

A new asymptotic representation for $\zeta(\frac{1}{2} + it)$ and quantum spectral determinants

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By analytic continuation of the Dirichlet series for the Riemann zeta function $\zeta(s)$ to the critical line $s = \frac{1}{2} + it$ (t real), a family of exact representations, parametrized by a real variable K , is found for the real function $Z(t) = \zeta(\frac{1}{2} + it) \exp\{i\theta(t)\}$, where θ is real. The dominant contribution $Z_0(t, K)$ is a convergent sum over the integers n of the Dirichlet series, resembling the finite ‘main sum’ of the Riemann–Siegel formula (RS) but with the sharp cut-off smoothed by an error function. The corrections $Z_3(t, K), Z_4(t, K) \dots$ are also convergent sums, whose principal terms involve integers close to the RS cut-off. For large K , Z_0 contains not only the main sum of RS but also its first correction. An estimate of high orders $m \gg 1$ when $K < t^{\frac{1}{2}}$ shows that the corrections Z_k have the ‘factorial/power’ form familiar in divergent asymptotic expansions, the least term being of order $\exp\{-\frac{1}{2}K^2t\}$.

Graphical and numerical exploration of the new representation shows that Z_0 is always better than the main sum of RS, providing an approximation that in our numerical illustrations is up to seven orders of magnitude more accurate with little more computational effort. The corrections Z_3 and Z_4 give further improvements, roughly comparable to adding RS corrections (but starting from the more accurate Z_0). The accuracy increases with K , as do the numbers of terms in the sums for each of the Z_m .

By regarding Planck’s constant \hbar as a complex variable, the method for $Z(t)$ can be applied directly to semiclassical approximations for spectral determinants $\Delta(E, \hbar)$ whose zeros $E = E_j(\hbar)$ are the energies of stationary states in quantum mechanics. The result is an exact analytic continuation of the exponential of the semiclassical sum over periodic orbits given by the divergent Gutzwiller trace formula. A consequence is that our result yields an exact asymptotic representation of the Selberg zeta function on its critical line.

1. Introduction

Riemann’s celebrated function $\zeta(s)$ arises not only in connection with prime numbers (Edwards 1974) but also as a model for spectral determinants in quantum chaology (Berry 1986, 1991; Berry & Keating 1990; Keating 1992*a, b*). It is often necessary to be able to represent $\zeta(\frac{1}{2} + it)$ in a simple way high in the critical strip ($|\text{Im } t| < \frac{1}{2}$, $|\text{Re } t| \gg 1$) and calculate it there with great accuracy. Particularly important is the critical line t real, where, according to the Riemann hypothesis, the non-trivial zeros lie. Our purpose here is to describe a way of doing this which has some advantages over the method currently used, and which can be applied directly to the analogous functions in quantum mechanics.

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The method is an extension of the formal approximating scheme introduced in Keating (1992*a*) for semiclassical formulae, and applied to $\zeta(s)$ in Keating (1992*b*). Here we go further; first, by eliminating the formal aspect of this approach; second, by pursuing it to its natural conclusion to obtain a complete asymptotic expansion; and third, by fine-tuning a parameter to improve convergence.

It follows from the functional equation for $\zeta(s)$ that the function defined by

$$Z(t) \equiv \exp\{i\theta(t)\} \zeta\left(\frac{1}{2} + it\right) \quad (1)$$

with
$$\exp\{i\theta(t)\} = \left[\frac{\Gamma\left(\frac{1}{4} + \frac{1}{2}it\right)}{\Gamma\left(\frac{1}{4} - \frac{1}{2}it\right)} \right]^{\frac{1}{2}} \exp\left\{-\frac{1}{2}it \ln \pi\right\} \quad (2)$$

is an even function of t (θ is odd). Moreover, it is real when t is real, as is $\theta(t)$. The simplest representation for $\zeta(s)$, namely the Dirichlet series

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad (3)$$

converges only when $\text{Re } s > 1$, and so fails when used in (1) for real t , generating a $Z(t)$ that is neither obviously real nor obviously even.

Computation of $Z(t)$ for real t using (3) requires analytic continuation. A powerful method, now universally used when t is large (Haselgrove 1963; Brent 1979; Odlyzko 1987), is the Riemann–Siegel formula (Edwards 1974; Titchmarsh 1986), hereinafter called RS:

$$Z(t) = 2 \sum_{n=1}^{N(t)} \frac{\cos\{\theta(t) - t \ln n\}}{\sqrt{n}} - (-1)^{N(t)} \left(\frac{2\pi}{t}\right)^{\frac{1}{4}} \sum_{j=0}^k \left(\frac{2\pi}{t}\right)^{j/2} \Phi^{(j)}\{p(t)\} + R^{(k)}(t). \quad (4)$$

Here $N(t)$ and $p(t)$ are defined by

$$N(t) \equiv \text{Int} \sqrt{\frac{t}{2\pi}}, \quad p(t) \equiv \sqrt{\frac{t}{2\pi}} - \text{Int} \sqrt{\frac{t}{2\pi}} \quad (5)$$

and the functions $\Phi^{(j)}(p)$ are combinations of derivatives of

$$\Phi^{(0)}(p) = \cos\left\{2\pi\left(p^2 - p - \frac{1}{16}\right)\right\} / \cos\{2\pi p\}. \quad (6)$$

To understand what follows, it is helpful to consider the following interpretation of RS. The sum over n (the ‘main sum’), which usually dominates $Z(t)$, follows from substituting (3) into (1), truncating the resulting divergent series at the term $N(t)$ whose phase is stationary, and adding the complex conjugate of this truncated series as an approximate resummation of the divergence (Titchmarsh 1986, ch. IV; Berry 1986; Keating 1992*a, b*). As an approximation to $Z(t)$, the main sum suffers from the defect of being a discontinuous function of t because of the discontinuous upper limit $N(t)$. It is the role of the correction terms, in the sum over j , to remedy this by removing, one by one, the discontinuities in successive derivatives at the truncation point.

Probably, the sum of all these corrections is an asymptotic expansion of $Z(t)$, but we know of no proof. And there appear to have been no studies of the high orders of the expansion, such as would be necessary to estimate the accuracy with which $Z(t)$ could be computed by choosing k in (4) to be the least term. Bounds do exist, however, for some of the remainders $R^{(k)}(t)$, a particularly useful one being (Gabcke 1979)

$$|R^{(4)}(t)| < 0.017/t^{\frac{11}{4}} \quad (t > 200). \quad (7)$$

The representation we derive here (§§2 and 3) superficially resembles RS in being dominated by a sum over n , similar to the main sum in (4), and possessing a series of correction terms. It has, however, several advantages over RS. First, all its terms are analytic functions of t : there are no discontinuities. Second, it is formally exact, unlike RS whose remainders $R^{(k)}(t)$ contain an unspecified exponentially small integral (Edwards 1974). Third, the size of the late terms can be estimated explicitly (§§4 and 5), showing that they have the ‘factorial divided by power’ form familiar in asymptotic expansions (Dingle 1973). Fourth, numerical studies (§6) suggest that term by term the new series is more accurate than RS. And fifth, the derivation generalizes (§7) directly to the series encountered in the determination of eigenvalues of wave operators associated with chaotic dynamical systems, an example of which is the Selberg zeta function (Balazs & Voros 1986). We emphasize this, because such series also suffer from fundamental convergence problems, and no analogue of RS is known for them.

Although the new formula looks like RS with its discontinuities smoothed away term by term, this appearance is misleading. Our formula involves an additional parameter. Moreover it contains RS in a complicated way; indeed we show (§4) that there is a limiting régime in which our dominant series contains not only the main sum of RS but at least its first correction term as well.

Before embarking on the analysis, we make two remarks. First, according to (2) the function $Z(t)$ has square-root branch points at the zeros of the gamma functions in $\exp\{i\theta(t)\}$. These points complicate the analysis slightly, and it might be thought preferable to work with a different combination of ζ and Γ , namely $\Xi(t)$ (eq. (2.1.16) in Titchmarsh 1986), which as well as being real for real t , and even, is also an entire function. In fact much of the argument to follow can be applied equally to $\Xi(t)$, but the final formulae are numerically far less effective than those for $Z(t)$. The reason is probably that the asymptotics must also be flexible enough to accommodate the rapidly decreasing amplitude factor by which the modulus $|\Xi(t)|$ differs from $|\zeta(t)|$ when t is real, a factor which is uninteresting in studies of the zeros, and which we never encounter because $|Z(t)| = |\zeta(t)|$ when t is real.

The second remark is that for simplicity of exposition we shall restrict ourselves to writing formulae valid for real t , that is on the critical line. However, continuation to complex t in the analyticity strip of $Z(t)$ is not difficult.

