be our principal concern. In correcting the main sum, the expansion removes the discontinuities where the upper limit jumps, that is at $t = 2\pi N^2$ (N integer), and interpolates between these points: as t increases from $2\pi N^2$ to $2\pi(N+1)^2$, z decreases from 1 to -1 , with $z = 0$ corresponding to points $2\pi(N + \frac{1}{2})^2$.

Riemann's technique for obtaining the coefficients $C_r(z)$ (explained for example by Edwards (1974) and Titchmarsh (1986)) is an intricate application of the saddle-point method to an integral representation of $Z(t)$, with the subtlety that the saddle lies on a line containing a string of poles. By contrast, the formalism I use in §2 is wholly elementary and based on the Dirichlet series $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ ($\text{Re } s > 1$). Since this series does not converge on the critical line, the method is formal and so cannot be regarded as a substitute for the customary derivation which gives the same results. However, the method has the advantages of exposing the essential algebra of the expansion, in a way that enables new results to be found later, and of generating a series for $Z(t)$ that is automatically real in spite of not explicitly using the functional equation. The coefficient $C_r(z)$ involves derivatives (up to the 3rd) of the function

$$F(z) = \frac{\cos(\frac{1}{2}\pi(z^2 + \frac{3}{4}))}{\cos(\pi z)}. \quad (6)$$

In §3 the elementary formalism is used to calculate high orders of the expansion, that is $C_r(z)$ for large r . The main result is

$$C_r(z) = \frac{\Gamma(\frac{1}{2}r)}{(\pi\sqrt{2})^{r+1}} f(r, z), \quad (7)$$

where f is bounded and given by the rapidly convergent series

$$f(r, z) \approx \sum_{m=0}^{\infty} (-1)^{m(m-1)/2} \exp\{-(m + \frac{1}{2})^2\} \\ \times \begin{cases} \sin\{(2m+1)\sqrt{r}\} \cos\{(m + \frac{1}{2})\pi z\} & (r \text{ even}) \\ \cos\{(2m+1)\sqrt{r}\} \sin\{(m + \frac{1}{2})\pi z\} & (r \text{ odd}) \end{cases} \quad \text{when } r \gg 1. \quad (8)$$

These formulae show that the Riemann–Siegel expansion (5) diverges, with the divergence dominated by the ‘factorial divided by a power’ typical of asymptotic series. For large t the terms in (5) get smaller before they increase, with the minimum near $r = r^* = \text{Int}(2\pi t)$. This familiar divergence is multiplied by the factor $f(r, z)$, whose oscillations are slow in comparison with the growth of $\Gamma(\frac{1}{2}z)$. Therefore the expansion falls in the class of ‘decorated factorial series’ now beginning to be encountered in asymptotics; another example is saddle-point expansions whose divergence is dom-

inated by coalescing distant saddles (Berry & Howls 1993). In the Riemann–Siegel case, however, the decoration f has an unfamiliar form.

These results are used in §4 to estimate the remainder when the Riemann–Siegel series is truncated at some large order R . The remainder is $S_R(t)$, where

$$R(t) = \frac{(-1)^{N+1}}{a^{1/2}} \sum_{r=0}^R \frac{C_r(z)}{a^r} + S_R(t). \quad (9)$$

I give two heuristic arguments leading to the expectation that $S_R(t)$ is of order $\exp(-\pi t)$. Then a direct calculation, using a variant of Borel summation, gives

$$S_R(t) \approx \frac{(-1)^N e^{-\pi t}}{a^{1/2} \sqrt{2}} \left\{ \left[-i \operatorname{erf}(i\sigma) + \frac{1}{3\sqrt{(\pi R)}} (4\sigma^2 + \tfrac{1}{2}) e^{\sigma^2} \right] [f(R+2, z) + f(R+1, z)] \right. \\ \left. + \frac{1}{2\sqrt{(\pi R)}} e^{\sigma^2} [f(R+2, z) - f(R+1, z)] \right\}, \quad (10)$$

where

$$\sigma = (\tfrac{1}{2}R - \pi t)/\sqrt{R}. \quad (11)$$

Optimal truncation, that is truncation of the Riemann–Siegel series near $R = r^*$ (where $\sigma \approx 0$), thus yields an error of the expected order $\exp(-\pi t)$. This shows that the Riemann–Siegel expansion is less accurate than that of Berry & Keating (1992), whose error is bounded by $\exp(-t^{4/3})$ (now we conjecture that this can be reduced to $\exp(-t^2)$).

The arguments leading to the asymptotic formulae (7) and (10) are formal and non-rigorous, so it is desirable to test them by comparison with direct calculations of the $C_r(z)$ and the remainders $S_R(t)$. This requires high derivatives of $F(z)$ (equation (6)), which are difficult to evaluate. In §5 methods are given for evaluating these derivatives exactly for the special cases $z = 0$, $z = \pm \frac{1}{2}$ and $z = \pm 1$ (§5a), and asymptotically for any z (§5b).

In §6a numerical comparisons are given between the first 50 ‘experimental’ Riemann–Siegel coefficients $C_r(z)$ and the ‘theoretical’ prediction (7) and (8) for a range of z values. The theory works very well, with the decoration $f(r, z)$ reproducing fine details of the coefficients, even for r as small as 5. In §6.2 comparisons are given between the ‘experimental’ and ‘theoretical’ remainders $S_R(t)$ as functions of truncation R , for several values of t . The theoretical formula (10) passes this highly discriminating test very well. It shows that the Riemann–Siegel formula is capable of astonishing accuracy, even for $t < 2\pi$, when there are no terms in the main sum (i.e. $N = 0$ in (4)). For example, when $t = \pi$ the Riemann–Siegel series (5) starts to diverge when $r \approx 20$ and can generate $Z(t)$ to one part in 10^5 . All computations were carried out using MATHEMATICA (Wolfram 1991).

In previous numerical applications (e.g. computations of the zeros by Brent (1979), van de Lune *et al.* (1986), Odlyzko (1987, 1990), Odlyzko & Schönhage (1988)), only a few terms of the Riemann–Siegel series were needed, and the questions addressed here, of the asymptotics for large r , did not arise. The most extensive theoretical study of the Riemann–Siegel formula was by Gabcke (1979). He gave explicit formulae for the $C_r(z)$ for $r \leq 12$, and derived strict (and realistic) error bounds for the $S_R(t)$ for $R \leq 10$ (e.g. $|S_{10}(t)| < 25\,966t^{-23/4}$). He speculated that the series diverges, and proved this for the special case of the coefficients $C_{2m}(1)$, using a direct method (Appendix B) that sidesteps the complications of the general formalism. We explore this further in Appendix D by determining the explicit form of these partic-

ular coefficients for $2m$ large (using a result about asymptotic series established in Appendix C). As it turns out, this special case is misleading, in the sense that the divergence of the $C_{2m}(1)$ is weaker than in the general case and is not captured by the leading-order theory (indeed (8) predicts zero for $C_{2m}(1)$).

2. Derivation of the series

In the function defined by (1) we can formally substitute the Dirichlet series for $\zeta(s)$, and obtain

$$Z(t) = \exp(i\theta(t)) \sum_{n=1}^{\infty} \frac{\exp(-it \log n)}{n^{1/2}}. \quad (12)$$

The sum does not converge and its terms are not real. However, we note that the main sum in (4) comprises the first N terms of the Dirichlet series, together with their complex conjugates. (These complex conjugate terms can be obtained (Berry 1986; Titchmarsh 1986) from the resummation of the divergent tail of (12).) Thus the remainder in (4) can be written as

$$R(t) = \sum_{n=N+1}^{\infty} \frac{\exp\{i[\theta(t) - t \log n]\}}{n^{1/2}} - \sum_{n=1}^N \frac{\exp\{-i[\theta(t) - t \log n]\}}{n^{1/2}}. \quad (13)$$

The Riemann–Siegel expansion (5) will be obtained by expanding the terms in the two sums about the limits $N+1$ and N . This ingenious procedure, devised by Keating (1993) to calculate the lowest coefficient $C_0(z)$, will be the basis of all that follows.

To obtain the expansion, it is necessary to make use of the asymptotic expansion of $\theta(t)$. Gabcke (1979) shows from (2) that

$$\theta(t) = \frac{1}{2}t(\log(t/\pi) - 1) - \frac{1}{8}\pi + \chi(t), \quad (14)$$

where $\chi(t)$ has the formal expansion

$$\chi(t) = \sum_{m=1}^{\infty} \frac{b_m}{t^{2m-1}}, \quad \text{where } b_m = \frac{(2^{2m-1} - 1)|B_{2m}|}{2^{2m+1}m(2m-1)}, \quad (15)$$

in which B_{2m} are the Bernoulli numbers. For the first sum in (13), we define the new variable K by

$$n = N + 1 + K = a(1 + Q(K, z)/a), \quad 0 \leq K \leq \infty, \quad (16)$$

where a and z are defined in (3) and

$$Q(K, z) \equiv \frac{1}{2}(1 + z) + K. \quad (17)$$

The analogous definition for the second sum is

$$n = N - K = a(1 - Q(K, -z)/a), \quad 0 \leq K \leq N - 1. \quad (18)$$

Now the phase in the first sum in (13) is expanded using (14) and (16). A short calculation gives

$$\begin{aligned} [\theta(t) - t \log n]_{(\text{mod } 2\pi)} &= (N + 1 + K)\pi + \frac{3}{8}\pi + \chi(2\pi a^2) - \frac{1}{2}\pi z^2 \\ &\quad + 2\pi z Q(K, z) + 2\pi a^2 \sum_{m=3}^{\infty} \frac{1}{m} \left(-\frac{Q(K, z)}{a} \right)^m. \end{aligned} \quad (19)$$

