

Semiclassical Calculation of Scars for a Smooth Potential

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Bogomolny's formula for energy-smoothed scars is applied to a nonspecific, nonscalable Hamiltonian, a two-dimensional anharmonic oscillator. The semiclassical theory reproduces well the exact quantal results over a large spatial and energy range.

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The scars left on stationary state wave functions by unstable classical periodic orbits were discovered by McDonald and Kaufman [1]. They were named and further studied by Heller [2]. The paradox of the scars is that they occur in an energy region where a generic classical trajectory covers the energy shell uniformly; in spite of this, many quantal wave functions like to concentrate in the vicinity of one or several periodic orbits. Obviously, an understanding of this paradox requires a semiclassical theory.

Such a semiclassical theory of scars in the usual, coordinate space wave functions was given by Bogomolny [3]. There are also semiclassical theories of scars in the Wigner distribution [4] and in the Husimi distribution [5]. We present here some results from an extensive comparison of the exact quantal scars with the Bogomolny scars [3] for an ordinary smooth potential. Apart from an interesting qualitative discussion [6], we do not know of any other detailed comparison for a sufficiently "generic" Hamiltonian.

The famous Gutzwiller trace formula [7] can be obtained by integrating the Bogomolny formula over the space coordinates. Therefore our work leads also to a check of the Gutzwiller trace formula for our Hamiltonian. There have already been a few checks of similar quality for the Gutzwiller trace formula with general enough Hamiltonians, for instance, Ref. [8].

Our Hamiltonian is

$$H(p_x, p_y, x, y) = \frac{1}{2}(p_x^2 + p_y^2) + 0.05x^2 + (y - x^2/2)^2. \quad (1)$$

Its classical dynamics and periodic orbits have been studied in detail [9]. We had to continue the study of periodic orbits towards higher energy, using a totally new method for which there is no space here. Suffice it to say that this method ensures that no orbit below period 20 is missed. Figure 1 shows a contour plot of the potential $V(x, y) = H - \frac{1}{2}p^2$ for energies of interest. The transition from mostly regular to mostly chaotic motion happens for energies of order 0.1. Islands of regularity remain, however, no matter how high in energy one goes. But at the energies of our numerical comparisons, they are very tiny.

We took $\hbar = 0.05$. The calculation of the exact quantal wave functions and energies was done with the basis $\phi_m^{(x)}(x)\phi_n^{(y)}(y - x^2/2)$, where $\phi_m^{(x)}$ and $\phi_n^{(y)}$ are harmonic oscillator wave functions appropriate for the bottom of the well. We used 240 oscillator states for the x direction and 26 for the y direction. A sensitive test of the sufficiency of this basis comes from a comparison with the smooth Thomas-Fermi density of states, including the corrections [10] of order \hbar^2 . The test shows that our basis begins to fail for an energy somewhere between 0.80 and 0.85, and consequently we stopped our comparisons there.

Bogomolny's formula is [3]

$$\Delta(\mathbf{q}, E; \epsilon) = \frac{2}{(2\pi\hbar)^{3/2}} \sum_{\text{periodic orbits}} \tilde{f}_\epsilon(\tau) \frac{1}{|\dot{\mathbf{q}}_1|} \frac{1}{\sqrt{|m_{qp}|}} \times \cos \left[\frac{1}{\hbar} \left(\bar{S} + \frac{1}{2} \frac{\text{tr} \mathcal{M} - 2}{m_{qp}} q_2^2 \right) - \frac{\pi}{2} \mu - \frac{\pi}{4} \right]. \quad (2)$$

Δ is the oscillating part (as explained in the next sentence) of the energy-smoothed coordinate space probability density