2. Analytic continuation

By Cauchy’s theorem we have

$$Z(t) = \frac{1}{2\pi i} \int_{C_+ + C_-} \frac{dz}{z} \gamma(z, t) Z(z + t), \tag{8}$$

where C_{\pm} are the contours shown in figure 1, and γ is any function, analytic inside the integration strip, for which the integral converges and $\gamma(0, t) = 1$. Choosing $\gamma(z, t)$ even in z , and using the fact that $Z(t)$ is even, we obtain

$$Z(t) = \frac{1}{2\pi i} \int_{C_-} \frac{dz}{z} \gamma(z, t) [Z(z + t) + Z(z - t)]. \tag{9}$$

Except near the branch point $z = -t - \frac{1}{2}i$, the Dirichlet series (3) converges

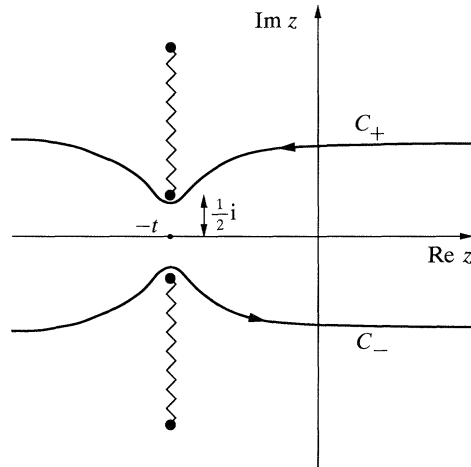


Figure 1. Integration contours C_+ and C_- in the z plane, with cuts (zigzags) connecting the square-root branch points of $Z(t)$.

everywhere on C_- , because $\text{Im } z < -\frac{1}{2}$ (corresponding to $\text{Re } s > 1$). However, the branch point gives a vanishing contribution. Therefore we can substitute (3), and obtain

$$Z(t) = \sum_{n=1}^{\infty} [T_n(t) + T_n(-t)], \tag{10}$$

where

$$T_n(t) = \frac{\exp\{i(\theta(t) - t \ln n)\}}{\sqrt{n}} \frac{1}{2\pi i} \int_{C_-} \frac{dz}{z} \gamma(z, t) \exp\{i[\theta(z+t) - \theta(t) - z \ln n]\}. \tag{11}$$

This analytic continuation gives $Z(t)$ on the critical line as a manifestly even function. The fact that $\theta(t)$ is odd leads (by an argument involving the deformation of C_- to the real axis plus an infinitesimal semicircle) to the relation

$$T_n(-t) = T_n^*(t) \tag{12}$$

and thence, via (10), to the (necessarily) real even function

$$Z(t) = 2 \text{Re} \sum_{n=1}^{\infty} T_n(t). \tag{13}$$

Of course these formulae make sense only if the sums and integrals converge. We achieve this by making the choice

$$\gamma(z, t) = \exp(-z^2 K^2 / 2|t|), \tag{14}$$

where K is a constant whose significance will become clear later. Convergence of the integrals (11) is obvious. In Appendix A we show that the sum over T_n converges too: after an initially rapid decrease as $\exp[-\ln^2(n/N)]$, the ultimate decrease of the terms is very slow, namely as $n^{-1} \ln^{-3} n$. This slow convergence of the n -sum will now be hastened by expanding each T_n as a series whose terms can be evaluated explicitly. The form (14) is chosen *ad hoc*. We have not explored the possibility of choosing γ to optimize convergence.

3. Series expansion

Henceforth we consider $t > 0$; this leads to no loss of generality because $z(t)$ is even. In (11) we expand $\exp\{i\theta(z+t)\}$ as

$$\exp\{i[\theta(z+t) - \theta(t)]\} = \exp\{i[z\theta'(t) + \frac{1}{2}z^2\theta''(t)]\} \left[1 + \sum_{m=3}^{\infty} z^m b_m(t) \right], \tag{15}$$

in which the functions $b_m(t)$ can be calculated recursively from $\theta(t)$ in terms of the polygamma functions $\psi^{(n)}(x)$ ($(n-1)$ st logarithmic derivative of $\Gamma(x)$),

$$\sum_{m=3}^{\infty} z^m b_m(t) = \exp\left\{ i \sum_{s=3}^{\infty} \left(\frac{1}{2}z\right)^s \frac{\text{Im } i^s \psi^{(s-1)}\left(\frac{1}{4} + \frac{1}{2}it\right)}{s!} \right\} - 1. \tag{16}$$

In the exponent of the integrand in (11) we now group the terms linear and quadratic in z by defining

$$\xi(n, t) \equiv \ln n - \theta'(t), \quad Q^2(K, t) \equiv K^2 - it\theta''(t). \tag{17}$$

For each term labelled by m in (15), we can now evaluate the integral in (11) and substitute into (13). In this way we obtain our main result:

$$Z(t) = Z_0(t, K) + Z_3(t, K) + Z_4(t, K) + \dots \tag{18}$$

The integral for Z_0 has a quadratic exponential and a first-order pole, and can be evaluated in terms of the complementary error function (eq. 7.1.4 of Abramowitz & Stegun 1964):

$$Z_0(t, K) = 2 \text{Re} \sum_{n=1}^{\infty} \frac{\exp\{i[\theta(t) - t \ln n]\}}{\sqrt{n}} \times \frac{1}{2} \text{Erfc} \left\{ \frac{\xi(n, t)}{Q(K, t)} \sqrt{\left(\frac{1}{2}t\right)} \right\}. \tag{19}$$

The integrals Z_m ($m \geq 3$) have quadratic exponentials multiplied by positive powers, and can be evaluated in terms of Hermite polynomials (eq. 8.951 of Gradshteyn & Ryzhik 1980):

$$Z_m(t, K) = \frac{2}{\sqrt{\pi}} \left(\frac{1}{2}t\right)^{m/2} \text{Re} \frac{(-i)^m b_m(t)}{Q^m(K, t)} \sum_{n=1}^{\infty} \frac{\exp\{i[\theta(t) - t \ln n]\}}{\sqrt{n}} \times \exp\left\{ \frac{-\xi^2(n, t) t}{2Q^2(K, t)} \right\} H_{m-1} \left\{ \frac{\xi(n, t)}{Q(K, t)} \sqrt{\left(\frac{1}{2}t\right)} \right\} \quad (m \geq 3). \tag{20}$$

(An earlier version of this theory failed to incorporate the quadratic term in the exponent of (15), so that the counterpart of the multiplying series began with b_2 rather than b_3 . This led to a slightly different representation for $Z(t)$, involving K rather than Q (whose first term – the counterpart of Z_0 – was obtained by Keating (1992*b*)). The low-order approximations to this representation were numerically much less accurate and their subsequent analysis proved more complicated than that of (18)–(20).)

The representation (18)–(20) gives Z , which is independent of K , as a series of contributions Z_m ; we call this the m -series. Z_0 is the main term, and $Z_3, Z_4 \dots$ are corrections. Each Z_m is a K -dependent sum of terms labelled n ; we call these the n -sums.

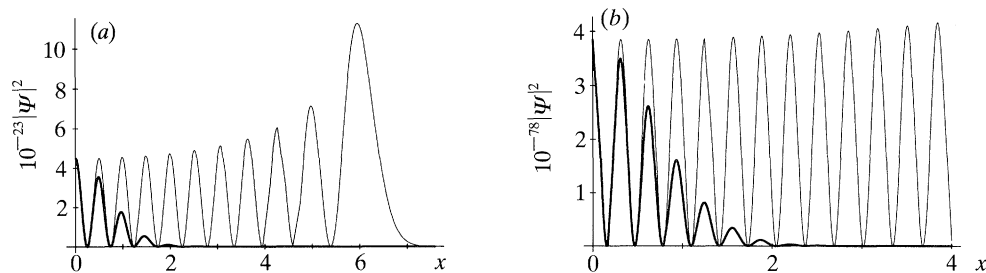


Figure 2. Comparison between squares of the functions $\psi_1 = \exp(-x^2)H_m(x)$ appearing in (20) (thick lines) and the squares of the Hermite functions $\psi_2 = \exp(-\frac{1}{2}x^2)H_m(x)$ (thin lines), for (a) $m = 20$, (b) $m = 50$.

The convergence of the n -sums is crucial to the usefulness of our representation, and depends on the smallness of

$$\exp\{-\xi^2(n, t)/2Q^2(K, t)\} \quad (21)$$

for the following reasons. In (19) the function Erfc is approximately proportional to this factor when ξ is large. And the Gauss–Hermite product in the second line of (20) is also dominated by the gaussian factor. This is not obvious. It follows from the fact that the ‘width’ of the product can be defined as

$$W_m \equiv \sqrt{\left[\int_0^\infty dx x^2 [\exp(-x^2)H_m(x)]^2 \right] / \left[\int_0^\infty dx [\exp(-x^2)H_m(x)]^2 \right]} = \frac{1}{2} \sqrt{\frac{(4m-1)}{(2m-1)}} \quad (22)$$

and is, asymptotically, independent of m and only $\sqrt{2}$ greater than W_0 (equation (22) can be derived from eq. 7.375.1 of Gradshteyn & Ryzhik (1980)). This behaviour is quite different from that of the widths of the harmonic oscillator functions, where (cf. eq. 7.375.2 of Gradshteyn & Ryzhik (1980))

$$W_m^{\text{osc}} \equiv \sqrt{\left[\int_0^\infty dx x^2 [\exp(-\frac{1}{2}x^2)H_m(x)]^2 \right] / \left[\int_0^\infty dx [\exp(-\frac{1}{2}x^2)H_m(x)]^2 \right]} = \sqrt{m + \frac{1}{2}}. \quad (23)$$

Here the Gaussian factor is weaker, and the widths increase with m . Figure 2 illustrates this striking difference between the functions appearing in (20) and the harmonic oscillator functions. The very useful consequence is that the convergence of the n -sums is the same for all the Z_m .