With these substitutions, the first sum in (13) becomes

$$\frac{(-1)^{N+1}}{a^{1/2}} T(a, z), \quad (20)$$

where

$$T(a, z) = \exp\left\{i\pi\left(\frac{3}{8} - \frac{1}{2}z^2\right) + i\chi(2\pi a^2)\right\} \\ \times \sum_{K=0}^{\infty} (-1)^K \frac{\exp\{i\pi Q(K, z)(2z + 2a - Q(K, z))\}}{(1 + Q(K, z)a)^{1/2+2\pi ia^2}}. \quad (21)$$

The second sum in (13) is given by a similar expression with the upper limit replaced by $K = N - 1$. This upper limit plays no part in the Riemann–Siegel expansion, and will henceforth be replaced by $K = \infty$ (this amounts to including terms with negative n in the second sum in (13), a point to which we will return). Thus we find

$$R(t) = \frac{(-1)^{N+1}}{a^{1/2}} [T(a, z) + T^*(-a, -z)]. \quad (22)$$

To generate the Riemann–Siegel expansion (5), it is necessary to expand T in powers of $1/a$, i.e.

$$T(a, z) = \sum_{r=0}^{\infty} \frac{T_r(z)}{a^r}. \quad (23)$$

Then the Riemann–Siegel coefficients are

$$C_r(z) = T_r(z) + (-1)^r T_r^*(-z). \quad (24)$$

We shall find that $T_r(-z) = (-1)^r T_r(z)$; thus the $C_r(z)$ are real, as they must be, and satisfy the symmetry relation

$$C_r(-z) = (-1)^r C_r(z). \quad (25)$$

The lowest coefficient is obtained directly from (21) (Keating 1993) as

$$C_0(z) = 2 \operatorname{Re} \left\{ \exp\left\{i\pi\left(\frac{3}{8} - \frac{1}{2}z^2\right)\right\} \sum_{K=0}^{\infty} (-1)^K \exp\{2i\pi Q(K, z)z\} \right\} \\ = \cos\left\{\frac{1}{2}\pi(z^2 + \frac{3}{4})\right\} / \cos(\pi z) \equiv F(z). \quad (26)$$

To get the general term in the expansion, it is convenient to use the operator notation

$$D \equiv \frac{\partial}{\partial z} \quad (27)$$

to bring (21) to a symbolic form where the K sum is the same as that in (26), namely

$$T(a, z) = \exp\left\{i\pi\left(\frac{3}{8} - \frac{1}{2}z^2\right) + i\chi(2\pi a^2)\right\} \\ \times \frac{\exp\{aD + iD^2/4\pi\}}{(1 + D/2\pi ia)^{1/2+2\pi ia^2}} \sum_{K=0}^{\infty} (-1)^K \exp\{2i\pi Qz\}. \quad (28)$$

Thus

$$T(a, z) = \exp\left\{i\pi\left(\frac{3}{8} + \frac{1}{2}z^2\right)\right\} \\ \times \exp(-i\pi z^2) \left[\left\{ \frac{\exp\{i\chi(2\pi a^2) + aD + iD^2/4\pi\}}{(1 + D/2\pi ia)^{1/2+2\pi ia^2}} \right\} \frac{\exp(i\pi z\zeta)}{2 \cos(\pi z)} \right]_{\zeta \rightarrow z}. \quad (29)$$

The operator in braces has an expansion in $1/a$ and D . It is easier to find this if the function is real, which we achieve with new variables x and y defined by

$$a \equiv (1/2y)\sqrt{(i/2\pi)}, \quad D \equiv \frac{1}{2}x\sqrt{(2\pi/i)}. \quad (30)$$

Then

$$\begin{aligned} & \left\{ \frac{\exp\{i\chi(2\pi a^2) + aD + iD^2/4\pi\}}{(1 + D/2\pi ia)^{1/2+2\pi ia^2}} \right\} \equiv g(x, y) \\ &= \frac{1}{(1 - xy)^{1/2-1/4y^2}} \exp\left\{i\chi\left(\frac{i}{4y^2}\right) + \frac{x}{4y} + \frac{x^2}{8}\right\} \\ &= \exp\left\{-\sum_{m=1}^{\infty} (-1)^m b_m (4y^2)^{2m-1} + \sum_{m=1}^{\infty} (xy)^m \left(\frac{1}{2m} - \frac{x^2}{4(m+2)}\right)\right\}. \end{aligned} \quad (31)$$

This has an expansion in powers of x and y , with the term in y^r multiplied by x^{3r} , x^{3r-2} , etc.:

$$g(x, y) = \sum_{r=0}^{\infty} \sum_{m=0}^{\text{Int}(3r/2)} g_{rm} x^{3r-2m} y^r. \quad (32)$$

Obviously, $g_{00} = 1$. In Appendix A it is shown that the coefficients satisfy the recurrence relation,

$$\begin{aligned} g_{r+1,m} &= \frac{1}{2(r+1)} \sum_{k=0}^{k_1(r,m)} g_{r-k,m-1-k} - \frac{1}{4(r+1)} \sum_{k=0}^{k_2(r,m)} \frac{(k+1)}{(k+3)} g_{r-k,m-k} \\ &+ \frac{1}{r+1} \sum_{p=0}^{p_1(m)} (-1)^p 2^{4p+2} (4p+2) b_{p+1} g_{r-4p-1,m-3(2p+1)}, \end{aligned} \quad (33)$$

where the limits of the sums are

$$\begin{aligned} k_1(r, m) &= \begin{cases} m-1 & (m \leq r+1), \\ 3r-2m+2 & (m \geq r+1), \end{cases} \\ k_2(r, m) &= \begin{cases} m & (m \leq r), \\ 3r-2m & (m \geq r), \end{cases} \\ p_1(m) &= \text{Int}(\tfrac{1}{6}m - \tfrac{1}{2}). \end{aligned} \quad (34)$$

With the expansion (32), after replacing x and y by D and a from (30), we find, for the coefficient of $1/a^r$ in (29),

$$\begin{aligned} T_r(z) &= \exp\{i\pi(\tfrac{3}{8} - \tfrac{1}{2}z^2)\} (-1)^r \frac{1}{\pi^{2r}} \sum_{m=0}^{\text{Int}(3r/2)} g_{rm} i^{-m} (\tfrac{1}{2}\pi)^m \\ &\times \left[D^{3r-2m} \frac{\exp(i\pi z \zeta)}{2 \cos(\pi z)} \right]_{\zeta \rightarrow z}. \end{aligned} \quad (35)$$

To evaluate the derivatives, we define

$$\Phi(z) \equiv \exp\{\tfrac{1}{2}i\pi(z^2 + \tfrac{3}{4})\} / 2 \cos(\pi z) \quad (36)$$

and use Leibniz's rule for differentiating a product. Thus

$$\begin{aligned} \exp\left\{\frac{1}{2}i\pi\left(\frac{3}{4} - z^2\right)\right\} \left[D^n \frac{\exp(i\pi z\zeta)}{2\cos(\pi z)} \right]_{\zeta \rightarrow z} \\ = \exp\left(-\frac{1}{2}i\pi z^2\right) [D^n \exp\{i\pi(z\zeta - \tfrac{1}{2}z^2)\} \Phi(z)]_{\zeta \rightarrow z} \\ = \sum_{s=0}^n \frac{n!}{s!(n-s)!} \Phi^{(n-s)}(z) [D^s \exp\{-\tfrac{1}{2}i\pi(z-\zeta)^2\}]_{\zeta \rightarrow z}, \end{aligned} \quad (37)$$

where $\Phi^{(m)}(z)$ denotes the m th derivative. The derivatives D^s are zero unless s is even. A little calculation now leads to

$$T_r(z) = \frac{(-1)^r}{\pi^{2r}} \sum_{q=0}^{\text{Int}(3r/2)} \left(\frac{1}{2}\pi\right)^q \frac{(-i)^q}{(3r-2q)!} \Phi^{(3r-2q)}(z) \sum_{m=0}^q \frac{(3r-2m)!}{(q-m)!} g_{rm}. \quad (38)$$

To get the Riemann–Siegel coefficients $C_r(z)$, this must be combined with $T_r^*(-z)$ according to (24). The fact that even and odd derivatives are, respectively, even and odd functions of z (cf. (36)) guarantees that the C_r are real. In (38) the terms with even q combine to give derivatives of

$$2 \operatorname{Re} \Phi(z) = F(z), \quad (39)$$

where Φ is defined by (6), and the terms with odd q combine to give derivatives of

$$2 \operatorname{Im} \Phi(z) = \sin\left\{\frac{1}{2}\pi\left(z^2 + \frac{3}{4}\right)\right\} / \cos(\pi z). \quad (40)$$

Now, $\operatorname{Im} \Phi(z)$ has poles at $z = \pm \frac{1}{2}$, whereas $\operatorname{Re} \Phi(z)$ is finite at these points (zeros of the numerator and denominator cancel). But $Z(t)$ is a smooth function, so that the poles cannot contribute to the Riemann–Siegel coefficients. Therefore the sum over m in (38) must vanish if q is odd. Extensive computations confirm that this is so, but I have not succeeded in finding a general proof.

Incorporating this observation, we obtain the Riemann–Siegel coefficients in their final form:

$$C_r(z) = \sum_{p=0}^{\text{Int}(3r/4)} \frac{F^{(3r-4p)}(z)}{\pi^{2(r-p)}} d_{rp}, \quad (41)$$

where

$$d_{rp} = \frac{(-1)^{r+p}}{2^{2p}(3r-4p)!} \sum_{m=0}^{2p} \frac{(3r-2m)!}{(2p-m)!} g_{rm}. \quad (42)$$

The multipliers d_{rp} are rational numbers, defined in terms of the g_{rm} which are calculated from the recurrence relation (33).

