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LETTER TO THE EDITOR

False singularities in partial sums over closed orbits

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Abstract. The contribution to the spectral density from all the repetitions of a single classical closed orbit can have singularities that are not eigenenergies of the system. Only by summing over all different topologies of orbits do these false singularities get replaced by δ peaks at the true eigenenergies. We illustrate this with an example where the expansion and sum over repetitions are exact rather than asymptotic.

In studies of the energy spectra of quantum systems much use has been made of the semiclassical expansion of the density of states as a sum over the closed orbits of the corresponding classical system (Gutzwiller 1967, 1969, 1970, 1971, 1978, Balian and Bloch 1972, Berry and Tabor 1976, Berry 1983). It is known that this series has peculiar convergence properties and that all the periodic orbits must be included if there is to be any hope of getting the correct structure of any one singularity. In this letter we consider a case for which the expansion is exact (i.e. there are no asymptotic approximations), non-trivial (i.e. there are infinitely many topologically different primitive periodic orbits) and for which the sum over repetitions of a given primitive orbit can be performed analytically.

The system is the billiard on a torus: a spinless particle moving freely in a rectangular cell with periodic boundary conditions. This is integrable and has eigenenergies given, in suitable units, by

$$E_{n,m} = n^2 + m^2/\alpha \qquad (m, n \in \mathbb{Z}^2) \tag{1}$$

where α is the ratio of the lengths of the sides of the rectangle. The density of states is

$$d(E) = \sum_{n,m} \delta(E - E_{n,m}) \tag{2}$$

which, using the Poisson summation formula, may be written

$$d(E) = \sum_{M,N=-\infty} \int\int \mathrm{d}n\, \mathrm{d}m\, \delta(E - n^2 - m^2/\alpha^2) \exp[2\pi\mathrm{i}(nN + mM)]. \tag{3}$$

Putting $(n, m/\alpha) \equiv \boldsymbol{r}$ and $(N, \alpha M) \equiv \boldsymbol{R}$, we obtain

$$d(E) = \alpha\, \mathrm{Re} \sum_{\boldsymbol{R}} \int_0^{\pi} \mathrm{d}\theta\, \exp(2\pi\mathrm{i}R\sqrt{E}\cos\theta). \tag{4}$$

Points in the lattice $\boldsymbol{R}$ represent classical closed orbits winding round the torus N times in one direction and M in the other.

The term $\boldsymbol{R}=(0,0)$ gives the Weyl average density of states (Berry and Tabor 1976) which we write as $\bar{d}(E)$. The sum over points $\boldsymbol{R}\neq(0,0)$ can be split into a sum over primitive closed orbits $\boldsymbol{R}_{\mathrm{p}}$ and repetitions m; primitive orbits have $\boldsymbol{R}_{\mathrm{p}}=(N,\alpha M)$ where N and M are relatively prime. Thus

$$d(E)=\bar{d}(E)+\alpha\ \mathrm{Re}\sum_{\boldsymbol{R}_{\mathrm{p}}\neq(0,0)}\sum_{m=1}^{\infty}\int_0^{\pi}\mathrm{d}\theta\ \exp(2\pi\mathrm{i}mR_{\mathrm{p}}\sqrt{E}\cos\theta). \tag{5}$$

Exchanging the sum over repetitions and the integral we find that this may be evaluated exactly as

$$d(E)=\bar{d}(E)+\alpha\sum_{\boldsymbol{R}_{\mathrm{p}}\neq(0,0)}\left(\frac{-\pi}{2}+\frac{1}{2R_{\mathrm{p}}\sqrt{E}}+\sum_{n=1}^{[R_{\mathrm{p}}\sqrt{E}]}\frac{1}{(R_{\mathrm{p}}^2E-n^2)^{1/2}}\right) \tag{6}$$

where $[x]\equiv\mathrm{Int}(x)$.

In this expression each contribution to $d(E)$ comes from one given primitive orbit $\boldsymbol{R}_{\mathrm{p}}$ and all its repetitions. Now by definition $d(E)$ consists simply of δ function singularities at the energies (1); on the other hand (6) consists of a smooth background with square-root singularities, which must therefore combine in a subtle way to give the correct form. Moreover the square-root singularities are at the energies of constructive interference for waves repeatedly traversing the orbit $\boldsymbol{R}_{\mathrm{p}}$, which are different from the energies (1); they are therefore *false* singularities. It seems miraculous that the false singularities associated with the different primitive orbits can combine to give the correct density of states. We emphasise that (6) is an identity, free from the asymptotic approximations normally underlying the closed orbit sum.