We now note that for the large t of interest here we may approximate $\theta(t)$ (and the derived quantities ξ , Q and the b_m) with Stirling’s asymptotic expansion for the gamma function:

$$\theta(t) = \frac{t}{2} \left(\ln \left\{ \frac{t}{2\pi} \right\} - 1 \right) - \frac{\pi}{8} + \frac{1}{48t} - \frac{7}{5760t^3} + \dots \quad (24)$$

In subsequent analysis we shall make extensive use of this formula.

In particular, we find, to lowest order,

$$\xi(n, t) \approx \ln \{n/\sqrt{(t/2\pi)}\} \approx \ln \{n/N(t)\}, \quad (25)$$

where $N(t)$ is the RS cut-off (5). Substituting this into (21) now shows that the n convergence depends on

$$\left| \exp \left\{ \frac{-[\ln(n/N)]^2 t}{2Q^2} \right\} \right| = \exp \left\{ \frac{-[\ln(n/N)]^2 t K^2}{2(K^4 + \frac{1}{4})} \right\}, \tag{26}$$

and so is faster than any power of n but slower than exponential. Note that this rapid convergence now holds for all n ; there is no drastic slowing-down for very large n , as with (13). The reason is that there the slowing-down was caused by a branch point of the integrand in (11) (see Appendix A), but there is no analogous contribution associated with the terms in the expansion (15). As we shall see in §5, the price to be paid for this is that the m -series is a divergent asymptotic expansion, but the least term is so small that the divergence has no effect on practical computations.

A consequence of (26) is that the upper limit guaranteeing that neglected terms are smaller than $\exp(-A)$ is

$$\begin{aligned} n = n^* &= \sqrt{\left(\frac{t}{2\pi}\right)} \exp \left\{ K \sqrt{\frac{2A(1+1/4K^4)}{t}} \right\} \\ &\approx N \exp \{ (K/N) \sqrt{[(A/\pi)(1+1/4K^4)]} \}. \end{aligned} \tag{27}$$

In what follows we shall make frequent use of this estimate. Note that n^* has a minimum value of $N \exp \{ \sqrt{(A/\pi)}/N \}$, when $K = 1/\sqrt{2}$.

For our representation to be a serious rival to RS when t is large, we require that the number of n -terms in each Z_m is not much larger than the number N in the main sum of RS. Therefore we impose upon K the restriction

$$K \ll N(t) \sim t^{\frac{1}{2}}. \tag{28}$$

Note that this is compatible with $K \gg 1$, a fact we exploit later. Then

$$n^* \approx N + K \sqrt{[(A/\pi)(1+1/4K^4)]} \tag{29}$$

revealing the meaning of K as proportional to the number of terms by which RS truncation has been smoothed, when t is large. Roughly, the leading sum Z_0 involves terms $n \leq N + K$, and the corrections $Z_{m \geq 3}$ involve terms $N - K \leq n \leq N + K$.

4. Quadratic phase approximation

In computations (§6), we shall use the series (18)–(20) with no approximations (except the replacement of $\theta(t)$ and its derivatives using the early terms of (24)), and it is these formulae which we shall generalize in §7. For $\zeta(s)$ we can, however, go much further, by studying the behaviour of the terms near the RS cut-off. By (25), this corresponds to $\xi = 0$. Therefore we write

$$n \equiv N(t) + k \tag{30}$$

and make use of

$$t = 2\pi[N(t) + p(t)]^2 \tag{31}$$

(cf. (5)) to expand $\theta(t) - t \ln n$ in the phases of the summands to second order in k . Thus for large t we have

$$[\theta(t) - t \ln n]_{\text{mod } 2\pi} = \pi N + \pi k + 2\pi p^2 - \frac{1}{8}\pi - 4\pi p k + O\{(p - k)^3/N\}. \tag{32}$$

Similarly, $\xi(n, t) = (k - p)/N + O\{(k - p)/N\}^2$. (33)

We use these approximations differently for Z_0 and $Z_{m \geq 3}$. In Z_0 the aim is to understand the connection with RS. First we write, in (19),

$$\frac{1}{2}\text{Erfc}(x) = \Theta(-x) + \frac{1}{2}\text{Erfc}(|x|)\text{sgn}(x), \tag{34}$$

where Θ denotes the unit step. To obtain the leading-order behaviour of the second term it is necessary in (19) to replace the phase by (32), and make the approximation $\xi = 0$. Then the dependence on K disappears, and we obtain (Keating 1992*b*)

$$\begin{aligned} Z_0(t) &\approx 2 \sum_{n=1}^N \frac{\cos\{\theta - t \ln n\}}{\sqrt{n}} + (-1)^N \left(\frac{2\pi}{t}\right)^{\frac{1}{4}} \\ &\times \text{Re exp}\left\{2i\pi\left(p^2 - \frac{1}{16}\right)\right\} \left(1 + \sum_{k=-\infty}^{\infty} \text{sgn}(k) (-1)^k \exp\{-4\pi i k p\}\right) \\ &= 2 \sum_{n=1}^N \frac{\cos\{\theta - t \ln n\}}{\sqrt{n}} - (-1)^N \left(\frac{2\pi}{t}\right)^{\frac{1}{4}} \Phi^{(0)}(p), \end{aligned} \tag{35}$$

which are precisely the main sum and first correction in RS (equation (4)). It is possible that more – perhaps all – terms of RS are contained in Z_0 and can be extracted by extending the expansion about $n = N$, but we have not pursued this.

In $Z_{m \geq 3}$ the ultimate aim will be to construct (§5) a theory of the high orders $m \geq 1$ of the m -series. First we replace the phase in (20) by (32) (this is valid under condition (38) below), but now it is necessary to replace ξ by (33) (rather than $\xi = 0$, which would give $Z_m = 0$). Thus after some reduction we find

$$\begin{aligned} Z_m(t, K) &\approx \frac{2(-1)^N}{\sqrt{\pi}} \left(\frac{t}{2}\right)^{m/2} \left(\frac{2\pi}{t}\right)^{\frac{1}{4}} \text{Re} \frac{(-i)^m b_m \exp\{2\pi i(p^2 - \frac{1}{16})\}}{Q^m} \\ &\times \sum_{k=-\infty}^{\infty} (-1)^k \exp\{-4\pi i p k\} \exp\left\{\frac{-\pi(k-p)^2}{Q^2}\right\} H_{m-1}\left\{\frac{(k-p)}{Q} \sqrt{\pi}\right\} \quad (m \geq 3). \end{aligned} \tag{36}$$

The sum over k can be transformed by the Poisson summation formula, giving a series of integrals which can be evaluated exactly (using eq. 7.374.6 of Gradshteyn & Ryzhik (1980), and $Q^2 \approx K^2 - \frac{1}{2}i$, which follows from (17) and the leading term of (24)). All phases cancel, and we obtain

$$\begin{aligned} Z_m(t, K) &\approx 2(-1)^N [\text{Im } b_m] \left(\frac{t}{2\pi}\right)^{m/2 - \frac{1}{4}} (2\pi)^{m-1} \\ &\times \sum_{l=-\infty}^{\infty} (-1)^{l(l+1)/2} (l + \frac{1}{2} - 2p)^{m-1} \exp\{-\pi K^2(2p - \frac{1}{2} - l)^2\} \quad (m \geq 3). \end{aligned} \tag{37}$$

This approximation will be valid if the neglected cubic terms in the expansion (32) of $\theta - t \ln n$ are small compared with π , that is if (cf. (29))

$$K \sqrt{[(A/\pi)(1 + 1/4K^4)]} < (\frac{3}{2}N)^{\frac{1}{3}} \sim t^{\frac{1}{6}}. \tag{38}$$

This condition supersedes (28) and therefore guarantees that the smoothing range of the n -sums is small compared with the size of the main sum of RS. Like (28), (38) is also compatible with $K \geq 1$ when t is large. A numerical test of this approximation will be presented in §6.

5. Late terms of the m -series

We can make use of (37) to estimate high orders ($m \gg 1$) of the expansion (18) if K is chosen to satisfy

$$1 \ll K \ll N^{\frac{1}{3}}. \tag{39}$$

This choice is a sensible compromise between K small (so that the n -sums are not too unwieldy) and K large, when as we shall see the corrections are small.