Table 1 shows some of the d_{rp} , extending the list of Gabcke (1979) which showed these multipliers for $r \leq 12$. For small m and p it is possible to calculate g_{rm} and

d_{rp} for all r ; the results are

$$\left. \begin{aligned} g_{r0} &= \frac{(-1)^r}{12^r r!}, & g_{r1} &= \frac{(-1)^{r+1} 3r(3r-1)}{12^r r!}, \\ g_{r2} &= \frac{27}{16} \frac{(-1)^r (15r^3 - 38r^2 + 29r - 6)}{12^r (r-1)!}, \\ d_{r0} &= \frac{1}{12^r r!}, & d_{r1} &= \frac{9}{5} \frac{(3r-1)}{12^r (r-2)!}. \end{aligned} \right\} \quad (43)$$

3. High orders

The coefficients $T_r(z)$ in (23) can be written as

$$T_r(z) = \frac{1}{2\pi i} \oint \frac{da}{a} a^r T(a, z), \quad (44)$$

in which the contour is a loop at infinity enclosing the origin. For T we substitute the series (21), treating each term separately. Thus we obtain

$$T_r(z) \equiv \sum_{K=0}^{\infty} U_{Kr}(z), \quad (45)$$

where

$$\begin{aligned} U_{Kr}(z) &= \exp\left\{i\pi\left(\frac{3}{8} - \frac{1}{2}z^2 + 2zQ - Q^2\right)\right\} \\ &\times \frac{(-1)^K}{2\pi i} \oint \frac{da}{a} a^r \frac{\exp\{i(2\pi aQ + \chi(2\pi a^2))\}}{(1 + Q/a)^{1/2+2\pi ia^2}}. \end{aligned} \quad (46)$$

The aim is to find the asymptotic form of this integral for large r , and then perform the summation over K .

Three preliminaries will enable the integral to be cast in a form suitable for asymptotic evaluation. First, the exponent $i\chi$ will be neglected; this seems drastic, but is justified by a calculation (Appendix D) of the asymptotic series (in $1/a$) for the corresponding exponential. This reveals that although the high orders diverge factorially, the divergence of the terms from the rest of (46) is exponentially larger and so dominates. It now follows from a result on the combination of asymptotic series (Appendix C) that the contribution of χ to the high-order Riemann–Siegel coefficients is negligible.

Second, we rearrange the exponent in (46) using

$$(-\pi Q^2 + 2\pi zQ - \frac{1}{2}\pi z^2)_{\text{mod } 2\pi} = +\pi Q^2 - \frac{1}{2}\pi. \quad (47)$$

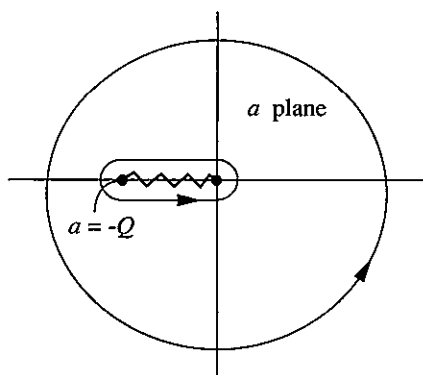
This is easily proved from the definition (17) of Q .

Third, we note that without χ the only singularities of the integrand in (46) are branch points at $a = 0$ and $a = -Q$. These can be connected with a cut, onto which the contour can be shrunk (figure 1). On the upper (lower) lip, the phase of $(1 + Q/a)$ is $-\pi$ ($+\pi$). With the natural change of variable $a = -Qu$, (46) now becomes

$$\begin{aligned} U_{Kr}(z) &= \exp\left\{i\pi\left(-\frac{1}{8} + Q^2\right)\right\} \frac{(-1)^{K+r}}{\pi} Q^r \\ &\times \int_0^1 \frac{du u^r}{\sqrt{u(1-u)}} \exp\{-2\pi i Q^2 u(1 + u \log(u^{-1} - 1))\} \cosh(2\pi^2 Q^2 u^2). \end{aligned} \quad (48)$$

Table 1. Lists of multipliers d_{rp} for $0 \leq r \leq 14$
(Calculated from equations (42) and (33); (a) $p \leq 3$, (b) $p \geq 4$; the first columns list the values of r .)

		(a)		(b)	
0	1				
1	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{128}$		
2	$\frac{1}{288}$	$\frac{1}{120}$	$\frac{1}{5}$		
3	$\frac{1}{10368}$	$\frac{1}{23040}$	$\frac{1}{384}$		
4	$\frac{1}{497664}$	$\frac{1}{414720}$	$\frac{1}{122880}$		
5	$\frac{1}{29859840}$	$\frac{1}{39813120}$	$\frac{1}{6649}$		
6	$\frac{1}{2149908480}$	$\frac{1}{119439360}$	$\frac{1}{23224320}$		
7	$\frac{1}{180592312320}$	$\frac{1}{171992678400}$	$\frac{1}{88651}$		
8	$\frac{1}{17336861982720}$	$\frac{1}{7223692492800}$	$\frac{1}{5573836800}$		
9	$\frac{1}{1872381094133760}$	$\frac{1}{1386948958617600}$	$\frac{1}{111476736000}$		
10	$\frac{1}{224685731296051200}$	$\frac{1}{4680952735334400}$	$\frac{1}{13759414272000}$		
11	$\frac{1}{29658516531078758400}$	$\frac{1}{513567385819545600}$	$\frac{1}{144473849856000}$		
12	$\frac{1}{4270826380475341209600}$	$\frac{1}{1186340661243150336000}$	$\frac{1}{6164217593856000}$		
13	$\frac{1}{666248915354153228697600}$	$\frac{1}{341666110438027296768000}$	$\frac{1}{374476218826752000}$		
14	$\frac{1}{1119298177949742421196800}$	$\frac{1}{9872610898319769600}$	$\frac{1}{10085920762063093760000}$		
7	$\frac{5}{81920}$	$\frac{41}{32768}$	$\frac{2603}{524288}$	$\frac{2603}{1048576}$	
8	$\frac{26405}{33030144}$	$\frac{2603}{393216}$	$\frac{5377}{983040}$	$\frac{1048576}{351937}$	
9	$\frac{21543701}{326998425600}$	$\frac{32851}{9437184}$	$\frac{7040165}{422785832}$	$\frac{351937}{50331648}$	
10	$\frac{2320279}{678218966800}$	$\frac{31587481}{47563407360}$	$\frac{71350619}{298969989120}$	$\frac{50331648}{422785832}$	
11	$\frac{413542091}{3296144130048000}$	$\frac{1681009907}{25113479086080}$	$\frac{3706405595341}{182826127746662400}$	$\frac{422785832}{15136141}$	
12	$\frac{8283026179}{2373223773634560000}$	$\frac{2927256839861}{68559797904984000}$	$\frac{1760589}{227026787}$	$\frac{15136141}{88645}$	
13	$\frac{733972733}{9492805094538240000}$	$\frac{1890353754197}{9872610898319769600}$	$\frac{1760589}{227026787}$	$\frac{88645}{12582912}$	
14	$\frac{965416409}{683488440806753280000}$			$\frac{12582912}{268435456}$	

Figure 1. Contours in the a plane for the integral (46).

This integral will be evaluated by the method of steepest descent. The main contribution comes from the part of the cosh function with the negative exponent. The corresponding exponent of the integrand has a stationary point between $u = 0$ and $u = 1$. The value of the exponent at this point depends on Q which is proportional to K . Since it will be necessary to sum over K , the most effective procedure is to determine the stationary point of the whole exponent in (48) with respect to both u and Q . This exponent is

$$E(u, Q; r) = r \log(Qu) - 2\pi Q^2 [\pi u^2 + i(-\frac{1}{2} + u + u^2 \log(u^{-1} - 1))]. \quad (49)$$

The stationary point (denoted by a superscript 's') is at

$$u^s = \frac{1}{2}, \quad Q^s = \sqrt{r/\pi}. \quad (50)$$

(Note that at this point $t = 2\pi a^2 = r/2\pi$, so that $\chi(2\pi a^2) \sim 1/r$, further justifying neglect of this quantity in (46).) The stationary values of E and its second derivatives (denoted by subscripts) are

$$\left. \begin{aligned} E^s &= \frac{1}{2}r \log(\frac{1}{2}r) - \frac{1}{2}r - r \log(\pi\sqrt{2}), \\ E_{uu}^s &= -8r(1 - 2i\pi), \quad E_{uQ}^s = -4\pi\sqrt{r}, \quad E_{QQ}^s = -2\pi^2. \end{aligned} \right\} \quad (51)$$

Thus we can write

$$E(u, Q; r) = E^s + \frac{1}{2}E_{uu}^s(u - \frac{1}{2})^2 + E_{uQ}^s(u - \frac{1}{2})(Q - \sqrt{r/\pi}) + \frac{1}{2}E_{QQ}^s(Q - \sqrt{r/\pi})^2 + \dots \quad (52)$$

Evaluating the u integral, and noting that

$$\exp(E^s) = \frac{1}{(\pi\sqrt{2})^r} (\frac{1}{2}r)^{r/2} \exp(-\frac{1}{2}r) \approx \frac{\sqrt{r}}{(\pi\sqrt{2})^r 2\sqrt{\pi}} \Gamma(\frac{1}{2}r) \quad (53)$$

leads, on reinstating K , to

$$U_{Kr}(z) \approx \frac{\Gamma(\frac{1}{2}r)}{(\pi\sqrt{2})^r} \exp(\frac{1}{8}i\pi) \frac{(-1)^{K+r}}{4\pi\sqrt{1-2i\pi^{-1}}} \exp\left\{-\frac{2\pi}{2\pi^{-1}+i}\left(K+\frac{1}{2}(1+z)-\frac{\sqrt{r}}{\pi}\right)^2\right\}. \quad (54)$$