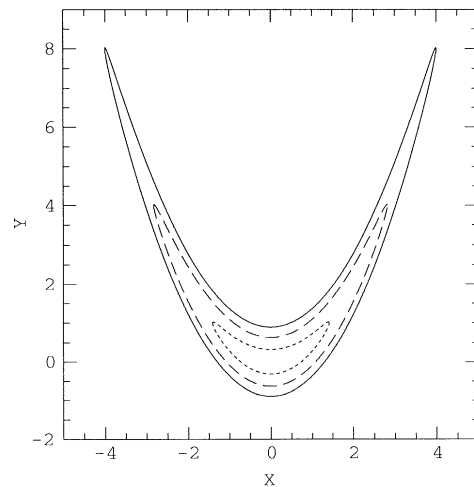
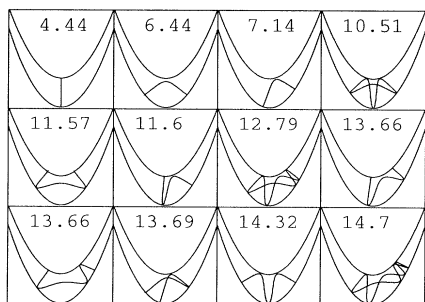


FIG. 1. Three contours of the potential $V(x, y)$: $E = 0.1$ (dots), $E = 0.4$ (dashes), and $E = 0.8$ (full).

FIG. 2. The 12 orbits with lowest periods for $E = 0.8$.

$$\sum_n f_\epsilon(E - E_n) |\langle \mathbf{q} | \psi_n \rangle|^2, \quad (3)$$

where f_ϵ is the smoothing function, which we take to be the normalized Gaussian

$$f_\epsilon(E) = (2\pi)^{-1/2} \epsilon^{-1} e^{-E^2/2\epsilon^2}. \quad (4)$$

Δ is obtained by subtracting from Eq. (3) the energy-smoothed Thomas-Fermi density. On the right-hand side of Bogomolny's formula, $\tilde{f}_\epsilon(\tau) = e^{-\epsilon^2 \tau^2 / 2\hbar^2}$ is the Fourier transform of $f_\epsilon(E)$, τ is the period of the periodic orbit, and \bar{S} is its action $\int \mathbf{p} \cdot d\mathbf{q}$. The coordinates q_1 and q_2 are chosen especially for each periodic orbit, q_1 being the distance along the orbit and q_2 being the perpendicular coordinate. \mathcal{M} is the 2×2 submatrix of the monodromy matrix involving coordinates q_2 and p_2 , and m_{qp} is one of its off-diagonal elements. Finally μ is equal to μ_m , the Maslov index of the orbit [11], when m_{qp} and $\text{Tr}\mathcal{M} - 2$ have the same sign; μ is equal to $\mu_m - 1$ when the signs are opposite.

In order that Eq. (2) be valid, it is also necessary to perform some smoothing over coordinate space on both sides of the equation. There are two reasons for this: (a) it is essential for reducing the semiclassical contribution to a sum over periodic orbits [3]; (b) the semiclassical theory is not valid near the points where $m_{qp} = 0$, which are the self-conjugate points, and the spatial smoothing minimizes this discrepancy. We smoothed with a Gaussian proportional to $e^{-(q_x^2 + q_y^2)/b^2}$. This is equivalent to calculating the coordinate space projection of the Husimi distribution. We chose $b = 0.2$; more about this later.

Gutzwiller's trace formula [7], obtained by integrating Eq. (2) over space, is

$$d(E; \epsilon) = \frac{1}{\pi\hbar} \sum_{\text{periodic orbits}} \tilde{f}_\epsilon(\tau) \frac{\tau_0}{\sqrt{|\text{tr}\mathcal{M} - 2|}} \cos\left(\frac{\bar{S}}{\hbar} - \frac{\pi}{2}\mu_m\right). \quad (5)$$

d is the oscillating part of the energy-smoothed density of states, calculated by subtracting the Thomas-Fermi density of states and its corrections [10] of order \hbar^2 . For orbits consisting of repeated traversals of a primitive periodic orbit, τ_0 is the period of the latter.

