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Resummation and the Turning-Points of Zeta Functions

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We review various periodic orbit formulae for the zeta function whose zeros represent semiclassical approximations to the energy levels of chaotic systems. In particular, we focus on the Riemann-Siegel-resummed expression. The emphasis is on the ability of such formulae to reproduce the analytic properties of the spectral determinant, whose zeros are the exact quantum levels. As an example, the distribution of turning points is investigated and compared.

Resummation and the turning-points of zeta functions

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Abstract. We review various periodic orbit formulae for the zeta function whose zeros represent semiclassical approximations to the energy levels of chaotic systems. In particular, we focus on the Riemann-Siegel-resummed expression. The emphasis is on the ability of such formulae to reproduce the analytic properties of the spetral determinant, whose zeros are the exact quantum levels. As an example, the distribution of turning points is investigated and compared.

One of the central aims of quantum chaology is to calculate approximations to the energy levels of chaotic systems using classical trajectories. Most recent studies of this problem have been based on the semiclassical zeta function (Voros 1988), whose zeros represent the levels to leading order as $\hbar \to 0$. Using the trace formula (Gutzwiller 1971), this zeta-function can be expressed as a product over all periodic orbits of the underlying classical dynamics, and hence these orbits can, at the least in principle, be used to compute the zeros. The difficulty is, however, that the product does not converge in the region where the zeros lie. The goal has therefore been to find a formula that provides an analytic continuation outside its domain of convergence.

The two main candidates purporting to provide such a continuation are the cycle expansion (Cvitanovic & Eckhardt 1989, Eckhardt 1993) and Riemann-Siegel-type formulae (Berry & Keating 1990, Keating 1992, Berry & Keating 1992). Both are based on resummations of the series obtained by expanding the orbit product. In the case of the cycle expansion, this involves exploiting the shadowing property of the orbits in hyperbolic systems to generate a conditionally convergent re-ordering of the series. The motivation behind the approach is thus firmly rooted in classical mechanics, and its success relies on the system in question being sufficiently hyperbolic to possess a complete symbolic dynamics. The Riemann-Siegel method is almost entirely complementary in these respects. It is based on the analytical imposition of quantum hermiticity, in the form of a functional equation, onto the semiclassical series representing the zeta function. The result is an asymptotic expansion, each term of which is given by an absolutely convergent orbit sum that is effectively truncated at half the Heisenberg time T_H ($= 2\pi\hbar$ divided by the mean level separation). In this case, the motivation and the success of the approach relies upon the ability of leading-order semiclassical approximations to capture the essentially quantum structure un-

1 Semiclassical zeta functions and resummation

For ease of presentation, I will consider the case of a 2-dimensional billard system corresponding to a domain Γ with boundary $\partial\Gamma$, although the results are much more general. The energy levels E_n are then the eigenvalues of the Laplacian in Γ with Dirichlet boundary conditions on $\partial\Gamma$; that is

$$\nabla^2\Psi_n = -E_n\Psi_n \tag{1}$$

in Γ, and $\Psi = 0$ on $\partial\Gamma$. These engergy levels are, by construction, the only zeros of the spectral determinant

$$\Delta(E) = \prod_n \left(1 - \frac{E}{E_n}\right)\exp(E/E_n), \tag{2}$$

where the product converges and defines an entire function in the complex E-plane. Alternatively, and more usefully for our purposes here, Δ can also be written as a function of the momentum k, where $E = k^2$, and the corresponding momentum eigenvalues k_n, defined by $E_n = k_n^2$:

$$\Delta(k^2) = \prod_n \left(1 + \frac{k}{k_n}\right)\left(1 - \frac{k}{k_n}\right)\exp(k^2/k_n^2). \tag{3}$$