This has a maximum near $K = \sqrt{r/\pi}$, so for large r the lower limit $K = 0$ of the sum in (45) can be replaced by $-\infty$ with an error that is exponentially small. Then the sum $T_r(z)$ is a theta-function series, which by the Poisson summation formula

can be transformed into another theta-function series that converges rapidly, namely

$$T_r(z) \approx \frac{(-1)^r \Gamma(\frac{1}{2}r)}{4(\pi\sqrt{2})^{r+1}} i \sum_{m=-\infty}^{\infty} (-1)^{m(m-1)/2} \exp\{-(m + \frac{1}{2})^2\} \\ \times \exp\{i[(m + \frac{1}{2})\pi z - (2m + 1)\sqrt{r}]\}. \quad (55)$$

Because of the symmetry about $m = -\frac{1}{2}$, the terms with negative and positive m can be combined, thus giving T_r as the real expression:

$$T_r(z) \approx \frac{(-1)^r \Gamma(\frac{1}{2}r)}{2(\pi\sqrt{2})^{r+1}} \sum_{m=0}^{\infty} (-1)^{m(m-1)/2} \exp\{-(m + \frac{1}{2})^2\} \\ \times \sin\{(2m + 1)\sqrt{r} - (m + \frac{1}{2})\pi z\}. \quad (56)$$

Finally, adding $T_r(-z)$ according to (24) gives high-order Riemann–Siegel coefficients as

$$C_r(z) = \frac{\Gamma(\frac{1}{2}r)}{(\pi\sqrt{2})^{r+1}} f(r, z), \quad (57)$$

where

$$f(r, z) \approx \sum_{m=0}^{\infty} (-1)^{m(m-1)/2} \exp\{-(m + \frac{1}{2})^2\} \\ \times \begin{cases} \sin\{(2m + 1)\sqrt{r}\} \cos\{(m + \frac{1}{2})\pi z\} & (r \text{ even}), \\ \cos\{(2m + 1)\sqrt{r}\} \sin\{(m + \frac{1}{2})\pi z\} & (r \text{ odd}), \end{cases} \quad \text{when } r \gg 1 \quad (58)$$

as claimed in §1.

Reinstating a , we see that the terms C_r/a^r in the Riemann–Siegel series (5) behave like

$$\frac{\Gamma(\frac{1}{2}r)}{(a\pi\sqrt{2})^r} = \frac{\Gamma(\frac{1}{2}r)}{(\pi t)^{r/2}}. \quad (59)$$

For fixed large t , the terms decrease rapidly and then increase, in the manner familiar in an asymptotic series (Dingle 1973). The least term is near $r^* = 2\pi t$.

The particular coefficients $C_{2m}(1)$ can be determined solely from the requirement that the discontinuities in the main sum in (4) are removed by the Riemann–Siegel expansion (5), leaving $Z(t)$ continuous as it must be. This argument, by Gabcke (1979), is elaborated in Appendix B, and extended in Appendix D to determine the high-order behaviour of these coefficients. The result is

$$C_{2m}(1) \approx \frac{\Gamma(m)}{(2\pi)^{2m}} \times \begin{cases} -\cos(\frac{1}{8}\pi)/48m & (m \text{ even}) \\ \sin(\frac{1}{8}\pi)2\pi & (m \text{ odd}) \end{cases} \quad \text{for } m \gg 1. \quad (60)$$

The powers in the denominator contain the factor 2, rather than $\sqrt{2}$ as in the general case (57). Therefore these special coefficients are smaller by a factor 2^{-m} than the even coefficients for $z \neq \pm 1$, consistent with (58) predicting zero for the high-order behaviour in this case.

4. Remainders

We seek the form of the remainders $S_R(t)$ of the Riemann–Siegel expansion, truncated at terms $r = R$ close to optimal, that is close to the least term $r \approx r^*$. The remainders are defined by (9). Before proceeding to a direct calculation, I give two heuristic arguments suggesting that they will be of order $\exp(-\pi t)$. The arguments are based on the observation that the divergence of an asymptotic series often originates in terms omitted in its derivation, so the size of these terms limits the accuracy that can be obtained with the expansion.

First, recall that in deriving the Riemann–Siegel expansion we included the terms with negative n in the second sum in (13) (see the remarks following equation (21)). These have the form

$$\exp\{it \log(-n)\} = \exp(-\pi t) \exp(it \log n) \quad (61)$$

and indeed involve the claimed exponential.

Second, the formal expansion (15) for the quantity $\chi(t)$ defined in (14) fails to capture the Stokes phenomenon for the gamma function (Berry 1991) that appears in the definition (2) of $\theta(t)$. Using the reflection and duplication formulae for the gamma function, Gabcke (1979) showed that $\theta(t)$ can be written in terms of $\Gamma(it)$ and $\Gamma(2it)$ through the identity

$$\theta(t) = \frac{1}{2}t(\log(t/2\pi) - 1) - \frac{1}{8}\pi + \frac{1}{2}\operatorname{Im}[\mu(2it) - \mu(it)] + \frac{1}{2}\arctan\{\exp(-\pi t)\}, \quad (62)$$

where $\mu(z)$ is defined by

$$\Gamma(z) \equiv \sqrt{2\pi} z^{z-\frac{1}{2}} \exp\{-z + \mu(z)\}. \quad (63)$$

The formal expansion (15), which contributes to the Riemann–Siegel expansion, is obtained by applying Stirling's series to $\mu(it)$ and $\mu(2it)$ in (62). The term involving $\exp(-\pi t)$ in (62) is beyond all orders of the expansion and so does not contribute to the calculation of its terms, although it is of course part of the function $Z(t)$ being approximated. $\exp(-\pi t)$ is the first in a string of small exponentials in the asymptotics of $\zeta(\frac{1}{2} + it)$; elsewhere I will pursue the idea that these correspond to complex periodic orbits ('instantons') in the conjectured associated dynamics.

With this expectation that the remainders will be of order $\exp(-\pi t)$, we now proceed to a direct calculation. $S_R(t)$ can be written formally as the divergent tail of the series (5). If R is large, the asymptotic formulae (57) and (58) can be substituted for the terms, giving (cf. (59))

$$S_R(t) \approx \frac{(-1)^{N+1}}{\pi\sqrt{2a}} \sum_{R+1}^{\infty} \frac{\Gamma(\frac{1}{2}r)}{(\pi t)^{r/2}} f(r, z). \quad (64)$$

Because this is divergent, it must be interpreted. This will be achieved using a variant of Borel summation (Dingle 1973). If the terms with r even and r odd are separated, the functions $f(r, z)$ are slowly varying and can be replaced by their values at the lower limit of the sums. Thus

$$S_R(t) \approx \frac{(-1)^{N+1}}{\pi\sqrt{2a}} \left\{ \frac{f(R+1, z)}{(\pi t)^{(R+1)/2}} \sum_{m=0}^{\infty} \frac{\Gamma(\frac{1}{2}(R+1) + m)}{(\pi t)^m} + \frac{f(R+2, z)}{(\pi t)^{R/2+1}} \sum_{m=0}^{\infty} \frac{\Gamma(\frac{1}{2}R + 1 + m)}{(\pi t)^m} \right\}. \quad (65)$$

Replacing the gamma functions by their integral representations, and then evaluating the sums, gives, after an elementary change of variable, the convergent representation

$$S_R(t) \approx \frac{(-1)^{N+1}}{\pi\sqrt{2a}} \{f(R+1, z) I(R-1, \pi t) + f(R+2, z) I(R, \pi t)\}, \quad (66)$$

where

$$I(R, w) = \oint_0^\infty du \frac{\exp(-wu)u^{R/2}}{1-u}. \quad (67)$$

The principal value is chosen to ensure that $S_R(t)$ is real for real t . We seek to evaluate this when R is large and close to the least term $2\pi t = 2w$. Then the integrand has a saddle close to the pole at $u = 1$, and it is natural to expand about $u = 1$. To third order, we obtain

$$\begin{aligned} I(R, w) &= -e^{-w} \int_{-\infty}^\infty \frac{ds}{s} \exp\{-\tfrac{1}{4}Rs^2 + (\tfrac{1}{2}R - w)s\}(1 + \tfrac{1}{6}Rs^3 + \dots) \\ &= -e^{-w} \int_{-\infty}^\infty \frac{dv}{v} \exp\{-v^2 + 2\sigma v\}(1 + \tfrac{4}{3\sqrt{R}}v^3 + \dots), \end{aligned} \quad (68)$$

where

$$\sigma(R, w) \equiv (\tfrac{1}{2}R - w)/\sqrt{R}. \quad (69)$$

The first integral in (68) can be transformed into an error function

$$\int_{-\infty}^\infty \frac{dv}{v} e^{-v^2} \sinh(2\sigma v) = 2\sqrt{\pi} \int_0^\sigma d\sigma e^{\sigma^2} = -i\pi \operatorname{erf}(i\sigma) \quad (70)$$

(which of course is real) and the second integral is elementary.

Incorporating the difference between $I(R, w)$ and $I(R-1, w)$ in (66) into the term of order $1/\sqrt{R}$, we finally obtain

$$\begin{aligned} S_R(t) &\approx \frac{(-1)^N \exp(-\pi t)}{\sqrt{2a}} \left\{ (-i \operatorname{erf}(i\sigma) + \frac{\exp(\sigma^2)}{3\sqrt{R}\pi} (4\sigma^2 + \tfrac{1}{2})) \right. \\ &\quad \times (f(R+1, z) + f(R+2, z)) + \frac{\exp(\sigma^2)}{2\sqrt{R}\pi} (f(R+2, z) - f(R+1, z)) \left. \right\}. \end{aligned} \quad (71)$$

This is the result (10) claimed in §1. It indeed has the expected leading-order dependence $\exp(-\pi t)$. Moreover it is easily confirmed from (57) that $S_R(t)$ is of the same order as the first term omitted in the truncated Riemann–Siegel series, consistent with Gabcke's rigorous bounds for the first few terms, and asymptotics folklore.