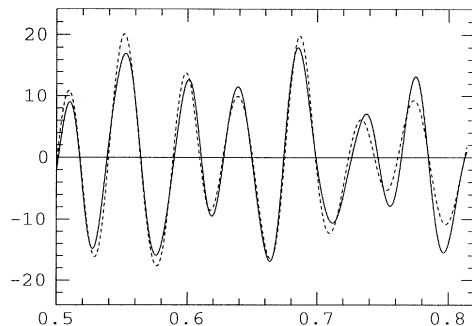


FIG. 3. The smoothed energy level density, with $\epsilon = 0.01$, minus the Thomas-Fermi density. The full line is the exact quantal calculation, the dashed line is Eq. (5) with 5 orbits. The Thomas-Fermi density at $E = 0.65$ is $\simeq 290$. Hence the average number of stationary states inside one ϵ is 2.9.

It has long been everybody's dream to get rid of the energy smoothing, to let $\epsilon \rightarrow 0$ and to use Eqs. (2) and (5) to predict individual stationary states. We avoided this limit, as the process seems to diverge. Instead, we chose our ϵ so that relatively few periodic orbits would contribute.

Figure 2 shows pictures of the first 12 orbits in order of increasing period, again at $E = 0.8$. We have worked in the range $0.5 \leq E \leq 0.85$ and, for $E \neq 0.8$, the order might be slightly different from that in Fig. 2. In the distribution of periods, the three lowest (4.44, 6.44, 7.14) are clearly separated from those above (10.51, 11.57, 11.60, ...). Hence we expect that, by choosing ϵ large enough, many features can be described in terms of 3 periodic orbits only. This turns out to be true indeed. Figure 3 shows the oscillations in the smoothed energy level density, as given by the Gutzwiller formula, Eq. (5), calculated with $\epsilon = 0.01$ and 5 periodic orbits, but it is only slightly better than that calculated with 3 orbits. On the other hand, it is radically different from that calculated with only 1 or 2 orbits. In the case of 3 or more orbits, the agreement with the exact quantal calculation can be termed very good for this value of ϵ .

Figure 4 shows the most striking scar we have found:

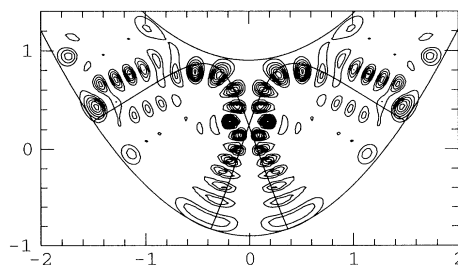


FIG. 4. Contours of the exact coordinate space probability density for odd state 145, showing striking scarring by the 3 periodic orbit and its mirror reflection $x \rightarrow -x$.

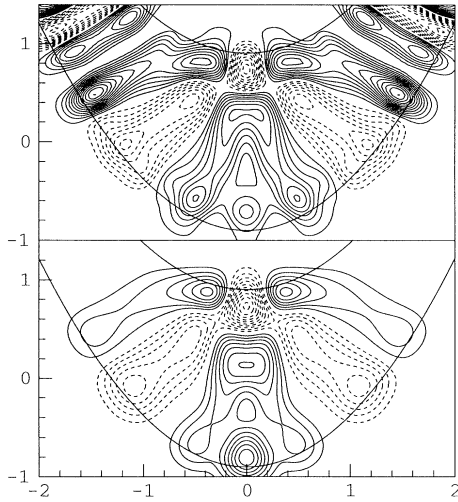


FIG. 5. The oscillating part, Δ , of the energy- and space-smoothed coordinate space density. Energy smoothing parameter $\epsilon = 0.01$. Top: exact quantal. Bottom: Eq. (2) with 5 orbits. Solid contours are positive, dashed are negative. The contour spacing is 0.5 in all Figs. 5, 6, and 7. Contour 0 is not drawn. The Thomas-Fermi density is $\frac{1}{2}\pi\hbar^2 = 63.7$. The energy is $E = 0.814$.

odd (in x) state 145, with $E = 0.814$, scarred by the third periodic orbit, a simple asymmetric libration. Our calculation of energy-smoothed scars according to the Bogomolny formula, Eq. (2), is illustrated in Figs. 5, 6, and 7 and compared with the exact result. For lack of space, we concentrate here on the energy range $0.726 \leq E \leq 0.814$, which is typical of other energies. Figure 5 is for the same energy as Fig. 4, and the scar is still prominent. Figures 6 and 7 are two other examples. They all show some combination of scarring by the first three orbits.

