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Quantum signature of a periodic orbit family in a Hamiltonian system

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Abstract. The periodic orbit family with the shortest period in a two-dimensional anharmonic oscillator is responsible for oscillations in the smoothed density of states. We have computed the energy spectrum for a specific potential and compared the oscillations of the smoothed density of states with those predicted by semiclassical theory. We also verify that the 'scarred' intensity profile for these orbits is not affected by the period-doubling bifurcation cascade that breaks up the surrounding tori.

1. Introduction

The formal semiclassical theory for the quantum energy spectrum, developed by Gutzwiller (1971), ascribes to each periodic orbit a term in the density of states. Generically, these orbits are embedded in families parametrised by the energy (or the period) and the phase of each contribution is basically the action S measured in units of Planck's constant $\hbar$. Balian and Bloch (1974) obtained similar results for the smoothed density of states, with the difference that in this case not all the periodic orbits contribute but only those having periods up to a finite value T, reciprocal to the energy smoothing δE according to the uncertainty principle $T\delta E \simeq h$. It follows that by increasing sufficiently the smoothing δE we can eliminate the contribution of all the periodic orbits so that only the average (or Weyl) density of states remains (see, e.g., Berry (1983) or Ozorio de Almeida (1988) for reviews of these topics). By decreasing δE we can then incorporate the contribution of the family of periodic orbits with shortest period. The resulting smoothed density of states should exhibit, superposed on the averaged background, a nearly sinusoidal oscillation in energy with frequency $1/\tau$, where

$$\tau = \mathrm{d}S/\mathrm{d}E \tag{1}$$

is the period of the orbit.

The wavefunctions for these quantum states may also display 'scars' in the neighbourhood of the periodic orbits, as discovered by Heller (1984). These scars become particularly sharp if we superpose the intensity of all the wavefunctions in a range δE. Heller's theory for wave intensities was cast in a form quite analogous to the one for the spectrum by Bogomolny (1988) (see also Ozorio de Almeida 1988). However, so far it is not certain whether the intensity peaks at a scar depend on the combined contribution of the many states that are in the range δE or whether they can be ascribed to a single strong state in this interval.

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The formal semiclassical results that we are discussing cannot be completely verified by a calculation using a basis of states and a given value of Planck's constant. Conversely, the semiclassical results are useful only if they describe the approximate features of each particular quantum systems. It is therefore important to verify computationally which are the features of these theories that can be relied on in less than ideal conditions. So far most work has been concentrated on the easily accessible periodic orbits of billiard systems (as in Heller 1984, Bogomolny 1988). However, nonlinear oscillators,

$$H(x, y, p_x, p_y) = (p_x^2 + p_y^2)/2 + V(x, y) \tag{2}$$

provide more realistic examples. Of these, the Hénon-Heiles potential is the most studied, but here we work with

$$V(x, y) = (x^2 + 3y^2)/2 - x^2 y + x^4/12. \tag{3}$$

This potential (codename MARTA) has a minimum at zero energy and two saddles at an energy of 0.75. The symmetry in x implies that $x = 0$, $p_x = 0$ is an invariant plane in phase space; hence this is foliated by the family of 'vertical' (y direction) periodic orbits. The potential along this plane is quadratic, so these orbits have constant period $\tau = 2\pi/\sqrt{3}$. Numerical studies of this system by de Aguiar *et al* (1987), show that this is the orbit with the lowest period below the saddle energy. Furthermore, this family generates a period-doubling bifurcation cascade starting at $E \simeq 0.103$. Below this energy the motion in its neighbourhood is mainly regular, becoming locally chaotic at higher energies, though the system still exhibits invariant tori (Aguiar and Baranger 1988).

The spectrum and the eigenfunctions of the MARTA potential can be calculated by diagonalising the quantum MARTA Hamiltonian in the harmonic oscillator basis corresponding to the quadratic terms in the potential. In the following section we display the smoothed density of states of the spectrum corresponding to 595 states in the energy range [0.0797, 0.1997] with $\hbar = 0.0029$, which thus includes the chaotic transition near the symmetry plane. Our numerical results are then compared with the predictions of periodic-orbit theory.