To illustrate the way in which the primitive closed orbits combine it is convenient to consider not $d(E)$ but its integral, the spectral staircase $N(E)$, namely

$$N(E)\equiv\sum_i\theta(E-E_i)=\int_0^E d(E)\,\mathrm{d}E \tag{7}$$

$$=\bar{N}(E)+\alpha\sum_{\boldsymbol{R}_{\mathrm{p}}\neq(0,0)}\left(\frac{-\pi E}{2}+\frac{\sqrt{E}}{R_{\mathrm{p}}}+\frac{2}{R_{\mathrm{p}}^2}\sum_{M=1}^{[R_{\mathrm{p}}\sqrt{E}]}(R_{\mathrm{p}}^2E-M^2)^{1/2}\right) \tag{8}$$

where, for this billiard

$$\bar{N}(E)=\int_0^E\bar{d}(E)\,\mathrm{d}E=\pi\alpha E. \tag{9}$$

The singularities of the individual terms are now discontinuities in slope, rather than divergences.

Now we can compute (8) and study how the form of $N(E)$ changes with the number of primitive closed orbits included in the sum. We take $\alpha=1$ (square billiard) and the energy range from $E=39$ to $E=42$ which includes two eigenenergies ($40=6^2+2^2$, $41=5^2+4^2$), each eight-fold degenerate. In figure 1 we plot $N(E)$ with an increasing number of primitive orbits (each of which of course now includes the contributions from all repetitions). In figure 1(a) one sees that the singularities are at points which are not eigenenergies of the system; these are the false singularities. However, as more orbits are included it is evident that singularities begin to accumulate to form steps where the two correct energies are. The form of $N(E)$ when the shortest 250 primitive orbits are included begins to approximate the correct spectral staircase rather well.

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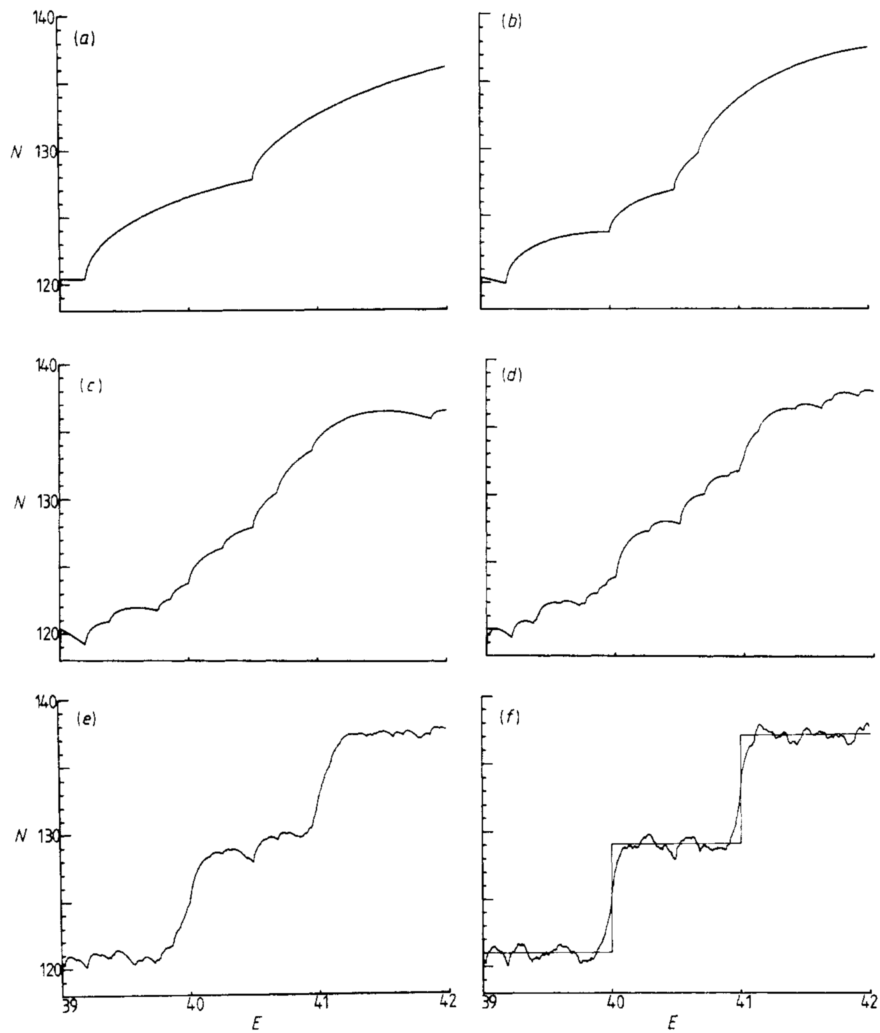

Figure 1. Spectral staircase, $N(E)$, when the number of primitive orbits included in the sum is (*a*) 3, (*b*) 5, (*c*) 10, (*d*) 20, (*e*) 40 and (*f*) 250. The sharp steps in (*f*) show the exact staircase.

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