Finally, we consider briefly the case where t is complex, that is when the zeta function is being calculated off the critical line. For optimal truncation, that is $R = \operatorname{Int}(2\pi \operatorname{Re} t)$, the remainder (71) consists, to leading order, of $\exp(-\pi t)$ times a multiplier involving

$$-i \operatorname{erf}\left(\frac{\operatorname{Im} \pi t}{\sqrt{R}}\right) \approx -i \operatorname{erf}\left(\frac{\operatorname{Im} \pi t}{\sqrt{2 \operatorname{Re} \pi t}}\right). \quad (72)$$

This is precisely the universal multiplier describing the smooth switching of the sign of a subdominant exponential across a Stokes line (Berry 1989). Here the subdominant exponential is $\exp(-\pi t)$ (the dominant exponential being unity), and the Stokes line is the critical line t real. An interesting fact is that the 'half-width' of the Stokes

line, that is the range over which the argument of the error function increases by unity, is $\text{Im } t \sim \sqrt{(2t/\pi)}$, which is larger than the half-width $\text{Im } t = \frac{1}{2}$ of the critical strip.

5. Calculation of derivatives contributing to the coefficients

According to (41), the coefficient $C_r(z)$ involves the n th derivatives $F^{(n)}(z)$ of the function $F(z)$ (defined by (6)), for $n \leq 3r$. These derivatives are nonsingular functions of z , because the zeros of the numerator and denominator cancel. Direct evaluation is very inefficient, because it gives each high $F^{(n)}(z)$ in terms of powerful singularities that must cancel when summed. In this section I describe two effective methods for evaluating the derivatives, as alternatives, applicable for large r , to the Taylor expansions commonly used for small r (Edwards 1974).

(a) Special values of z

For $z = 0$, Leibniz's formula for the derivative of a product gives, for the even derivatives (the odd ones being zero)

$$F^{(2m)}(0) = (2m)! \text{Re} \exp\left(\frac{3}{8}i\pi\right) \times \sum_{s=0}^m \frac{1}{(2s)!(2m-2s)!} (\sec \pi z)_{z=0}^{(2s)} (\exp(\frac{1}{2}i\pi z^2))_{z=0}^{(2m-2s)}. \quad (73)$$

Use of

$$\sec \pi z = \sum_{n=0}^{\infty} (-1)^n E_{2n} \frac{(\pi z)^{2n}}{(2n)!}, \quad (74)$$

where E_{2n} are the Euler numbers, leads to

$$F^{(2m)}(0) = (2m)! \left(\frac{1}{2}\pi\right)^m \sum_{s=0}^m (-2\pi)^s E_{2s} \frac{\cos\{\frac{1}{2}\pi(m-s+\frac{3}{4})\}}{(2s)!(m-s)!}. \quad (75)$$

For $z = 1$, we note that

$$F(1+\zeta) = \sin\{\frac{1}{2}\pi(\zeta^2 + \frac{3}{4})\} + \cos\{\frac{1}{2}\pi(\zeta^2 + \frac{3}{4})\} \tan \pi\zeta. \quad (76)$$

The first (second) term is even (odd) in ζ , and so gives the even (odd) derivatives. Use of

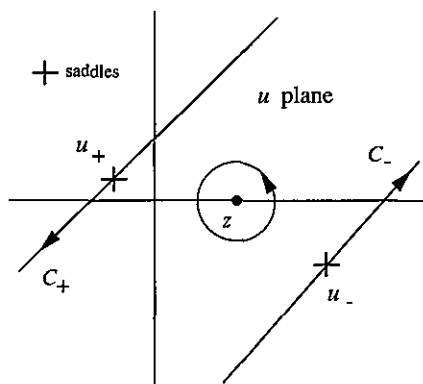
$$\tan \pi\zeta = \sum_{n=1}^{\infty} (-1)^{n-1} B_{2n} (\pi\zeta)^{2n-1} \frac{2^{2n}(2^{2n}-1)}{(2n)!}, \quad (77)$$

where B_{2n} are the Bernoulli numbers, leads to

$$\left. \begin{aligned} F^{(2m)}(1) &= \pi^{-1/2} (m - \frac{1}{2})! (2\pi)^m \sin\{\frac{1}{2}\pi(m + \frac{3}{4})\}, \\ F^{(2m+1)}(1) &= 4\pi(2m+1)! \left(\frac{1}{2}\pi\right)^m \\ &\quad \times \sum_{s=0}^m (-8\pi)^s B_{2s+2} \frac{(2^{2s+2}-1) \cos\{\frac{1}{2}\pi(m-s+\frac{3}{4})\}}{(2s+2)!(m-s)!}. \end{aligned} \right\} \quad (78)$$

For $z = \frac{1}{2}$, we note that

$$F(\frac{1}{2} + \zeta) = \frac{1}{2} \cos(\frac{1}{2}\pi\zeta^2) \sec(\frac{1}{2}\pi\zeta) + \frac{1}{2} \sin(\frac{1}{2}\pi\zeta^2) \text{cosec}(\frac{1}{2}\pi\zeta). \quad (79)$$

Figure 2. Contours in the u plane for the integral (82).

Again, the first (second) term is even (odd) in ζ , and so gives the even (odd) derivatives. Use of (74) and

$$\operatorname{cosec}(\tfrac{1}{2}\pi\zeta) = 2 \sum_{n=0}^{\infty} (-1)^{n+1} B_{2n} (\tfrac{1}{2}\pi\zeta)^{2n-1} \frac{(2^{2n-1} - 1)}{(2n)!} \quad (80)$$

leads to

$$\left. \begin{aligned} F^{(4m)}(\tfrac{1}{2}) &= \tfrac{1}{2}(-1)^m (4m)! (\tfrac{1}{2}\pi)^{2m} \sum_{s=0}^m \frac{E_{4s}(-1)^s (\tfrac{1}{2}\pi)^{2s}}{(4s)!(2m-2s)!}, \\ F^{(4m+1)}(\tfrac{1}{2}) &= (-1)^{m+1} (4m+1)! (\tfrac{1}{2}\pi)^{2m} \sum_{s=0}^m \frac{B_{4s}(-1)^s (\tfrac{1}{2}\pi)^{2s} (2^{4s-1} - 1)}{(4s)!(2m-2s+1)!}, \\ F^{(4m+2)}(\tfrac{1}{2}) &= \tfrac{1}{2}(-1)^{m+1} (4m+2)! (\tfrac{1}{2}\pi)^{2m+2} \sum_{s=0}^m \frac{E_{4s+2}(-1)^s (\tfrac{1}{2}\pi)^{2s}}{(4s+2)!(2m-2s)!}, \\ F^{(4m+3)}(\tfrac{1}{2}) &= (-1)^m (4m+3)! (\tfrac{1}{2}\pi)^{2m+2} \sum_{s=0}^m \frac{B_{4s+2}(-1)^s (\tfrac{1}{2}\pi)^{2s} (2^{4s+1} - 1)}{(4s+2)!(2m-2s+1)!}. \end{aligned} \right\} \quad (81)$$

(b) Asymptotics of high derivatives

A familiar dogma of asymptotics is the invocation of Darboux's theorem (Dingle 1973) to infer that high derivatives of a function at a regular point are determined by the nearest singularity. This fails for $F(z)$, which has no finite singularities. Therefore it is necessary to use a different method. From (6), Cauchy's theorem gives

$$F^{(n)}(z) = \frac{n!}{2\pi} \operatorname{Re} \exp(-\tfrac{1}{8}i\pi) \oint \frac{du}{(u-z)^{n+1}} \frac{\exp(\tfrac{1}{2}i\pi u^2)}{\cos(\pi u)}, \quad (82)$$

where the contour is a small loop surrounding $u = z$.

The poles at the zeros of the cosine do not contribute: they are cancelled when the real part is taken. Instead, the integral is dominated by saddles. Their contributions can be extracted by expanding the contour into lines C_+ and C_- connecting infinity in the first and third quadrants (figure 2), where the exponential converges. Saddles lie in the second (fourth) quadrants on C_+ (C_-), where the negative (positive)

exponential in the cosine dominates. Therefore we can write

$$\frac{1}{\cos(\pi u)} = 2 \sum_{p=0}^{\infty} (-1)^p \exp\{\pm i\pi u(2p+1)\} \quad (83)$$

(upper sign: on C_+ , in upper half-plane; lower sign: on C_- , in lower half-plane) and express the derivatives as

$$F^{(n)}(z) = \frac{n!}{\pi} \operatorname{Re} \exp(-\tfrac{1}{8}i\pi) \sum_{p=0}^{\infty} (-1)^p [I_{np}^+(z) + I_{np}^-(z)]. \quad (84)$$

Here
$$I_{np}^{\pm}(z) \equiv \int_{C_{\pm}} du \exp\{-\phi_{np}^{\pm}(u, z)\}, \quad (85)$$

where
$$\phi_{np}^{\pm}(u, z) = (n+1) \log(u-z) - \tfrac{1}{2}i\pi u^2 \mp i\pi u(2p+1). \quad (86)$$

Each integral is dominated by a single saddle, at

$$u = u_{np}^{\pm}(z) \tfrac{1}{2} \{ \mp e^{-i\pi/4} \sqrt{[(4/\pi)(n+1) + i(z \pm (2p+1))^2]} + z \mp (2p+1) \}. \quad (87)$$

Then the saddle-point method, including the first correction term, gives the approximations

$$I_{np}^{\pm}(z) \approx \sqrt{\frac{2\pi}{\partial_u^2 \phi_{np}^{\pm}}} \exp(-\phi_{np}^{\pm}) \left\{ 1 + \frac{1}{8} \left[\frac{5(\partial_u^3 \phi_{np}^{\pm})^2}{3(\partial_u^2 \phi_{np}^{\pm})^3} - \frac{\partial_u^4 \phi_{np}^{\pm}}{(\partial_u^2 \phi_{np}^{\pm})^2} \right] \right\} \quad (88)$$

in which all quantities are evaluated at u_{np}^{\pm} . Substitution into (84) gives the derivatives. For large n , the contributions from higher p in (84) and from the saddle-point correction (in square brackets in (88)) diminish rapidly, making this an effective method for computing the high derivatives.