When K and m are large, the sum over l in (37) is dominated by its biggest term, namely

$$l = \text{nearest integer to } 2p - \frac{1}{2} \pm \sqrt{[(m-1)/2\pi K^2]}. \tag{40}$$

As m increases, the summand will equal

$$\pm x^{m-1} \exp\{-\pi K^2 x^2\} \tag{41}$$

with $x (= l - 2p + \frac{1}{2})$ varying irregularly over unit ranges including $x^* \equiv \pm \sqrt{[(m-1)/2\pi K^2]}$. Therefore we can estimate the sum by the average of its biggest term, namely

$$\begin{aligned} \sum_{l=-\infty}^{\infty} (-1)^{l(l+1)/2} (l + \frac{1}{2} - 2p)^{m-1} \exp\{-\pi K^2 (2p - \frac{1}{2} - l)^2\} \\ \approx \pm \int_{x^* - \frac{1}{2}}^{x^* + \frac{1}{2}} dx x^{m-1} \exp\{-\pi K^2 x^2\} \approx \pm \frac{(\frac{1}{2}m)!}{mK^m \pi^{m/2}}. \end{aligned} \tag{42}$$

We also require the form of the high expansion coefficients $b_m(t)$ defined by (16). In Appendix B we show that

$$b_m(t) \approx \left(\frac{2}{\pi^3 e m^2 t}\right)^{\frac{1}{4}} \frac{(-1)^m}{(t + \frac{1}{2}i)^m} \exp\{\frac{1}{8}i(2t - \pi)\} \quad (m \gg t). \tag{43}$$

Substituting (42) and (43) into (37), we obtain the estimate that on average

$$Z_m(t, K) \xrightarrow{m \rightarrow \infty} \pm (-1)^N \left(\frac{2}{tm^3 \pi^3 \sqrt{e}}\right)^{\frac{1}{2}} \sin\{\frac{1}{4}t - \frac{1}{8}\pi\} \frac{(\frac{1}{2}m)!}{F^m}, \tag{44}$$

where

$$F = -K \sqrt{\frac{1}{2}t}. \tag{45}$$

For large t , these terms decrease and then increase in typical ‘factorial/power’ fashion. It therefore appears that the m -series is a divergent asymptotic expansion, and we can expect (Dingle 1973) that the error is of the same order as the first omitted term. This is smallest when

$$\frac{1}{2}m = |F|^2, \quad \text{i.e. } m = m^* \approx K^2 t. \tag{46}$$

Thus the accuracy with which $Z(t)$ could be approximated by our representation (18)–(20), considered as a bare asymptotic series (that is without resummation), is

$$|Z_{m^*}(t, K)| \sim (tm^*)^{-\frac{1}{2}} \exp(-\frac{1}{2}m^*) \sim (1/t^2 K^3) \exp\{-\frac{1}{2}K^2 t\}. \tag{47}$$

We have encountered this ‘small exponential’ before. As shown in Appendix A, it is approximately the size of the term T_n in the series (13) for which the rapid decrease $\exp(-\ln^2 n)$ yields to the slow decrease $n^{-1} \ln^{-\frac{3}{2}} n$. This slow decrease, and the form of the divergence responsible for the least term (47), both originate in the branch

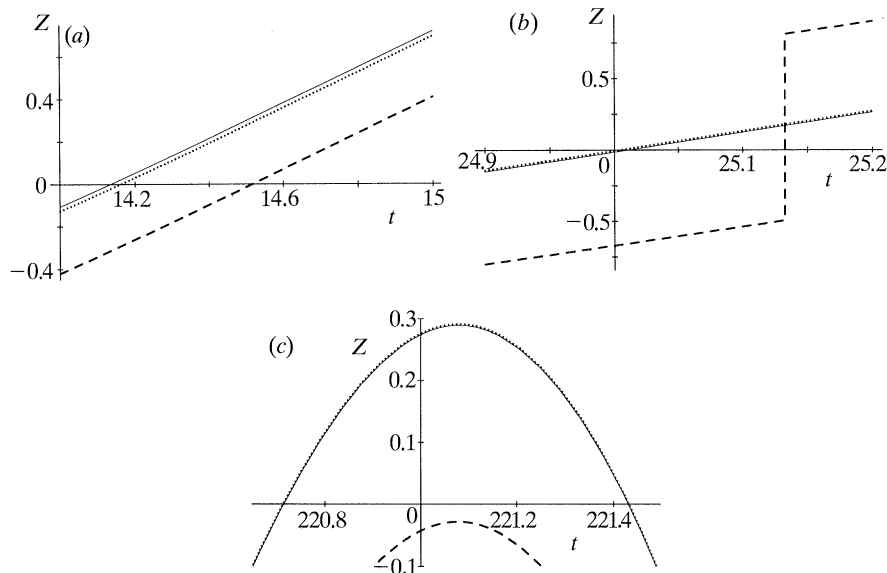


Figure 3. Comparison of lowest term Z_0 (equation (19)) for $K = 1/\sqrt{2}$ (dotted lines), the main sum of RS (dashed lines), and the exact Z (full lines), for different ranges of t . The number of terms used to compute Z_0 were (a) $n^* = 4$, (b) $n^* = 4$, (c) $n^* = 8$.

point of the integrand in (11). Now we can see that the influence of this branch point has been transformed: from the slow convergence of (13), via the expansion (16) whose n -sums (19) and (20) converge much faster, into a divergence of the m -series.

The least term (47) is smallest if K is as large as it can be, consistent with the restriction (38) implied by the quadratic approximation, so

$$|Z_{m^*}(t, K)| \gtrsim t^{-\frac{5}{2}} \exp(-t^{\frac{4}{3}}). \tag{48}$$

We do not expect to be able to achieve this enormous accuracy in practice, because the number m^* of terms in the m -series that would be required is, from (46),

$$m^* \sim N^{\frac{2}{3}} t \sim t^{\frac{4}{3}} \sim N^{\frac{8}{3}}, \tag{49}$$

i.e. much larger than the number N of terms in the n -sum in Z_0 (or the main sum of RS).

We would like to compare (48) with the best accuracy that could be achieved with RS by summing the j -series in (4) to its least term, but are frustrated by lack of knowledge of the late terms $\Phi^{(j)}(p)$.

6. Numerical illustrations

First we present (figure 3) pictorial comparisons between $Z(t)$ and the two lowest-order approximations: $Z_0(t)$ from our representation (19), and the main sum of RS. To make the n -sums as short as possible, we chose $K = 1/\sqrt{2}$ (cf. (27)), and for the convergence exponent we chose $A = 10$ (i.e. accuracy $\exp(-10) = 5 \times 10^{-5}$, which was adequate for pictures). The differences between Z_0 and the RS main sum were obvious under low magnification, but considerable magnification of small t -ranges was necessary to visually separate Z_0 from the exact Z .

Table 1. Computations of $Z(t)$ for t_1

t	$Z(t)$	$N(t)$	$p(t)$
18	2.336 7997	1	0.693
	Z_{approx}	$Z - Z_{\text{approx}}$	
RS main sum	1.993 457 1	3.4×10^{-1}	
+ $\Phi^{(0)}$	2.339 656 5	-2.8×10^{-3}	
+ $\Phi^{(1)}$	2.335 475 8	1.3×10^{-3}	
+ $\Phi^{(2)}$	2.336 816 0	-1.6×10^{-5}	
+ $\Phi^{(3)}$	2.336 765 9	3.4×10^{-5}	
+ $\Phi^{(4)}$	2.336 796 2	-3.5×10^{-6}	
$K = 0.5, n^* = 14$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	2.303 184 5	3.4×10^{-2}	
$Z_0 + Z_3$	2.288 540 6	4.8×10^{-2}	
$Z_0 + Z_3 + Z_4$	2.311 417 9	2.5×10^{-2}	
$K = 1.0, n^* = 14$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	2.329 718 3	7.1×10^{-3}	
$Z_0 + Z_3$	2.333 847 0	3.0×10^{-3}	
$Z_0 + Z_3 + Z_4$	2.336 161 0	6.4×10^{-4}	
$K = 1.5, n^* = 32$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	2.335 505 1	1.3×10^{-3}	
$Z_0 + Z_3$	2.336 631 5	1.7×10^{-4}	
$Z_0 + Z_3 + Z_4$	2.336 702 8	9.7×10^{-5}	

We chose three ranges which included Riemann zeros. Even as low as the first zero (figure 3a), Z_0 gives an excellent approximation. The superiority of Z_0 is particularly striking near the second zero (figure 3b), where the main sum of RS has a discontinuity. The RS main sum misses two zeros near the 90th (figure 3c), but these are captured by Z_0 , which is barely distinguishable from $Z(t)$.

For a more detailed exploration of the representation (18)–(20), we chose three values of t :

$$t_1 = 18, \quad t_2 = 7005.081\,86, \quad t_3 = 2\pi(200.15)^2 = 251\,704.544\,777\,28. \quad (50)$$

For each, we computed Z_0 and the first two corrections Z_3 and Z_4 , for several values of K . We used the asymptotic approximation (24) in $\theta(t)$ and in the quantities $Q(K, t)$, $\xi(n, t)$, $b_3(t)$ and $b_4(t)$ dependent upon it (cf. (B 4)). For convenience we show the explicit formulae for Z_3 and Z_4 :

$$Z_3(t, K) = -\frac{1}{12\pi} \left(\frac{2\pi}{t}\right)^{\frac{1}{2}} \operatorname{Re} \frac{1}{Q^3(K, t)} \sum_{n=1}^{n^*} \frac{\exp\{i[\theta(t) - t \ln n]\}}{\sqrt{n}} \left[1 - \frac{\xi^2(n, t) t}{Q^2(K, t)}\right] \exp\left\{\frac{-\xi(n, t)^2 t}{2Q^2(K, t)}\right\},$$

$$Z_4(t, K) = \frac{1}{8\pi} \left(\frac{2\pi}{t}\right)^{\frac{1}{2}} \operatorname{Re} \frac{1}{Q^5(K, t)} \sum_{n=1}^{n^*} \frac{\exp\{i[\theta(t) - t \ln n]\}}{\sqrt{n}} \times \xi(n, t) \left[1 - \frac{\xi^2(n, t) t}{3Q^2(K, t)}\right] \exp\left\{\frac{-\xi(n, t)^2 t}{2Q^2(K, t)}\right\}. \quad (51)$$