In section 3 we display wave intensities, averaged over y, as functions of x. These can be compared with the wave intensities given by the hypothesis of Voros (1976, 1977) and Berry (1977) at the same energy, that is the hypothesis which results from the assumption that the Wigner function is a delta function over the energy shell. Comparison with this average background reveals that individually scarred states are still present above the period-doubling bifurcation that destroys the neighbouring tori.

2. Density of states

Below the saddle energy (0.75), the eigenvalue problem of the MARTA quantum system,

$$H\psi_i(x, y) = E_i\psi_i(x, y) \tag{4}$$

was solved by using the expansion

$$\psi_i(x, y) = \sum_{n=0}^{2N}{}' \sum_{m=0}^{N} C_{nm}^i \varphi_n(x)\varphi_m(y) \tag{5}$$

where $\varphi_n(x)$ and $\varphi_m(y)$ are eigenfunctions of the one-dimensional harmonic oscillator

Hamiltonians H_x and H_y,

$$H_x = (p_x^2 + x^2)/2$$
$$H_y = (p_y^2 + 3y^2)/2. \tag{6}$$

The prime in the summation means that only even n (even parity) or only odd n (odd parity) are included.

The value $n = N$, at which the expansion (5) is truncated, is chosen according to the energy interval to be investigated, which, of course, has to be much below the saddle point energy. In this region we can neglect the connection with the continuum through tunnelling under the saddles.

As already mentioned, one of the families of periodic orbits of the classical MARTA Hamiltonian (de Aguiar *et al* 1987) is the so-called vertical family, which consists of harmonic oscillations of period $2\pi/\sqrt{3}$ in the y direction. This family undergoes a first period-doubling bifurcation at $E \simeq 0.103$ and, in order to verify its effect on the level density, we calculated this level density in the energy interval [0.0797, 0.1977]. This range of energy is much below the saddle energy, therefore the expansion method with truncation can be safely used. Semiclassical results are obtained by using a small value of $\hbar$. However, too small a value of $\hbar$ implies the diagonalisation of too large a matrix, so the value $\hbar = 0.0029$ chosen by us represents a compromise. With this value the level spacing of the vertical harmonic oscillator is $\hbar\omega_y \simeq 0.005$ and the above energy interval contains 595 states. We made the truncation of expansion (5) at $N = 40$.

The density of states (histograms) as a function of energy has been calculated in the above energy interval using $\delta E = 0.001$ and $\delta E = 0.002$. For the value of $\hbar$ we are using, the number of states contained in such small δE is small, which gives rise to spurious fluctuations, but this problem can be circumvented by making a Gaussian smoothing. We have used normalised Gaussians of half width equal to δE, and the resulting smoothed level densities for $\delta E = 0.001$ and $\delta E = 0.002$ are displayed in figures 1 and 2, respectively. These densities were numerically obtained at energy points separated by 0.0005 and a line was drawn joining these points.

According to the periodic-orbit theory, the density of states may be separated into two terms (Berry 1983, Ozorio de Almeida 1988),

$$d(E) = d_{\text{av}}(E) + d_{\text{osc}}(E) \tag{7}$$

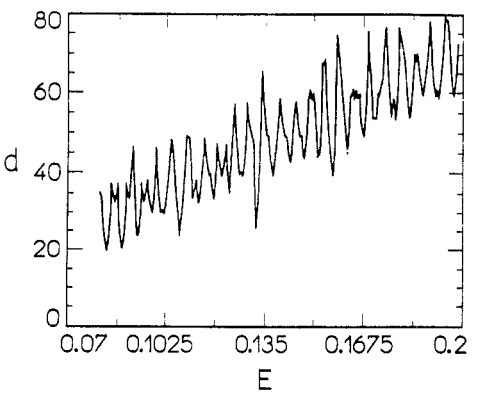

Figure 1. Gaussian smoothed density of states $d(E)$ with $\delta E = 0.001$.