6. Numerical tests of the formulae

(a) Riemann-Siegel coefficients

Here we compare the 'experimental' $C_r(z)$ computed from the exact formulae (41) and (42), using coefficients g_{rm} obtained from the recurrence relation (33), with the 'theory' represented by the asymptotic formulae (57) and (58). The coefficients were computed for $0 \leq r \leq 50$.

For the 'experiment' it is necessary to evaluate the derivatives $F^{(n)}(z)$ up to $n = 150$. This was done using the saddle-point approximations of §5b with $0 \leq p \leq 3$. It is convenient to present the data by factoring out the dominant dependence in (57). Therefore the 'experimental' graphs show $f(r, z)$ defined by (57), that is

$$f(r, z) \equiv \frac{(\pi\sqrt{2})^{r+1}}{\Gamma(\frac{1}{2}r)} C_r(z) \quad (89)$$

and the 'theoretical' curves show the large- r approximation (58).

Figures 3 and 4 are synoptic comparisons for a range of z values between 0 and 1, for r even and r odd. Evidently the theory works well, even for r as small as 5. Figure 5 shows comparisons for some individual z values.

It is necessary to check the unlikely possibility that the good agreement in figures

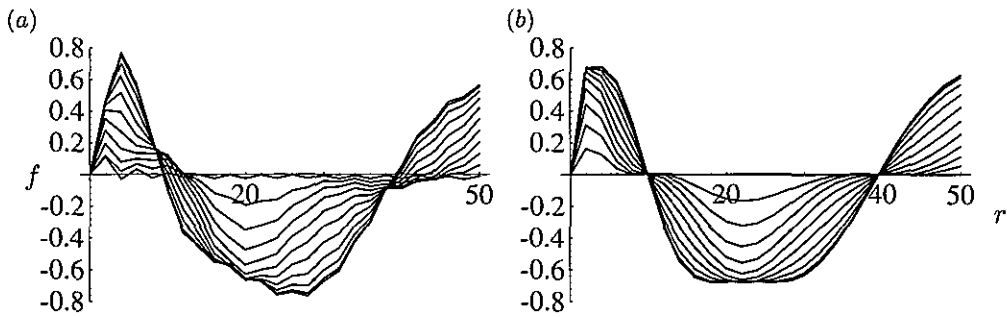


Figure 3. Decoration function $f(r, z)$ (defined by (90)) multiplying factorials in the Riemann-Siegel coefficients, for even r . The curves show $z = 0 [0.1] 1$. (a) 'Experimental' coefficients (41) and (42) with derivatives approximated by the saddle-point method of §5b; (b) 'theory' (58).

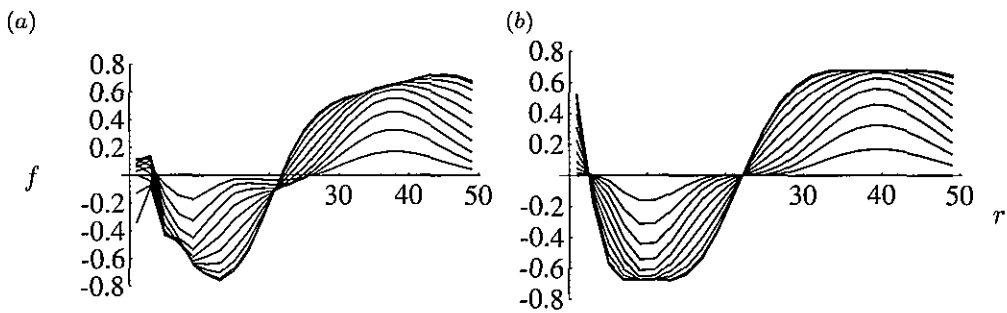


Figure 4. As figure 3, with r odd.

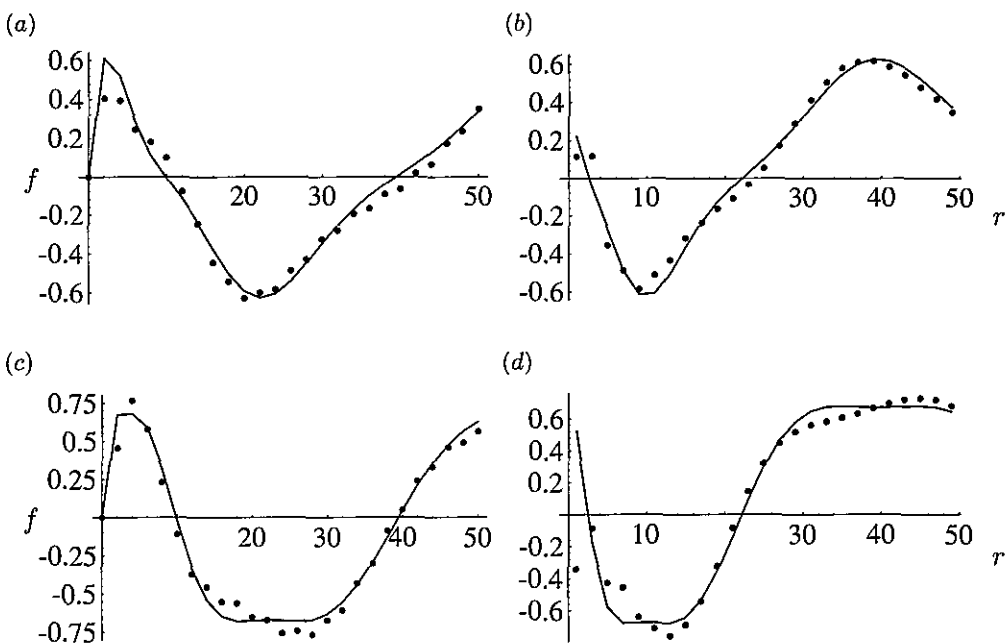


Figure 5. As figure 3, for (a) $z = 0.5$, even r ; (b) $z = 0.5$, odd r ; (c) $z = 0$, even r ; (d) $z = 1$, odd r . Dots, 'experiment'; full lines 'theory'.

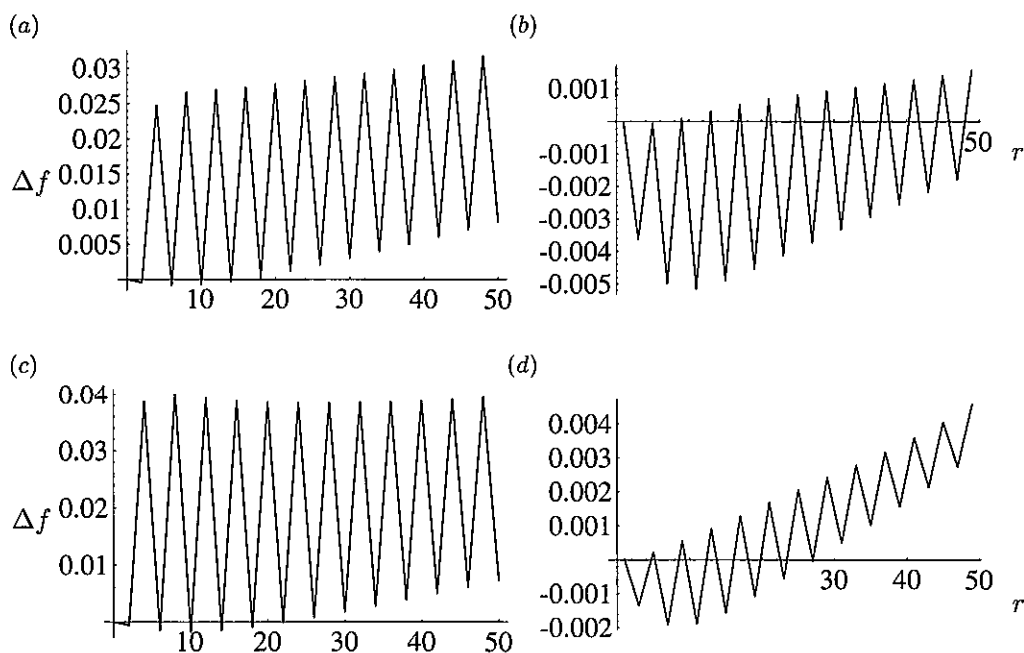


Figure 6. Test of saddle-point approximation of §5*b* with $0 \leq p \leq 3$, for derivatives of $F(z)$, with $\Delta f(r, z) = f_{\text{exact}}(r, z) - f_{\text{saddle}}(r, z)$, for (a) $z = 0.5$, even r ; (b) $z = 0.5$, odd r ; (c) $z = 0$, even r ; (d) $z = 1$, odd r .

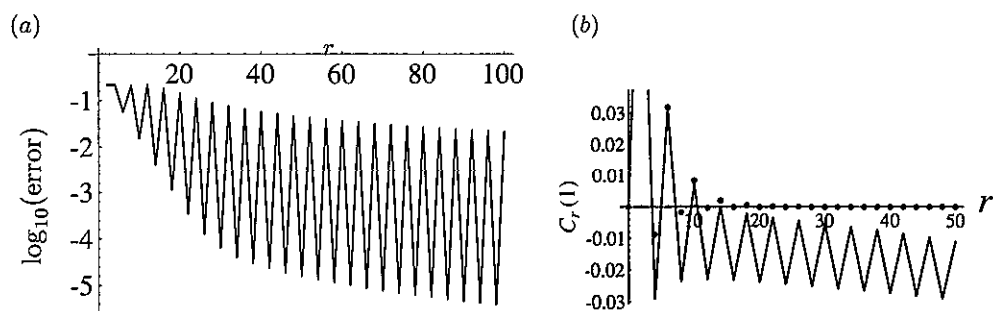


Figure 7. Coefficients $C_r(1)$ against r for r even. (a) $\log_{10}(\text{error})$ in the high-order approximation (60), where error = (approximate C /exact C) - 1; (b) coefficients calculated exactly (dots), and via saddle-point approximation for the derivatives (full line).