Table 2. Computations of $Z(t)$ for t_2

t	$Z(t)$	$N(t)$	$p(t)$
7005.08186	0.00396735727731	33	0.390
	Z_{approx}	$Z - Z_{\text{approx}}$	
RS main sum	-0.06600396768502	7.0×10^{-2}	
+ $\Phi^{(0)}$	0.00393683499809	3.1×10^{-5}	
+ $\Phi^{(1)}$	0.00396655239702	8.0×10^{-7}	
+ $\Phi^{(2)}$	0.00396735603114	1.2×10^{-9}	
+ $\Phi^{(3)}$	0.00396735721927	5.8×10^{-11}	
+ $\Phi^{(4)}$	0.00396735727731	$< 4.4 \times 10^{-13}$	
	Z_{approx}	$Z - Z_{\text{approx}}$	
$K = 1, n^* = 37$			
Z_0	0.00399124165286	-2.4×10^{-5}	
$Z_0 + Z_3$	0.00396599955999	1.4×10^{-6}	
$Z_0 + Z_3 + Z_4$	0.00396736308864	-5.8×10^{-9}	
	Z_{approx}	$Z - Z_{\text{approx}}$	
$K = 3, n^* = 44$			
Z_0	0.00396145445096	5.9×10^{-6}	
$Z_0 + Z_3$	0.00396733343461	2.4×10^{-8}	
$Z_0 + Z_3 + Z_4$	0.00396735718159	9.6×10^{-11}	
	Z_{approx}	$Z - Z_{\text{approx}}$	
$K = 10, n^* = 88$			
Z_0	0.00396747696881	-1.2×10^{-7}	
$Z_0 + Z_3$	0.00396735693288	3.4×10^{-10}	
$Z_0 + Z_3 + Z_4$	0.00396735728143	-4.1×10^{-12}	

The upper limits n^* were chosen according to (27) with $A = 33$, thereby ensuring convergence of the sums to $\exp(-33) = 5 \times 10^{-15}$. For t_1 , we also evaluated Z_0 , Z_3 and Z_4 using the exact formula (2) for $\theta(t)$, and confirmed that even for this small value the errors introduced by (24) are small compared with the deviations from the exact $Z(t)$ of Z_0 , $Z_0 + Z_3$ and $Z_0 + Z_3 + Z_4$.

For comparison, we computed $Z(t)$ by RS, including the main sum and five corrections (that is, $\Phi^{(0)}$ through $\Phi^{(4)}$ in (4)). The bound (7) ensured that in all cases the errors of RS were small compared with those of Z_0 , Z_3 and Z_4 , and we confirmed this with a more accurate evaluation of $Z(t_1)$.

Tables 1–3 show the results of these computations, which we now discuss. The first value t_1 is very low; it lies between the first two Riemann zeros. As table 1 shows, the RS improves quite slowly as more terms are included. The same is true of our series, especially for $K = 0.5$; this is the only case where we approach the least term of the m -series as predicted by (46), which gives $m^* \sim 4.5$. For the higher values, $K = 1$ and $K = 1.5$, Z_3 and Z_4 do improve significantly on Z_0 , which is itself better than the main sum of RS in all three cases. There is a price for this improvement: because t_1 is so small, the number n^* of terms in the n -sums of Z_m is always much bigger than the number of terms in the main sum of RS (here $N = 1$), i.e. the condition (28) is violated.

The value of t_2 is chosen between two close Riemann zeros, where Z is very small

Table 3. Computations of $Z(t)$ for t_3

t	$Z(t)$	$N(t)$	$p(t)$
251 704.544 777 283 6	-1.463 773 120 222 623	200	0.15
	Z_{approx}	$Z - Z_{\text{approx}}$	
RS main sum	-1.419 501 811 072 478	-4.4×10^{-2}	
+ $\Phi^{(0)}$	-1.463 770 667 363 168	-2.5×10^{-6}	
+ $\Phi^{(1)}$	-1.463 773 114 608 635	-5.6×10^{-9}	
+ $\Phi^{(2)}$	-1.463 773 120 222 490	-1.3×10^{-13}	
+ $\Phi^{(3)}$	-1.463 773 120 222 619	-4.6×10^{-15}	
+ $\Phi^{(4)}$	-1.463 773 120 222 623	$< 2.4 \times 10^{-17}$	
$K = 1, n^* = 203$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	-1.463 766 937 951 2	-6.1×10^{-6}	
$Z_0 + Z_3$	-1.463 773 108 489 4	-1.2×10^{-8}	
$Z_0 + Z_3 + Z_4$	-1.463 773 120 211 0	-1.2×10^{-11}	
$K = 3, n^* = 210$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	-1.463 772 335 497 91	-7.8×10^{-7}	
$Z_0 + Z_3$	-1.463 773 120 583 50	3.6×10^{-10}	
$Z_0 + Z_3 + Z_4$	-1.463 773 120 221 83	-9.9×10^{-13}	
$K = 10, n^* = 235$	Z_{approx}	$Z - Z_{\text{approx}}$	
Z_0	-1.463 773 124 118 41	3.9×10^{-9}	
$Z_0 + Z_3$	-1.463 773 120 220 92	-1.7×10^{-12}	
$Z_0 + Z_3 + Z_4$	-1.463 773 120 222 64	1.7×10^{-14}	

(this is a near counterexample to the Riemann hypothesis). The main sum of RS misses both zeros by predicting (table 2) the wrong sign for Z (cf. figure 3c, which shows a similar occurrence for a smaller t); the first correction $\Phi^{(0)}$ gives a much better approximation, and with higher corrections the errors decrease rapidly. For all three values of K , Z_0 is much more accurate than the main sum of RS, and Z_3 and Z_4 give much better approximations still. Note that for $K = 1$ and $K = 3$ the number of terms n^* is not much larger than the value $N(t_2) = 33$ for RS; both satisfy (28), and $K = 1$ also satisfies the condition (38) for the validity of the quadratic approximation.

To represent what we expect to happen in the truly asymptotic region, t_3 is chosen so that the main sum of RS has $N(t_2) = 200$ terms. The main sum gives an error of a few percent. For all K in table 3, n^* is not much larger than N , yet Z_0 is better than the main sum of RS by between four and seven orders of magnitude. The improvements with Z_3 and Z_4 are each between two and three orders of magnitude, which is comparable to the improvement with extra terms of RS. All three K values satisfy (28), and $K = 1$ and $K = 3$ also satisfy the condition (38) for the validity of the quadratic approximation.

In all cases, except when $t = t_1$ and $K = 0.5$, the already accurate approximation provided by Z_0 was greatly improved by including Z_3 and Z_4 . Consistent with this rapid convergence, we noticed that each error was very close to the next omitted term.

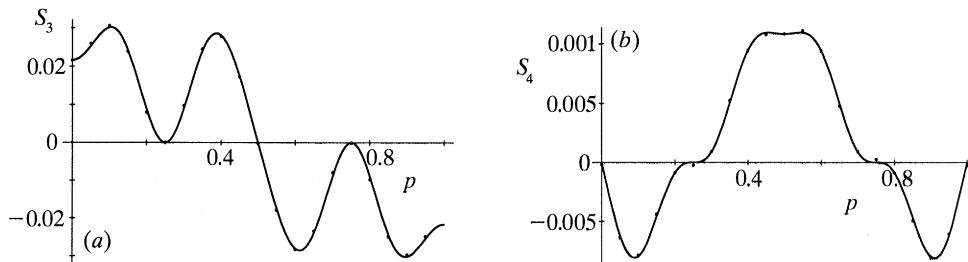


Figure 4. Comparison of S_m (points), defined by the second member of (52), with the quadratic approximation S_m^{quad} (full lines), defined by the third member of (52), with $N = 200$ and $K = 2$, for (a) $m = 3$, (b) $m = 4$.

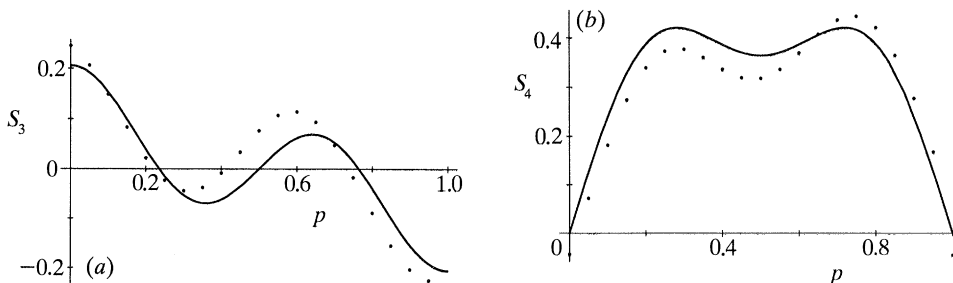


Figure 5. As figure 4, with $N = 2$ and $K = 1/\sqrt{2}$.