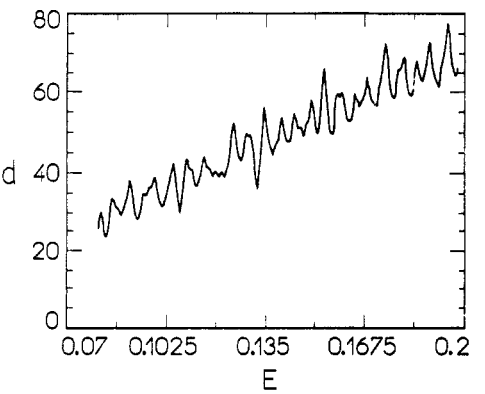

Figure 2. Gaussian smoothed density of states $d(E)$ with $\delta E = 0.002$.

where d_{av} is the average density of states (the so-called Weyl term) corresponding to zero-period orbits, and d_{osc} is the oscillatory term that incorporates the contribution of periodic orbits of period greater than zero.

Numerically, the Weyl term d_{av} is obtained by using a sufficiently large value of δE in the calculation of the density. The term d_{osc} is then obtained by subtracting the Weyl term from the total density $d(E)$. Therefore, the contribution to d_{osc} of the lowest period orbits may be analysed by appropriately choosing the value of δE used in the calculation.

The Weyl term has been approximated by the Gaussian smoothed level density calculated using $\delta E = 0.04$ (see figure 3). Thus, using this approximation for d_{av} we obtained d_{osc} for $\delta E = 0.001$ and $\delta E = 0.002$. These results are displayed in figures 4 and 5, respectively (full curves).

In theory, each periodic orbit and all its repetitions contribute to d_{osc}. When a period n-upling occurs, new orbits are generated and the summation will include the nth repetition of the original orbit plus all the new period n-upled orbits generated at the bifurcation. The vertical family is the family of periodic orbits of the classical MARTA potential (3) having the lowest period in the energy range under consideration.

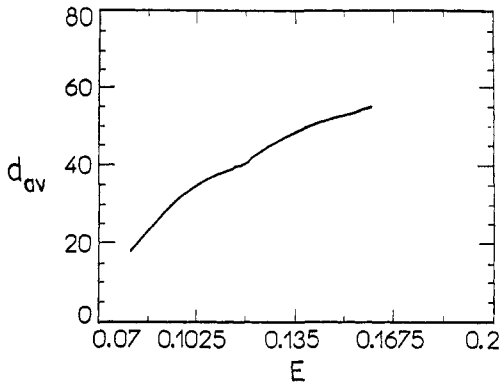

Figure 3. The Weyl term $d_{av}(E)$, corresponding to the Gaussian smoothed density of states calculated with $\delta E = 0.04$.

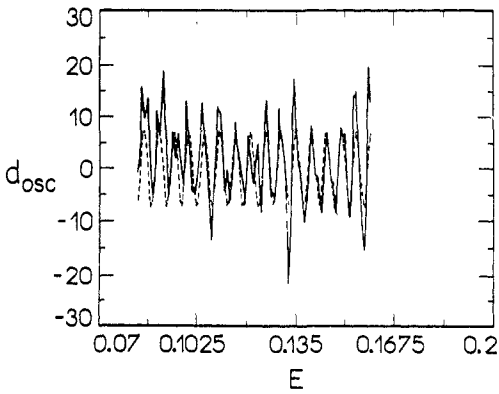

Figure 4. The full curve is $d_{osc}(E)$ with $\delta E = 0.001$ and the broken curve is the approximation (8) with $A = -7.290$ (standard deviation 0.653) and $B = -0.695$ (standard deviation 0.089), obtained by a least-squares nonlinear fit.