In the semiclassical limit, as $|k| \to \infty$, the density of momentum states

$$d_k(x) = \sum_n \{\delta(x - k_n) + \delta(x + k_n)\} \tag{4}$$

has a leading order asymptotic representation as a sum over all periodic orbits of the classical hamiltonian flow in Γ (Gutzwiller 1971). This in turn implies (Voros 1988, Keating & Sieber 1994) that in the same limit

$$\Delta(k^2) \approx B(k^2)\exp\left(-i\pi\bar{N}_k(k)\right)\frac{\zeta_s(k)}{\zeta_s(0)}, \tag{5}$$

where B is real and non-zero when k is real; $\bar{N}_k(x)$ is the mean of the momentum staircase N_k, defined by

$$N_k(x) = \int_0^x d_k(x')dx', \tag{6}$$

and so is an odd function of x (since d_k is even); and ζ_s is the semiclassical zeta function defined by

$$\zeta_s(k) = \prod_p \prod_{m=0}^{\infty}\left(1 - \sigma_p^m \exp\left\{-(\tfrac{1}{2} + m)\lambda_p l_p + ikl_p - \tfrac{1}{2}i\pi\mu_p\right\}\right) \tag{7}$$

where l_p is the length and λ_p the Liapunov exponent of the pth periodic orbit, μ_p is a Maslov-type index (Robbins 1991), and σ_p is the sign of the eigenvalues of orbits have no intrinsic knowledge of quantum hermiticity. This is clearly related to the subtle convergence properties of the expansions involved, since, for example, if the orbit product (7) is substituted into (10) the two sides will not both converge simultaneously at any given point in the complex plane. It is in this observation that one sees the first hint that solving the hermiticity problem may also lead to a solution of the convergence problem.

The functional equation may be imposed upon the pseudo-orbit sum in the following way (for full details see Berry and Keating 1992). First

$$Z(k) = \exp\left(-i\pi\bar{N}_k(k)\right)\zeta_s(k) \tag{11}$$

is written in the form

$$Z(k) = \oint Z(k+s)\exp\left(-s^2\alpha^2/2|k|\right)\frac{ds}{2\pi i s}, \tag{12}$$

where the contour contains the origin, but no other singularities. This holds for any real α. Choosing the contour to be symmetric with respect to reflection through the origin, using the fact that the functional equation implies that $Z(-s) = Z(s)$, and assuming that Z is analytic in a strip about the real axis, we then have that

$$Z(k) = \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon}\{Z(s+k)+Z(s-k)\}\exp\left(-s^2\alpha^2/2|k|\right)\frac{ds}{2\pi i s}. \tag{13}$$

Finally, lifting the contour up into the region where the pseudo-orbit sum converges (assuming this is possible) and integrating term-by-term leads to the main result, namely that to leading semiclassical order when k is real

$$Z(k) = Z_0(k,\alpha) + \sum_{m=3}^{\infty} Z_m(k,\alpha), \tag{14}$$

where if

$$\gamma_n(k) = L_n - \pi\bar{N}'_k(k), \tag{15}$$

$$Q^2(k,\alpha) = \alpha^2 + i\pi k\bar{N}''_k(k), \tag{16}$$

and $b_m(k)$ is defined by

$$\exp\left\{-i\pi\bar{N}_k(k+x) + i\pi\bar{N}_k(k) + i\pi x\bar{N}'_k(k) + \tfrac{1}{2}i\pi x^2\bar{N}''_k(k)\right\} = 1+\sum_{m=3}^{\infty} b_m(k)x^m, \tag{17}$$

then

$$Z_0(k,\alpha) = 2\mathrm{Re}\left[\exp\left(-i\pi\bar{N}_k(k)\right)\sum_n C_n\exp\left(ikL_n\right)\tfrac{1}{2}\,\mathrm{erfc}\left(\frac{\gamma_n(k)}{Q(k,\alpha)}\sqrt{\frac{k}{2}}\right)\right] \tag{18}$$

is only a leading order semiclassical object, and so it is important to test the predictions explicitly in indiviual chaotic systems. One obvious way of doing this is to compare the contributions directly by summing up the corresponding sets of orbits. This has been done for the hyperbola billiard (Keating & Sieber 1994), and the results provide a detailed confirmation of the relationship. Another test is to use the resummed expression (14) to compute approximations to the energy levels. Here too the numerical support is strong. For example, in the case of the hyperbola billiard the first 46 levels were computed and the modulus of the error relative to the exact quantum values found to have an average of 3.4% and a standard deviation of 4.7% of the mean level spacing. Similar results have been reported for the wedge billard (Szeredi & Goodings 1993). However, as noted above, the ability to locate the positions of the zeros of the zeta function does not represent a particularly strict benchmark for the method of calculation employed. Indeed, good numerical results have also been obtained using unresummed formulae. It is for this reason that we now turn to the analytic structure of Z in order to provide a more discriminating test of the ideas associated with resummation.