3–5 is a fortuitous consequence of the saddle-point approximation for the F derivatives. That this is not the case is clear from figure 6, which shows the difference between the coefficients computed with the exact and approximate derivatives, for the particular cases (§5*a*) where the derivatives can be computed exactly. The errors never exceed 4% and would barely be perceptible in figures 3–5. It is interesting to note that the errors are smaller when r has the form $4m$ than for $r = 4m + 2$, and much smaller still when r is odd.

Figure 7 concerns the particular coefficients $C_{2m}(1)$, which can easily be computed exactly (Appendix B). Figure 7*a* confirms that the formula (60) for the high orders is better for larger r , and also shows that the relative error is much smaller for $r = 4m + 2$ than for $r = 4m$. Figure 7*b* shows that for these coefficients (which are

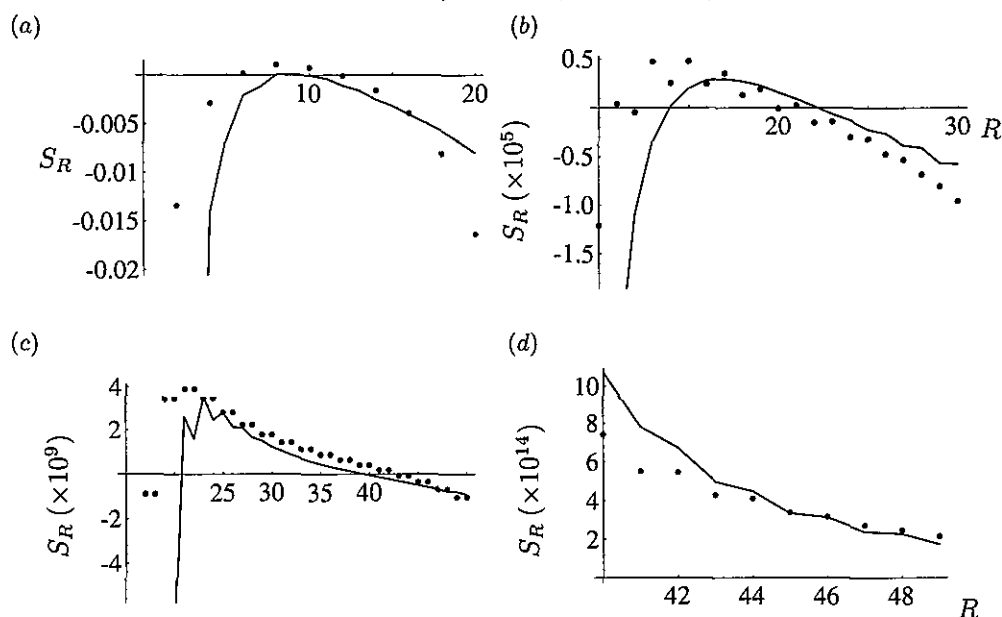


Figure 8. Riemann–Siegel remainders $S_R(t)$, computed exactly from (9) (dots), and from the theory (71) (full lines), for the following values of t (table 2): (a) $t = \frac{1}{2}\pi$ (least term near $R = 10$); (b) $t = \frac{9}{8}\pi$ (least term near $R = 22$); (c) $t = 2\pi$ (least term near $R = 40$); (d) $t = \frac{25}{4}\pi$ (least term near $R = 62$).

exponentially smaller than in the general case) large errors result from using the saddle-point approximation to calculate the derivatives.

(b) Exact and approximate remainders

To test the theory (71) it is necessary to calculate the remainders $S_R(t)$ defined by (9), by subtracting from $Z(t)$ the first $R + 1$ terms of the Riemann–Siegel expansion. As explained by Edwards (1974), $Z(t)$ can be computed with arbitrary accuracy, albeit not very efficiently, by a method based on the Euler–Maclaurin sum formula. When calculating the remainders, the Riemann–Siegel coefficients must be evaluated with an accuracy $\exp(-\pi t)$. This cannot be achieved by calculating the F derivatives with the saddle-point approximation of § 5 *b*. Therefore I restricted the tests to $z = 0$, $z = \frac{1}{2}$ and $z = 1$, for which the derivatives can be calculated exactly as explained in § 5 *a*.

Even so, the comparison was necessarily restricted to low values of t ; otherwise, the fact that the optimal truncation is near $R = 2\pi t$ would have required the evaluation of very high derivatives. For these, the methods of § 5 *a*, although exact, are inefficient and require very high numerical accuracy. For example, $R = 50$ requires the Euler and Bernoulli numbers up to order 150, and E_{150} is an integer of order 10^{233} and B_{150} is a ratio of integers with numerator of order 10^{149} . Table 2 shows the values of t for which the theory of the remainders was tested.

Figure 8 shows the ‘experimental’ and ‘theoretical’ remainders as functions of truncation R . Evidently the theory (71) works well for a large range of near-optimal truncations (including, it seems, figure 8*d*, where $R = r^* = 62$ is out of range of the computations).

Table 2. *Special values of t*

t	N	z	$r^* \approx 2\pi t$	$\Gamma(\frac{1}{2}r^*)/(\frac{1}{2}r^*)^{(r^*+1)/2}$
$\frac{1}{2}\pi$	0	0	10	3.7×10^{-3}
$\frac{9}{8}\pi$	0	$-\frac{1}{2}$	22	3.4×10^{-6}
2π	0	-1	39	3.4×10^{-10}
$\frac{25}{8}\pi$	1	$+\frac{1}{2}$	62	3.3×10^{-15}

It should be noted that although these t values are large in the sense that the optimum order r^* of Riemann–Siegel truncation is large, they are all smaller than the lowest Riemann zero (near $t = 14.1$), and for all except one ($t = 25\pi/8 \approx 9.8$) the main sum is empty. For the lowest Riemann zero, $r^* = 89$, which is out of reach of our computations.

The extraordinary accuracy of the Riemann–Siegel expansion is achieved at a high computational cost. To attain the optimal accuracy $\exp(-\pi t)$, the number of terms that must be included is $2\pi t$; this is $4\pi^2 N^2$ and so increases faster than the number of terms in the main sum in (4). Nevertheless, it is interesting to speculate that it might be possible to attain still higher accuracy, by extending ‘hyperasymptotics’ (Berry & Howls 1991) to the Riemann–Siegel expansion.

I thank Dr Jonathan Keating and Professor Michael Morgan for very helpful conversations, and useful comments based on their careful reading of the manuscript.

Appendix A. Recurrence relation for g_{rm}

This is the derivation of (33). The first step is to expand $g(x, y)$, defined by (31), in terms of y . Thus we write

$$g(x, y) = \exp\left(\sum_{r=1}^{\infty} \gamma_r(x) y^r\right) = \sum_{r=0}^{\infty} g_r(x) y^r \quad (\text{A } 1)$$

with $g_0(x) = 1$. Differentiating the second equation with respect to y and identifying terms in y gives

$$g_{r+1}(x) = \frac{1}{r+1} \sum_{m=0}^r (m+1) \gamma_{m+1}(x) g_{r-m}(x). \quad (\text{A } 2)$$

Now we note that, from (31),

$$\gamma_r(x) = \frac{x^r}{2r} - \frac{x^{r+2}}{4(r+2)} - [(-1)^{(r+2)/4} 2^r b_{(r+2)/4}] \text{ when } (r+2)/4 \text{ is integer.} \quad (\text{A } 3)$$

The next step is to expand $g_r(x)$ in powers of x (cf. (32)):

$$g_r(x) = \sum_{s=0}^{\text{Int}(3r/2)} g_{rs} x^{3r-2s}. \quad (\text{A } 4)$$

Substitution into (A 2) and identifying terms now gives, ignoring for the moment the upper limits of the sums,

$$(r+1)g_{r+1,m} = \frac{1}{2} \sum_{k=0}^{k_1(r,m)} g_{r-k,m-1-k} - \frac{1}{4} \sum_{k=0}^{k_2(r,m)} \frac{(k+1)}{(k+3)} g_{r-k,m-k} \\ + \left[\sum_k 2^{k+1} (-1)^{(k-1)/4} (k+1) b_{(k+3)/4} g_{r-k,m-3(k+1)/2} \right]_{(k+3)/4 \text{ integer}} \quad (\text{A } 5)$$

In the last sum we change the variable to $k = 4p + 1$ and thereby obtain (33).

The upper limits (34) of the sums are determined by the requirement that in each g_{rm} the indices must satisfy $0 \leq m \leq \text{Int}(3r/2)$. Thus in the first sum, $k_1(r, m)$ follows from

$$0 \leq m - 1 - k \leq \text{Int}(\tfrac{3}{2}(r - k)) \quad (\text{A } 6)$$

and similarly for k_2 . For the third sum, the same principle gives

$$0 \leq m - 3(2p + 1) \leq \text{Int}(\tfrac{3}{2}(r - 4p - 1)) \quad (\text{A } 7)$$

and $p(m)$ follows from the first inequality.