The estimates in §5 of late terms in the series Z_m depended on the quadratic phase approximation of §4. In figures 4 and 5 we illustrate this approximation for Z_3 and Z_4 as $p(t)$ ranges from 0 to 1, that is (31) as t ranges from $2\pi N^2$ to $2\pi(N+1)^2$. From (37) and (B 4), the quadratic approximation can be written

$$\begin{aligned}
 S_m(N, p, K) &\equiv 6(-1)^{N+1} (m-3) (N+p)^{m-\frac{3}{2}} Z_m(2\pi(N+p)^2, K) \\
 &\approx \sum_{l=-\infty}^{\infty} (-1)^{l(l+1)/2} (2p-l-\frac{1}{2})^{m-1} \exp\{-\pi K^2(2p-\frac{1}{2}-l)^2\} \\
 &\equiv S_m^{\text{quad}}(p, K) \quad (m = 3, 4).
 \end{aligned}
 \tag{52}$$

Figure 4 shows S and S^{quad} for $N = 200$ ($t \approx 250000$), and $K = 2$, which lies comfortably within the expected range of validity (38) of the quadratic approximation (for $A = 33$, (37) requires $K < 2.6$). As expected, the approximation is excellent over the whole range of p .

More surprising is figure 5, which shows S and S^{quad} for $N = 2$ ($25.1 < t < 56.5$). For these low values of t there is no K satisfying (38); nevertheless for $K = 1/\sqrt{2}$, where the left-hand side of (38) is smallest, the quadratic approximation still gives a good qualitative fit for all p .

7. Generalization to quantum spectral determinants

In the study of the spectra of quantum systems whose classical counterparts have chaotic trajectories (Berry 1987; Eckhardt 1988; Gutzwiller 1990), divergent or conditionally convergent series occur which are closely analogous to the Dirichlet series (3) for $\zeta(s)$. Our purpose in this section is to show that, remarkably, precisely

the resummation method we have used for $Z(t)$ can be applied directly, to yield an asymptotic series of convergent contributions for an analogous function in quantum mechanics.

This is the *quantum spectral determinant* $\Delta(E, \hbar)$, constructed as follows. In quantum mechanics the energy levels $E_j(\hbar)$ are the (necessarily real) eigenvalues of a hermitian operator (the quantum hamiltonian), obtained by quantizing, with Planck's constant \hbar , a classical hamiltonian function $H(\mathbf{q}, \mathbf{p})$ of phase space variables

$$\mathbf{q} = \{q_1, \dots, q_D\}, \quad \mathbf{p} = \{p_1, \dots, p_D\}. \tag{53}$$

Here D is the number of classical freedoms. We confine ourselves to chaotic systems, where the orbits generated by $H(\mathbf{q}, \mathbf{p})$ are all unstable. The spectral determinant of the hamiltonian operator is

$$\Delta(E, \hbar) \equiv \prod_j \{A\{E, E_j(\hbar)\} [E - E_j(\hbar)]\}, \tag{54}$$

where A , whose role is to make the product converge (Voros 1987), is a zero-free function which is real for real E and \hbar . Thus $\Delta(E, \hbar)$ is real for real E and \hbar , and its zeros are the quantum energies $E_j(\hbar)$. In this context, quantum chaology (Berry 1987) is the study of the small- \hbar , or semiclassical, asymptotics of the E_j , and is obviously related to the small- \hbar asymptotics of the real quantum spectral determinant $\Delta(E, \hbar)$.

For wide classes of system, E and \hbar are related by scaling, so that Δ depends only on one variable. Examples are the quantum mechanics of billiards, motion on compact curved surfaces, and particles in potentials which are homogeneous functions of \mathbf{q} . In such cases, the small- \hbar asymptotics and the large- E asymptotics are the same. In general, however, there is no scaling relation between E and \hbar , and the semiclassical and high-energy limits are not the same. Then we shall regard $\Delta(E, \hbar)$ as a function of complex \hbar with E fixed and real. In the analogy with $\zeta(\frac{1}{2} + it)$, the variable corresponding to t is $1/\hbar$. This choice of variable might seem odd but is in fact natural, because then we are quantizing a system with fixed classical mechanics, an important simplification for non-scaling systems, where the dynamics depends non-trivially on E (the same procedure has been used by Balian & Bloch (1974) and Berry & Tabor (1977)).

By semiclassical techniques based on the trace formula of Gutzwiller (1971) for $\ln \Delta$, Berry & Keating (1990) obtained the following semiclassical expression for the quantum spectral determinant,

$$\Delta(\hbar, E) \approx \Delta^{\text{sc}}(\hbar, E) \equiv B(E, \hbar) \exp\{i\pi \bar{\mathcal{N}}(E, \hbar)\} \sum_{n=0}^{\infty} C_n(E) \exp\{-i\mathcal{S}_n(E)/\hbar\} \tag{55}$$

in which the quantities have the following meanings. The sum is over pseudo-orbits, that is linear combinations of (primitive and repeated) periodic classical orbits (all unstable) with energy E ; n labels pseudo-orbits in increasing (pseudo) period \mathcal{T} . \mathcal{S}_n is the action of the n th pseudo-orbit, that is the sum of the actions of the periodic orbits of which it is composed. The coefficients C_n involve the stability exponents of the periodic orbits (which do not depend on \hbar), and the Maslov phases (Maslov & Fedoriuk 1981; Robbins 1991). The exponent $\bar{\mathcal{N}}(E, \hbar)$ is the smoothed spectral staircase, counting the mean number of levels with $E_j < E$. Semiclassical approximation (see Berry 1983) provides an asymptotic series (the analogue of (24)) for this quantity, whose leading term is

$$\bar{\mathcal{N}}(E, \hbar) \approx \Omega(E)/(2\pi\hbar)^D, \tag{56}$$

where Ω is the classical phase-space volume with energy less than E , namely

$$\Omega(E) = \iint dq dp \Theta\{E - H(q, p)\}. \quad (57)$$

Finally, $B(E, \hbar)$ is real and non-zero when E and \hbar are real. The quantum analogue of $Z(t)$ is $-\Delta(E, \hbar)/B(E, \hbar)$.

For real \hbar , the representation (55) is divergent (or, at best, only conditionally convergent (Sieber & Steiner 1991)). A simplified argument (Eckhardt & Aurell 1988; Keating 1992*b*) revealing the nature of the divergence is that the exponential decrease of the C_n for long orbits, namely

$$C_n(E) \sim \exp\{-\frac{1}{2}\lambda(E)\mathcal{T}_n(E)\} \quad \text{as } \mathcal{T}_n \rightarrow \infty, \quad (58)$$

where λ denotes the metric entropy, is dominated by the exponential proliferation of periodic (and pseudo) orbits, whose number $\nu(E) d\mathcal{T}$ between \mathcal{T} and $\mathcal{T} + d\mathcal{T}$ is

$$\nu(E) \sim \exp\{+\lambda(E)\mathcal{T}(E)\} \quad \text{as } \mathcal{T} \rightarrow \infty \quad (59)$$

(we are here assuming for simplicity that the metric and topological entropies are equal). Thus the sum diverges like the integral over \mathcal{T} of

$$\exp\{+\frac{1}{2}\lambda(E)\mathcal{T}(E)\}. \quad (60)$$

By making \hbar complex, (55) can be made absolutely convergent, the condition being that for long orbits

$$\text{Im } 1/\hbar < -\lambda\mathcal{T}/2\mathcal{S}. \quad (61)$$

Now, for the long-period orbits and pseudo-orbits of an ergodic system, \mathcal{S} and \mathcal{T} are proportional (Hannay & Ozorio de Almeida 1984), the precise relationship being

$$\mathcal{S} \approx \mathcal{T} D\Omega/\Omega'. \quad (62)$$

(This follows from

$$S = \int \mathbf{p} \cdot d\mathbf{q} = \int dt \mathbf{p} \cdot d\mathbf{q}/dt \rightarrow T \langle \mathbf{p} \cdot d\mathbf{q}/dt \rangle,$$

where $\langle \dots \rangle$ denotes ergodic averaging over the energy surface.) Thus the convergence condition (61) becomes

$$\text{Im } 1/\hbar < -\lambda(E)\Omega'(E)/2D\Omega(E). \quad (63)$$

This is the familiar ‘entropy barrier’, here expressed in terms of complex $1/\hbar$ rather than the more usual complex E .

For real \hbar , (55) fails, not only by diverging but by being not obviously real as the exact Δ must be. The analogy between this situation and that for the function $Z(t)$ defined by (1) has already been employed by Berry (1986) and Berry & Keating (1990) to conjecture for Δ^{sc} a manifestly real and finite approximate resummation of (55), analogous to the main sum of RS. Keating (1992*a*) has given a formal argument supporting this conjecture, as has Bogomolny (1992), and there is some computational support for the relation (Sieber & Steiner 1991). Now we can go much further, and give an *exact* resummation of (55), analogous to the representation of $Z(t)$ obtained in §3.

To demonstrate this, we use analytic continuation as in §2, in the variable $1/\hbar$. This requires an analogue of the functional equation $Z(t) = Z(-t)$. The analogue is the exact relation

$$\Delta(E, \hbar) = \Delta(E, -\hbar), \tag{64}$$

which holds because the eigenvalues E_j are independent of the sign of \hbar . This is true even for a system without time-reversal symmetry: \hbar -reversal changes the hermitian operator to its conjugate, leaving the eigenvalues unchanged. Cauchy's theorem can now be used as in (8) and (9), to yield the analogues of (10) and (11). The contour C_- can be taken to lie outside the entropy barrier (63), so (55) (the analogue of (3)) may be used as a valid semiclassical approximation to obtain an analytic continuation to real $1/\hbar$.