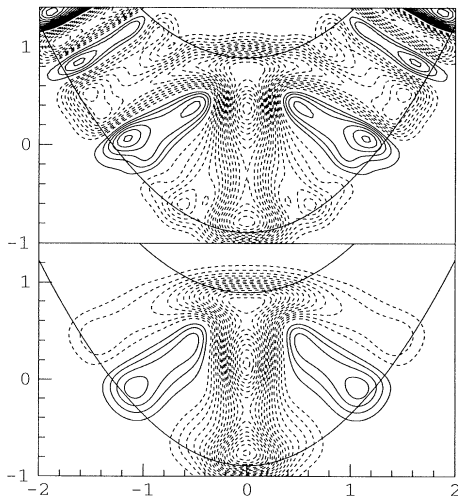


FIG. 6. Same as Fig. 5 for $E = 0.794$.

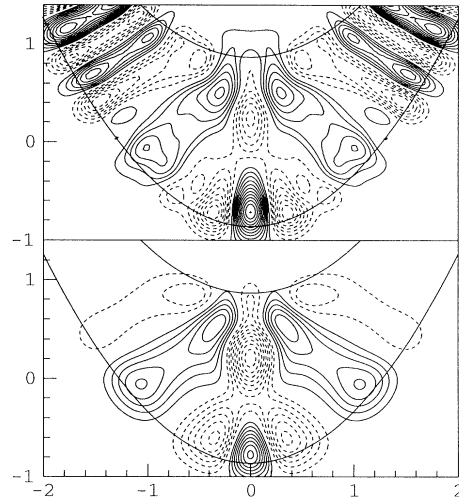


FIG. 7. Same as Fig. 5 for $E = 0.746$.

The agreement between the exact quantal and the semiclassical pictures can be described as following the main trends very well, but quantitatively inaccurate. By “main trends,” we mean in particular the way that the density fluctuation in the vicinity of each orbit (the “scar” of that orbit) oscillates and changes sign as a function of energy. This is better seen in Fig. 8, which shows the scar strength (both exact and semiclassical) as a function of energy for three points in the x - y plane.

The agreement between Eq. (2) and the exact quantal density is limited to the central part of our potential, exclusive of the two “arms” (see Fig. 1). This is because, in the arms, the motion is approximately integrable, consisting of fast transverse oscillations whose

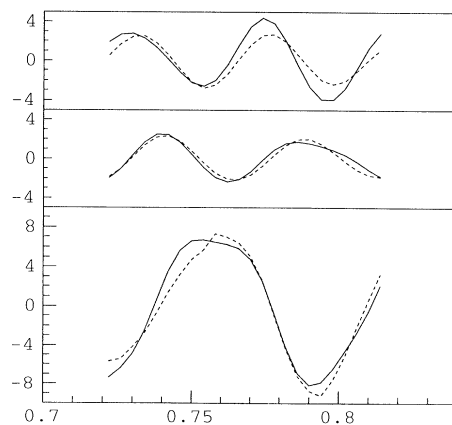


FIG. 8. The exact scar strength Δ (full line) and the semiclassical one calculated with 5 orbits (dashed), as a function of energy, at three points of coordinate space. Bottom: $x = 0$, $y = -0.65$, emphasizing orbit 1. Middle: $x = 0.8$, $y = 0$, emphasizing orbit 2. Top: $x = 0.75$, $y = 0.75$, emphasizing orbit 3.

action is an adiabatic invariant for the slower longitudinal motion [12]. As a result, the exact density in the arms exhibits a very simple pattern, visible in the upper corners of Figs. 5, 6, and 7, and consisting mostly of wide longitudinal oscillations whose wavelength can be calculated very simply with the above adiabatic picture. The short-period classical orbits, on the other hand, are found only in the central, chaotic region. It is possible to increase the value of b , the spatial smoothing width, so as to wash out the oscillations in the arms, but then this would also wash out many interesting features in the center. The value chosen, $b = 0.2$, is a reasonable compromise.

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