Appendix B. $C_{2m}(1)$ from discontinuities in the main sum (Gabcke 1979)

Continuity of $Z(t)$ at $t = 2\pi N^2$, in spite of the discontinuity of the main sum in (4), implies that the Riemann-Siegel coefficients in (5) must satisfy

$$0 = \lim_{\varepsilon \rightarrow 0} [Z(2\pi N^2 + \varepsilon) - Z(2\pi N^2 - \varepsilon)] \\ = 2N^{-1/2} \cos\{\theta(2\pi N^2) - 2\pi N^2 \log N\} + \frac{(-1)^{N+1}}{N^{1/2}} \sum_{r=0}^{\infty} \frac{C_r(+1) + C_r(-1)}{N^r}. \quad (\text{B } 1)$$

The symmetry relation (25), together with (14), gives

$$\sum_{m=0}^{\infty} \frac{C_{2m}(+1)}{N^{2m}} = (-1)^N \cos\{\theta(2\pi N^2) - 2\pi N^2 \log N\} \\ = \cos(\tfrac{1}{8}\pi) \cos\{\chi(2\pi N^2)\} + \sin(\tfrac{1}{8}\pi) \sin\{\chi(2\pi N^2)\}. \quad (\text{B } 2)$$

Noting the expansion (15) for χ , and defining

$$x \equiv i/N^2, \quad d_m \equiv (-1)^m b_m / (2\pi)^{2m-1} \quad (\text{B } 3)$$

we see that the desired $C_{2m}(1)$ depend on the real coefficients e_l (with $e_0 = 1$) in the expansion

$$\exp\{i\chi(2\pi N^2)\} = \exp\left(-\sum_{m=1}^{\infty} d_m x^{2m-1}\right) \equiv \sum_{l=0}^{\infty} e_l x^l. \quad (\text{B } 4)$$

From (B 2), the coefficients are

$$C_{4l}(1) = (-1)^l \cos(\tfrac{1}{8}\pi) e_{2l}, \quad C_{4l+2}(1) = (-1)^l \sin(\tfrac{1}{8}\pi) e_{2l+1}. \quad (\text{B } 5)$$

The e_l can be found from the following recurrence relation, which follows from differentiating (B 4):

$$e_{l+1} = -\frac{1}{l+1} \sum_{s=0}^{\text{Int}(l/2)} (2s+1) d_{s+1} e_{l-2s}. \quad (\text{B } 6)$$

Gabcke's argument can be extended by requiring that derivatives of $Z(t)$ are continuous at $t = 2\pi N^2$. This leads to (rather cumbersome) equations determining the n th derivatives of the Riemann-Siegel coefficients C_r at $z = 1$, where $n + r$ is even.

Appendix C. Two results on late terms in asymptotic series

These results (which are probably 'well known to those who know well', and are given here for completeness) will be used in Appendix D. The first concerns the exponential of an asymptotic series. If

$$s(x) = \sum_{n=1}^{\infty} s_n x^n \quad (\text{C } 1)$$

is a factorially divergent formal asymptotic series, we seek the high-order coefficients e_n defined by

$$\exp \left(\sum_{n=1}^{\infty} s_n x^n \right) \equiv \sum_{n=0}^{\infty} e_n x^n. \quad (\text{C } 2)$$

Clearly, $e_0 = 1$.

Differentiating (C 2) gives

$$\begin{aligned} e_{n+1} &= \frac{1}{n+1} \sum_{m=0}^n (1+m) s_{m+1} e_{n-m} \\ &= s_{n+1} + \frac{n}{n+1} s_n e_1 + \frac{n-1}{n+1} s_{n-1} e_2 + \dots \end{aligned} \quad (\text{C } 3)$$

For $n \gg 1$ the assumed factorial divergence of the s_n implies that the terms in this series diminish as powers of $1/n$. We include the first two terms, to allow for the circumstance (which will occur in Appendix D) that the first might vanish because of symmetry. Thus

$$e_{n+1} \approx s_{n+1} + s_n s_1 \quad \text{for } n \gg 1. \quad (\text{C } 4)$$

The second result concerns the product of two asymptotic series. If

$$s(x) = \sum_{n=0}^{\infty} s_n x^n \quad \text{and} \quad t(x) = \sum_{n=0}^{\infty} t_n x^n \quad (\text{C } 5)$$

are factorially divergent formal asymptotic series with $s_0 = 1$ and $t_0 = 1$, we seek the high-order coefficients p_n defined by

$$s(x)t(x) = \sum_{n=0}^{\infty} s_n x^n \sum_{n=0}^{\infty} t_n x^n \equiv \sum_{n=0}^{\infty} p_n x^n. \quad (\text{C } 6)$$

Clearly, $p_0 = 1$.

Collecting terms with the same power of x gives

$$p_n = \sum_{k=0}^n s_k t_{n-k} = t_n + s_1 t_{n-1} + \dots + s_n + t_1 s_{n-1} + \dots \quad (\text{C } 7)$$

For $n \gg 1$ the assumed factorial divergence of the s_n and t_n implies that the terms in the two series following t_n and s_n in (C 7) diminish as powers of $1/n$. Therefore

$$p_n \approx \max(s_n, t_n) \quad \text{for } n \gg 1. \quad (\text{C } 8)$$

In words, the high orders in the product series are simply the high orders of the dominant of the two component asymptotic series.

Appendix D. Two results for the gamma series $\exp(i\chi)$

The first result is the derivation of the formula (60) for the high coefficients $C_{2m}(1)$. This is an application of the ‘exponential’ formula (C 4) to the high orders of the series (B 4) generating $C_{2m}(1)$. Identification of the middle member of (B 4) with the first member of (C 2) gives

$$s_{2m} = 0, \quad s_{2m+1} = -d_{m+1}. \quad (\text{D } 1)$$

For the high d_m , we use the definitions (B 3) and (15), together with asymptotics of the Bernoulli numbers, to obtain

$$d_m = \frac{(-1)^m (2^{2m-1} - 1) |B_{2m}|}{(2\pi)^{2m-1} 2^{2m} 2m(2m-1)} \approx \frac{(-1)^m (2m-2)!}{(2\pi)^{4m-1}} \quad \text{for } m \gg 1. \quad (\text{D } 2)$$

Equation (C 4) now gives

$$\left. \begin{aligned} e_{2m} &\approx s_{2m-1} s_1 = -\frac{|B_2|}{16\pi} d_m \approx \frac{(-1)^{m+1} (2m-2)!}{96\pi (2\pi)^{4m-1}} \\ e_{2m+1} &\approx s_{2m+1} = -d_{m+1} \approx \frac{(-1)^m (2m)!}{(2\pi)^{4m+3}} \end{aligned} \right\} \quad \text{for } m \gg 1. \quad (\text{D } 3)$$

Substitution into (B 5) gives the claimed formulae (60).

The second result is the justification, promised in the second paragraph of § 3, for ignoring terms generated by the factor $\exp(i\chi)$ when calculating the high orders of the Riemann–Siegel series. From (B 3) and (B 4) we find

$$\exp\{i\chi(2\pi a^2)\} = \sum_{l=0}^{\infty} \frac{e_l i^l}{a^{2l}} \quad (\text{D } 4)$$

From (D 4) we have the high-order behaviour

$$\frac{e_l}{a^{2l}} \sim \frac{\Gamma(l)}{(2\pi)^{2l} a^{2l}} \quad (\text{D } 5)$$

so the coefficient of $1/a^r$ in the expansion of $\exp(i\chi)$ is proportional to

$$\frac{\Gamma(\frac{1}{2}r)}{(2\pi)^r}. \quad (\text{D } 6)$$

This is smaller by $2^{-r/2}$ than the leading dependence found for the C_r in (57) and

so, by the result (C8), the factor $\exp(i\chi)$ does not contribute to the asymptotics of the Riemann–Siegel coefficients. Another way to see this is to reinstate t and note that the terms in the expansion of $\exp(i\chi)$ diverge as

$$\frac{\Gamma(\frac{1}{2}r)}{(2\pi t)^{r/2}}, \quad (\text{D7})$$

which is smaller than (59) and by Borel summation generates a remainder of order $\exp(-2\pi t)$, rather than the $\exp(-\pi t)$ found in §4.

References

- Berry, M. V. 1986 In *Quantum chaos and statistical nuclear physics* (ed. T. H. Seligman & H. Nishioka), pp. 1–17. Springer Lecture Notes in Physics No. 263.
- Berry, M. V. 1989 *Proc. R. Soc. Lond. A* **422**, 7–21.
- Berry, M. V. 1991 *Proc. R. Soc. Lond. A* **434**, 465–472.
- Berry, M. V. & Howls, C. J. 1991 *Proc. R. Soc. Lond. A* **434**, 657–675.
- Berry, M. V. & Howls, C. J. 1993 *Proc. R. Soc. Lond. A* **443**, 107–126.
- Berry, M. V. & Keating, J. P. 1992 *Proc. R. Soc. Lond. A* **437**, 151–173.
- Brent, R. P. 1979 *Math. Comp.* **33**, 1361–1372.
- Dingle, R. B. 1973 *Asymptotic expansions: their derivation and interpretation*. New York and London: Academic Press.
- Edwards, H. M. 1974 *Riemann's zeta function*. New York and London: Academic Press.
- Gabcke, W. 1979 Neue Herleitung und Explizite Restabschätzung der Riemann–Siegel-Formel. Ph.D. thesis, Göttingen.
- Keating, J. P. 1993 In *Quantum chaos* (ed. G. Casati, I. Guarneri & U. Smilansky), pp. 145–185. Amsterdam: North-Holland.
- Odlyzko, A. M. 1987 *Math. Comp.* **48**, 273–308.
- Odlyzko, A. M. 1990 The 10^{20} th zero of the Riemann zeta function and 175 million of its neighbours. AT&T Bell Laboratory preprint.
- Odlyzko, A. M. & Schönhage, A. 1988 *Trans. Am. math. Soc.* **309**, 797–809.
- Paris, R. B. 1994 *Proc. R. Soc. Lond. A* **446**, 565–587.
- Titchmarsh, E. C. 1986 *The theory of the Riemann zeta-function*, 2nd edn. Oxford: Clarendon Press.
- van de Lune, J., te Riele, H. J. J. & Winter, D. T. 1986 *Math. Comp.* **46**, 667–681.
- Wolfram, S. 1991 *Mathematica*. Addison-Wesley.

Received 16 November 1994; accepted 4 January 1995