To obtain the analogue of the manifestly real expression (13) we need the analogue of (12). This must be

$$C_n(E) \exp\{i[\pi\bar{\mathcal{N}}(E, \hbar) - \mathcal{S}_n(E)/\hbar]\} \rightarrow [C_n(E) \exp\{i[\pi\bar{\mathcal{N}}(E, \hbar) - \mathcal{S}_n(E)/\hbar]\}]^* \quad \text{if } \hbar \rightarrow -\hbar. \tag{65}$$

Mere substitution of $-\hbar$ for \hbar is inadequate to demonstrate the truth of this formula. That it is the correct continuation of terms in the time-independent semiclassical approximation (including $\bar{\mathcal{N}}(E, \hbar)$ and the Maslov phases incorporated in C_n) follows from the behaviour under \hbar -reversal of the time-dependent Schrödinger equation from which semiclassical approximations can be derived (see Berry 1991). (For the Selberg zeta function (Balazs & Voros 1986), (65) follows from standard formulae.)

Thus we find the exact semiclassical resummation for real \hbar :

$$\Delta^{\text{sc}}(E, \hbar) = 2B(E, \hbar) \operatorname{Re} \sum_{n=0}^{\infty} U_n(E, \hbar), \tag{66}$$

where (cf. (11))

$$U_n(E, \hbar) = C_n(E) \exp\{i(\pi\bar{\mathcal{N}}(E, \hbar) - \mathcal{S}_n(E)/\hbar)\} \frac{1}{2\pi i} \int_{C_-} \frac{dz}{z} \gamma(z, \hbar) \times \exp\{i[\pi\bar{\mathcal{N}}(E, (\hbar^{-1} + z)^{-1}) - \pi\bar{\mathcal{N}}(E, \hbar) - z\mathcal{S}_n(E)]\}. \tag{67}$$

To convert this into a usable formula we again begin by choosing (*ad hoc*) the function $\gamma(z, \hbar)$ (cf. (14)):

$$\gamma(z, \hbar) = \exp(-\frac{1}{2}z^2K^2|\hbar|). \tag{68}$$

Next we follow the procedure of §3 by considering $1/\hbar > 0$ and expanding the exponential in powers of z (cf. (15)), as follows:

$$\exp\{i\pi[\bar{\mathcal{N}}(E, (\hbar^{-1} + z)^{-1}) - \bar{\mathcal{N}}(E, \hbar)]\} = \exp\{i\pi[z\bar{\mathcal{N}}_1(E, \hbar) + \frac{1}{2}z^2\bar{\mathcal{N}}_2(E, \hbar)]\} \left[1 + \sum_{m=3}^{\infty} z^m\beta_m(E, \hbar)\right], \tag{69}$$

where the subscripts on $\bar{\mathcal{N}}$ denote derivatives with respect to $1/\hbar$. Now we collect together the terms in z and z^2 , defining (cf. (17))

$$\left. \begin{aligned} \xi(n, \hbar, E) &\equiv \mathcal{S}_n(E) - \pi\bar{\mathcal{N}}_1(E, \hbar) \left(\sim \mathcal{S}_n(E) - \frac{D\Omega(E)}{2(2\pi\hbar)^{D-1}} \right), \\ Q^2(K, \hbar, E) &\equiv K^2 - \frac{i\pi}{\hbar} \bar{\mathcal{N}}_2(E, \hbar) \left(\sim K^2 - i \frac{D(D-1)\Omega(E)}{2(2\pi\hbar)^{D-1}} \right). \end{aligned} \right\} \tag{70}$$

Finally, the integrals over z in (67) can be evaluated exactly, giving (cf. (18)–(20)) the m -series

$$\Delta^{\text{sc}}(E, \hbar) = \Delta_0(E, \hbar, K) + \Delta_3(E, \hbar, K) + \Delta_4(E, \hbar, K) + \dots, \tag{71}$$

where

$$\begin{aligned} \Delta_0(E, \hbar, K) &= 2B(E, \hbar) \operatorname{Re} \sum_{n=0}^{\infty} C_n(E) \\ &\times \exp \{i[\pi \bar{\mathcal{N}}(E, \hbar) - \mathcal{S}_n(E)/\hbar]\} \frac{1}{2} \operatorname{Erfc} \left\{ \frac{\xi(n, \hbar, E)}{Q(K, \hbar, E)} \sqrt{\left(\frac{1}{2\hbar}\right)} \right\} \end{aligned} \tag{72}$$

and

$$\begin{aligned} \Delta_m(E, \hbar, K) &= (2B(E, \hbar)/\sqrt{\pi})(1/2\hbar)^{m/2} \\ &\times \operatorname{Re} \frac{(-i)^m \beta_m(E, \hbar)}{Q^m(K, \hbar, E)} \sum_{n=0}^{\infty} C_n(E) \exp \{i[\pi \bar{\mathcal{N}}(E, \hbar) - \mathcal{S}_n(E)/\hbar]\} \\ &\times \exp \left\{ \frac{-\xi^2(n, \hbar, E)}{2\hbar Q^2(K, \hbar, E)} \right\} H_{m-1} \left\{ \frac{\xi(n, \hbar, E)}{Q(K, \hbar, E)} \sqrt{\left(\frac{1}{2\hbar}\right)} \right\} \quad (m \geq 3). \end{aligned} \tag{73}$$

Previously, the arguments of Keating (1992*a*) were used in Keating (1992*b*) and Aurich & Steiner (1992) to obtain an approximation to the first term Δ_0 , corresponding to replacing Q by K .

We will not comment in detail on these formulae, because their structure is so similar to (18)–(20) for $Z(t)$, which we have already explored, but we do wish to make two remarks. The first concerns Δ_0 . This is analogous to the main sum of RS with the sharp cut-off smoothed away. The smoothing is centred on the pseudo-orbit for which ξ , given in (70), is zero. Because of the factor $\hbar^{-(D-1)}$ in the second term, this is a long pseudo-orbit, so \mathcal{S} can be replaced by its approximation (62). Thus when \mathcal{T} is large

$$\begin{aligned} \xi(n, \hbar, E) &\approx \frac{\mathcal{T}_n(E) D\Omega(E)}{\Omega'(E)} - \frac{D\Omega(E)}{2(2\pi\hbar)^{D-1}} \\ &= (D\Omega(E)/\Omega'(E)) [\mathcal{T}_n(E) - \pi\hbar\bar{d}(E, \hbar)], \end{aligned} \tag{74}$$

where

$$\bar{d}(E, \hbar) \approx \Omega'(E)/(2\pi\hbar)^D \tag{75}$$

is the semiclassical smoothed level density. The centre of the smoothing is therefore the pseudo-orbit n^* whose period is

$$\mathcal{T}_{n^*}(E) = \pi\hbar\bar{d}(E, \hbar). \tag{76}$$

It is satisfying that this result, here derived by analytic continuation of $1/\hbar$, is exactly that previously guessed (Berry 1986; Berry & Keating 1990), or obtained by analytic continuation of E (Keating 1992*a*). Note that the above derivation involves the non-trivial result (62), which requires the classical motion to be ergodic.

The second remark is that it would be interesting to study the convergence of the m -series (71) by investigating its late terms (i.e. Δ_m for large m).

We emphasize that (71)–(73) is an exact analytic continuation of the semiclassical formula (55), which completely eliminates the difficulties caused by the lack of convergence of Gutzwiller's trace formula. But in general (71)–(73) does not provide

an exact representation for the quantum spectral determinant $\Delta(E, \hbar)$, because (55) is an approximation, valid to lowest order in \hbar . In particular, the zeros of (71)–(73) will be semiclassical approximations to the exact eigenvalues $E_j(\hbar)$. To improve the approximation, it would be necessary to incorporate higher \hbar -corrections into (55). If this were done, analytic continuation could be carried out as we have done here, for each successive order of semiclassical approximation.

However, there is at least one case where the Gutzwiller trace formula, and the semiclassical quantum spectral determinant (55) derived from it, are not semiclassical approximations but are exact (although of course not absolutely convergent within the entropy barrier). This is the spectral determinant for the Laplace–Beltrami operator on compact surfaces of constant negative curvature, for which the logarithm of (55) is the celebrated Selberg trace formula (Balazs & Voros 1986). For this system, our formulae (71)–(73) should provide an exact analytic continuation, enabling arbitrarily high eigenvalues to be determined from the periodic geodesics with no approximation (except the exponentially small error resulting from truncating the series of Δ_m (cf. (47) and (48)), which can be made arbitrarily small by increasing K). This procedure should converge much more rapidly than gaussian smoothing of the spectral density (logarithmic derivative of $\Delta(E, \hbar)$) as used by Aurich *et al.* (1988) (analogous to Delsarte’s (1966) regularization of $\ln \zeta(\frac{1}{2} + it)$), which requires approximately N^2 , rather than N , terms.

We do not wish to imply that the exact regularization of the semiclassical spectral determinant solves all problems in the quantum chaos of spectra. Several difficulties remain. First, there is the question of higher-order \hbar -corrections; we expect this to be crucial in resolving groups of close-lying eigenvalues. Second, there is the question of whether the regularization guarantees that the approximate eigenvalues will be real, like the exact ones; we believe it does not. Third, there is the difficulty caused by the fact that even with the (approximate) cut-off (76) the sums in the contributions Δ_m involve exponentially many pseudo-orbits and so are cumbersome; here the curvature expansions (Cvitanovic & Eckhardt 1989) and related ideas for pruning the pseudo-orbits (Bogomolny 1992) could prove important. Finally, there is the question of the statistics of the zeros of the semiclassical spectral determinant, and their relation to the universal statistics of random-matrix theory (Bohigas & Giannoni 1984; Berry 1985, 1988; Keating 1992*b*).