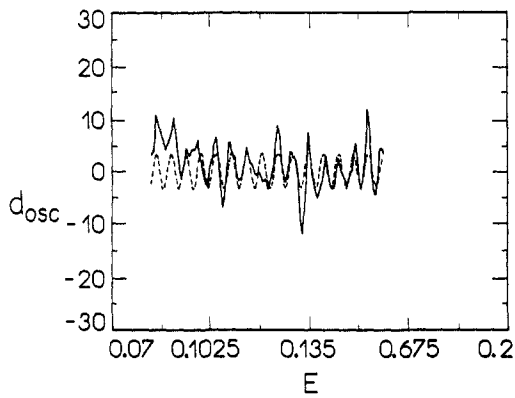

Figure 5. The full curve is $d_{osc}(E)$ with $\delta E = 0.002$ and the broken curve is the approximation (8) with $A = -3.364$ (standard deviation 0.440) and $B = -0.536$ (standard deviation 0.130), obtained by a least-squares nonlinear fit.

Thus, for the smoothing that we used, d_{osc} is basically obtained by considering only the contribution of the vertical family, without any repetition. In this approximation, d_{osc} is nearly a sinusoidal oscillation with the same period of the vertical family, therefore it can be approximated by

$$d_{osc}(E) = A \sin[(2\pi/\hbar\omega_y)E + B]. \tag{8}$$

The dominance of this period in d_{osc} is confirmed by the Fourier analysis shown in figure 6. The broken curves displayed in figures 5 and 6 were obtained by fitting the corresponding values of d_{osc} to the above sine function.

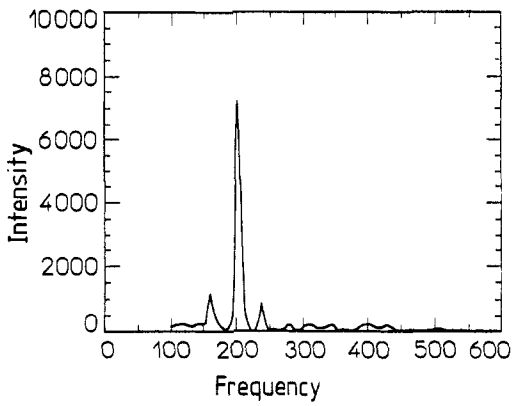

Figure 6. Fourier analysis of the smoothed density of states with $\delta E = 0.001$ (figure 1).

It is important to note that the amplitude of a bifurcating orbit goes through a sharp peak (Ozorio de Almeida and Hannay 1987). However, in this case of period doubling, the peak appears only for even repetitions, justifying the approximately constant amplitude over a narrow energy range in (8) for the first return of the orbit.

Now, d_{osc} obtained numerically incorporates the contributions of all periodic families having periods up to $h/\delta E$. It should be noted that, depending on the energy value, already for a period twice the period of the vertical orbit, there are several orbits contributing to the density of states in the energy interval considered by us (de Aguiar *et al* 1987). These contributions are not completely cancelled by the Gaussian smoothing in the period. Therefore, it is quite remarkable that there should be such close agreement between the frequency of oscillation of d_{osc} and that of the approximation given by (8). As for the amplitude of d_{osc}, it should vary smoothly in the semiclassical limit, according to the theory. Thus, the large variations in amplitude observed in figures 4 and 5 cannot be accounted for in the semiclassical approximation (8), though it may result from the influence of orbits with longer periods.

3. Averaged wave intensities

As we wanted to detect the existence of scars due to the vertical period family, we have calculated the state density distribution averaged over y, given by

$$\rho_i(x) = \int |\psi_i(x, y)|^2 \, dy \simeq \sum_{\substack{n,n'm=0 \\ \text{even}}}^{N} C^i_{nm} C^i_{n'm} \varphi_n(x) \varphi_{n'}(x). \tag{9}$$

(The odd-parity states are zero at the origin and therefore cannot exhibit any scar due to the vertical family.)