2 Turning Points

The turning points of the quantum spectral determinant have a simple distribution: when E is real $\Delta(E)$ has a single maximum or, alternatively, a single minimum between each pair of neighbouring zeros. This fact may be proved as follows. Differentiating (1) gives

$$\frac{d}{dE}\left(\frac{\Delta'}{\Delta}\right) = -\sum_n \frac{1}{(E-E_n)^2} \ , \tag{20}$$

which in turn implies that

$$\frac{d}{dE}\left(\frac{\Delta'}{\Delta}\right) < 0 \qquad \text{for} \qquad E \neq E_n. \tag{21}$$

Thus between consecutive zeros of $\Delta, \Delta'/\Delta$ is a monotonically decreasing function and so Δ' can itself have at most one zero. Obviously there must be either a maximum or a minimum in the range, and hence the result follows.

The question is, to what extend is the analytical behaviour just described respected by the various semiclassical formulae discussed in the previous section? This issue is important because it follows from (20) that any additional maxima and minima must be associated with complex zeros. It is thus related to the fundamental problem of how far quantum hermiticity is preserved in leading-order semiclassical formulae, since complex zeros represent complex, and hence spurious or unphysical, energy levels. A key point now is the fact that semiclassically it is more natural to calculate $Z(k)$, definded by (11), rather than Δ. It thus

Armed with these expressions for B it is a simple matter to repeat for F the analysis performed for Δ at the beginning of this section. Consider first the case of a general bounded billard. Clearly

$$\frac{d}{dE}\left(\frac{F'}{F}\right) = -\sum_n \frac{1}{(E-E_n)^2} - \left(\frac{A}{4\pi E} - \frac{C}{E^2}\right), \tag{29}$$

and so F'/F is a monotonically decreasing function provided the term in the brackets is positive. This is obviously the case for $E > \tilde{E}$, where

$$\tilde{E} = \frac{4\pi C}{A}. \tag{30}$$

Thus for $E > \tilde{E}$, F behaves in the same way as Δ in that it has only a single maximum or minimum between adjacent zeros. Typically $\tilde{E}$ is smaller than the value of the first energy level E_0 because, roughly speaking, $\bar{N}(E_0) \approx 1/2 \Rightarrow E_0 \approx 2\pi/A$, and for billiards with smooth boundaries $C = 1/6$. For $E < \tilde{E}$ there is a competition between the two terms on the left-hand-side in (29). Clearly as $E \to 0$ the second term wins, because it is unbounded. Hence there is the possibility that before the first energy level there may be both a maximum and a minimum, since the derivative of F'/F may, and generally will, change sign.

For the hypberbola billard

$$\frac{d}{dE}\left(\frac{F'}{F}\right) = -\sum_n \frac{1}{(E-E_n)^2} - \left(\frac{\log E}{8\pi E} + \frac{a+1}{8\pi E} - \frac{c^{\pm}}{E^2}\right). \tag{31}$$

Again, when the term in the brackets is positive, F'/F is a monotonically decreasing function and so F has only one maximum or one minimum between consecutive zeros. This is clearly the case for $E > \tilde{E}$, where

$$\frac{1}{8\pi}\log\tilde{E} + \frac{a+1}{8\pi} = \frac{c^{\pm}}{\tilde{E}}. \tag{32}$$

In the even symmetry there is no solution to this equation and so the behaviour just described persists down to $E = 0$. In the odd symmetry case there is one solution, which may be found numerically to be $\tilde{E} \approx 8.26$, that is, well below the first energy level $E_0 \approx 21.46$. Hence only below the first zero is the existence of two turning points possible. A detailed study of the balance between the terms in (31) shows that both a maximum and a minimum do indeed occur in this case.

3 Discussion

The distribution of the maxima and minima would not be of interest here if it did not distinguish between the resummed and unresummed formulae for the semiclassical approximation Z of F. Fortunately, it does. In particular, both functions have been studied in considerable detail for the hyperbola billiard

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