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Appendix A. Convergence of the analytically continued Dirichlet series

Here our aim is to estimate high orders in the n -sum (13), that is T_n for n much larger than the cutoff N in RS (equation (5)), and thereby investigate the convergence of (13). Thus we must study the integral

$$T_n(t) = \frac{\exp\{-it \ln n\}}{\sqrt{n}} \frac{1}{2\pi i} \int_{C_-} \frac{dz}{z} \exp\left\{-iz \ln n - \frac{K^2 z^2}{2t}\right\} \exp\{i\theta(z+t)\}. \quad (\text{A } 1)$$

There are two contributions, one of which dominates when $N \ll n \ll N \exp(K^2)$ and the other when $n \gg N \exp(K^2)$; they originate respectively from a saddle and a branch point in the z plane of integration.

A sufficiently good approximation to the position of the saddle can be found by including the first exponential in (A 1) and the term of first order in z in the second exponential, and then using Stirling's formula (24). With (5) we find

$$z_{\text{saddle}} \sim -i(t/K^2) \ln(n/N(t)). \tag{A 2}$$

Expanding to second order about this saddle and evaluating the resulting gaussian integral we obtain

$$|T_n|_{\text{saddle}} \approx \frac{K}{\ln(n/N) \sqrt{(2\pi nt)}} \exp \left\{ -\frac{t}{2K^2} \ln^2 \left(\frac{n}{N} \right) \right\} \\ \times \exp \left\{ \frac{1}{2} \operatorname{Re} [(t + z_{\text{saddle}}) \ln(1 + z_{\text{saddle}}/t) - z_{\text{saddle}}] \right\}. \tag{A 3}$$

The first exponential dominates the second.

Ultimately, convergence of (11) is determined not by this saddle contribution but by the nearest singularity to which the integration contour C_- can be deformed. This is the square-root branch point corresponding to one of the zeros of the gamma function in (2) namely

$$z_{\text{branch}} = -t - \frac{1}{2}i. \tag{A 4}$$

We write $z = z_{\text{branch}} - i\sigma$, expand the integrand to lowest order in σ , and integrate along both sides of the cut descending from z_{branch} . Thus we find, after a little reduction,

$$T_{n\text{branch}} = \frac{i \exp \left\{ -(K^2/2t) (t + \frac{1}{2}i)^2 \right\}}{n(t + \frac{1}{2}i) \pi \sqrt{2}} \int_0^\infty d\sigma \sqrt{\sigma} \exp \left\{ -\sigma \left(\ln n \sqrt{\pi} + iK^2 \left(1 + \frac{i}{2t} \right) \right) \right\} \\ \approx \frac{i \exp \left\{ -\frac{1}{2}K^2 t \right\}}{2 \sqrt{(2\pi) tn \ln^{\frac{3}{2}} n}}, \tag{A 5}$$

where the approximation requires $t \gg 1$. This decrease is very slow, but is sufficient to make the n -sum in (11) converge, because

$$\sum_{n=M}^\infty \frac{1}{n \ln^{\frac{3}{2}} n} \xrightarrow{M \rightarrow \infty} \frac{1}{2 \ln^{\frac{1}{2}} M}. \tag{A 6}$$

The crossover between the saddle and branch contributions to T_n occurs when their dominant exponentials are equal, that is when

$$(t/2K^2) \ln^2(n/N) = \frac{1}{2}K^2 t, \quad \text{i.e. } n = N \exp(K^2) \tag{A 7}$$

as asserted earlier. Summarizing, we have, retaining only leading orders,

$$\left. \begin{aligned} |T_n| &\sim \exp \left\{ -(t/2K^2) \ln^2(n/N) \right\} \quad (N \ll n \ll N \exp(K^2)), \\ |T_n| &\sim \exp \left\{ -\frac{1}{2}K^2 t \right\} / n \ln^{\frac{3}{2}} n \quad (n \gg N \exp(K^2)). \end{aligned} \right\} \tag{A 8}$$

Appendix B. Asymptotics of the expansion coefficients

We seek approximations for the quantities $b_m(t)$ defined by (15) and (16), for t large with m fixed, and also for t large with $m \gg t$. Defining

$$a_s(t) \equiv [\operatorname{Im} i^s \psi^{(s-1)}(\frac{1}{4} + \frac{1}{2}it)] / 2^s s! \tag{B 1}$$

our problem is to solve

$$\sum_{m=3}^\infty z^m b_m = \exp \left\{ i \sum_{s=3}^\infty z^s a_s \right\} - 1 \tag{B 2}$$

for b_m .

For low m this can easily be achieved by direct expansion of the exponential and use of the following approximation (Abramowitz & Stegun 1964) for polygamma functions:

$$\psi^{(n)}(w) \approx (-1)^{n+1} (n-1)!/w^n \quad (|w| \text{ large, } n \text{ fixed}). \tag{B 3}$$

We find

$$b_3 = ia_3 \approx -\frac{i}{12t^2}, \quad b_4 = ia_4 \approx \frac{i}{24t^3},$$

$$b_5 = ia_5 \approx -\frac{i}{40t^4}, \quad b_6 = ia_6 - \frac{1}{2}a_3^2 \approx \frac{i}{60t^5} - \frac{1}{288t^4}. \tag{B 4}$$

The direct calculation is much more difficult for large m . For a start, polygamma functions of high order have an asymptotic approximation different from (B 3) (in fact (B 3) must be multiplied by nw). And each high b_m is a complicated combination of many a_m , ranging from approximately

$$\frac{(ia_3)^{m/3}}{(\frac{1}{3}m)!} \approx \frac{(-\frac{1}{12}i)^{m/3}}{(\frac{1}{3}m)! t^{2m/3}} \tag{B 5}$$

to

$$ia_m \sim 1/t^m \tag{B 6}$$

and neither extreme dominates. Therefore we adopt a different strategy, based on Darboux's principle of the nearest singularity (Dingle 1973).

To apply this, we first write the solution of (15) as

$$b_m = G^{(m)}(0)/m!, \tag{B 7}$$

where the superscript denotes the m th derivative, and (cf. (2))

$$G(z) = \left[\frac{\Gamma\{\frac{1}{4} + \frac{1}{2}i(t+z)\}}{\Gamma\{\frac{1}{4} - \frac{1}{2}i(t+z)\}} \right]^{\frac{1}{2}} \exp\{i\chi(z)\} \tag{B 8}$$

with

$$\chi(z) = -[\frac{1}{2}(t+z) \ln \pi + \theta(t) + z\theta'(t) + \frac{1}{2}z^2\theta''(t)] \tag{B 9}$$

(we do not indicate the t dependence explicitly).

Darboux's principle asserts that the high derivatives $G^{(m)}(0)$ are determined by the singularities of $G(z)$ (this can be justified by writing b_m as a contour integral surrounding $z = 0$, and expanding the contour to hit the singularities). In (B 8) the singularities are square-root branch points at the poles of the gamma functions, namely

$$z = -t \pm \frac{1}{2}i(2n + \frac{1}{2}), \quad n = 0, 1, \dots \tag{B 10}$$

Of these, the dominant contribution comes from

$$z = -t + \frac{1}{2}i \tag{B 11}$$

(this can be confirmed by repeating for the other branch points the argument which follows).

Expanding about this point, we find

$$G(z) \xrightarrow{\text{as } z \rightarrow -t + \frac{1}{2}i} \frac{\sqrt{2} \exp\{-\frac{1}{4}i\pi\}}{\pi^{\frac{1}{2}} [z - (-t + \frac{1}{2}i)]^{\frac{1}{2}}} \exp\{i\chi(-t + \frac{1}{2}i)\}. \tag{B 12}$$

Differentiating m times, where m is large, swells the domain of applicability of this formula. Setting $z = 0$, using (B 7), and approximating the function χ for large t with the aid of (B 9) and (24), then leads to

$$b_m(t) \xrightarrow{m \rightarrow \infty} \left(\frac{2}{\pi^3 e m^2 t} \right)^{\frac{1}{4}} \frac{(-1)^m}{(t + \frac{1}{2}i)^m} \exp \left\{ \frac{1}{8}i(2t - \pi) \right\}. \quad (\text{B } 13)$$

We need to know how large m must be in order for this limiting form to be a good approximation. The answer requires knowledge of any competing contributions to b_m that are eventually dominated by (B 13). The relevant contribution comes from a saddle of the integrand (cf. Appendix A) of the loop integral representing b_m , namely

$$b_m = \frac{1}{2\pi i} \oint dz \frac{G(z)}{z^{m+1}}, \quad (\text{B } 14)$$

where the loop encircles the origin. The relevant saddle is close to $z \approx (t^2 m)^{\frac{1}{3}}$; it gives a contribution whose dominant factors differ from those in (B 13) by the replacement of t^{-m} by $(t^2 m)^{-m/3}$ (the contribution is the same as that given by (B 5)). The crossover, beyond which (B 13) dominates this saddle contribution, is therefore $m \sim t$. This is consistent with Darboux's principle: for $m < t$ the saddle is closer to $z = 0$ than the branch point $z = -t + \frac{1}{2}i$ which generates (B 13), and for $m > t$ the branch point is nearer.

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