Thus, this averaged wave intensity was calculated for those eigenstates with eigenvalues lying in the energy interval considered in section 2. The full curves in figures 7, 8 and 9 show $\rho_i(x)$ corresponding to the eigenstates of energies 0.1040, 0.1043 and 0.1044, respectively. The dotted curves shown in these figures are the corresponding state density distributions $\rho_i^c(x)$, resulting from the use of the ergodic assumption

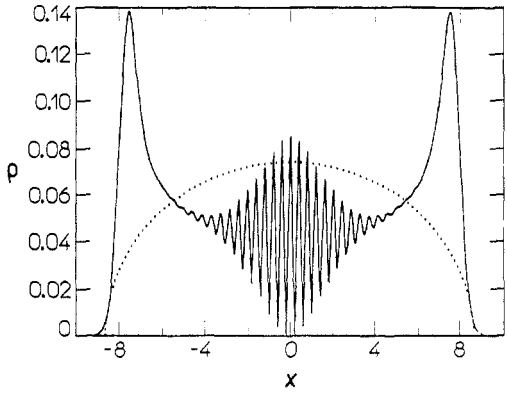

Figure 7. The full curve is $\rho_i(x)$ for the eigenstate with $E = 0.1040$, exhibiting the caustic peaks characteristic of quasiperiodic motion. The dotted curve is the corresponding $\rho_i^c(x)$.

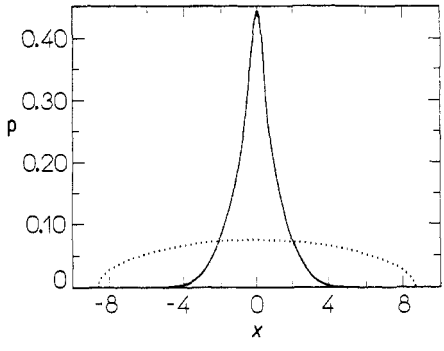

Figure 8. The full curve is $\rho_i(x)$ for the eigenstate with $E = 0.1043$, exhibiting a scar due to the vertical periodic family. The dotted curve is the corresponding $\rho_i^c(x)$.

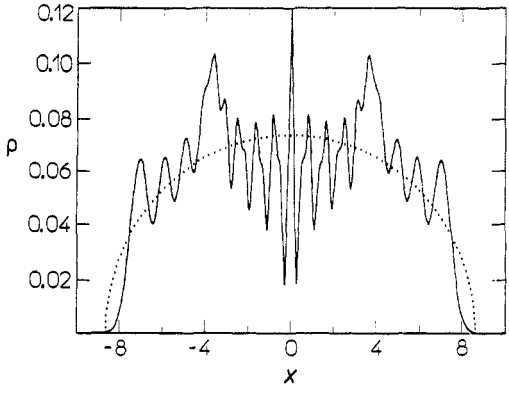

Figure 9. The full curve is $\rho_i(x)$ for the eigenstate with $E = 0.1044$, apparently exhibiting anticaustics with oscillations that follow $\rho_i^c(x)$ (dotted line).

(Voros 1976, 1977), which in the case of a Hamiltonian with two degrees of freedom of type (2) is given by (Berry 1977)

$$\rho_i^e(x) = \int \mathrm{d}y\, \Theta(E_i - V(x, y)) \tag{10}$$

with Θ the step function.

We see that the wave intensities displayed in figures 7, 8 and 9 exhibit completely different characteristics. The state distribution in figure 7 exhibits caustic peaks, which are the signature of quasiperiodic motion. The corresponding eigenvalue is just above 0.103, which is the energy value at which the vertical periodic family undergoes its first period-doubling bifurcation. The scarred wave intensity profile shown in figure 8 is virtually identical to the ones found below the bifurcation where the vertical orbit is stable. These scarred states are found near the quantised actions

$$\Delta S = n\hbar \tag{11}$$

as previously discovered by M Saraceno. The wave intensity displayed in figure 9 seems to exhibit anticaustics (Berry 1983), with the oscillations more or less following $\rho_i^e(x)$. However, as the classical underlying motion is not globally chaotic, further verification is required in order to confirm the presence of anticaustics.

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