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## Complex Periodic Orbits and Tunneling in Chaotic Potentials

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We derive a trace formula for the splitting-weighted density of states suitable for chaotic potentials with isolated symmetric wells. This formula is based on complex orbits which tunnel through classically forbidden barriers. The theory is applicable whenever the tunneling is dominated by isolated orbits, a situation which applies to chaotic systems but also to certain near-integrable ones. It is used to analyze a specific two-dimensional potential with chaotic dynamics. Mean behavior of the splittings is predicted by an orbit with imaginary action. Oscillations around this mean are obtained from a collection of related orbits whose actions have nonzero real part. [S0031-9007(96)01893-5]

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In this Letter we develop a method for computing tunneling effects in quantum states associated with chaotic regions of phase space. While the influence of chaotic dynamics has been actively studied in the context of chaos-assisted tunneling between Einstein-Brillouin-Keller- (EBK)-quantized tori [1], less attention has been paid to the problem of tunneling between chaotic states. This is presumably because there is, at present, no semiclassical theory for individual chaotic eigenstates. However, there does exist a well-developed theory for the spectral properties of such systems in terms of periodic orbits [2]. We will show how this can be extended to a calculation of spectral tunneling averages using complex periodic orbits.

Complex multidimensional trajectories were introduced in [3] to understand barrier-penetration problems as motivated by quantum field theories. Complex periodic orbits were first used by Miller [4] in one-dimensional potentials to derive splittings and resonance widths. These calculations were extended in [5] to the rotational spectrum of SF<sub>6</sub>. Splittings in chaotic potentials were related to complex trajectories in [6]. In the context of chaotic maps, complex periodic orbits were used to calculate band gaps [7]. Complex trajectories in chaotic maps have also been explored in the time domain [8].

A commonly used probe for tunneling effects is to study the spectra of two symmetric wells which have a barrier between them. When classical trajectories are

localized within one well or the other, one finds that energy levels come in symmetric-antisymmetric pairs  $E_n^\pm$ , with small splittings between them. Denote the splittings by  $\Delta E_n$  and the mean levels by  $E_n$ , so that  $E_n^\pm = E_n \mp \Delta E_n/2$ . A standard periodic orbit calculation using real orbits yields a set of doubly degenerate levels  $E_n^{\text{sc}}$ , approximating the mean levels  $E_n$ . The degeneracy arises because each periodic orbit has a symmetric partner in the opposing well. Therefore, the most naive use of periodic orbit theory fails to predict the existence of splittings. However, since including *complex* orbits does yield splittings in one dimension [4,5], we are motivated to pursue this approach in higher dimensions.

A literal extension of this work to chaotic problems is too difficult because it involves finding tiny differences between poles in traces or zeros in zeta functions. Instead, the splitting-weighted density of states,

$$f(E) = \sum_n \Delta E_n \delta(E - E_n), \quad (1)$$

will provide an effective vehicle for evaluating splittings directly from complex orbits. Analysis of  $f(E)$  in terms of periodic orbits follows from approximating it by the difference,

$$f(E) \approx N_+(E) - N_-(E), \quad (2)$$

between the staircase functions  $N_\pm(E)$  for even and odd states. The approximation is valid if we use a resolution

in energy that is much greater than  $\Delta E_n$ . We next note that  $N_{\pm}(E) = -(1/\pi) \text{Im} \int^E dE' g_{\pm}(E')$ , where  $g_{\pm}$  are traces of the symmetry-projected Greens functions [9]

$$g_{\pm}(E) = \sum_n \frac{1}{E - E_n^{\pm}} \approx \frac{1}{2} \sum_{\gamma} \chi_{\pm}(g_{\gamma}) A_{\gamma} e^{iS_{\gamma}/\hbar}. \quad (3)$$

The traces receive contributions from orbits  $\gamma$  which either close simply in phase space ( $g_{\gamma} = I$ ) or close after applying a reflection operation ( $g_{\gamma} = R_x$ ). The group characters are  $\chi_{\pm}(I) = 1$  and  $\chi_{\pm}(R_x) = \pm 1$ ,  $S_{\gamma}$  is the action and  $A_{\gamma}$  is obtained from the stability of the orbit. Real orbits cannot cross from one well to the other and necessarily correspond to  $g_{\gamma} = I$ . Their contribution vanishes when we calculate the difference, a fact which is true to all orders in  $\hbar$ .  $f(E)$  is then approximated by orbits corresponding to  $g_{\gamma} = R_x$ , which are necessarily complex, and from which we can extract the exponentially small splittings.

After substituting the contributions of complex orbits into the trace formula and integrating, we arrive at the following sum [10]:

$$f(E) \approx \frac{2}{\pi} \text{Im} \sum_{\gamma} \beta_{\gamma} \frac{e^{iS_{\gamma}/\hbar}}{\sqrt{-\det(M_{\gamma} - I)}}. \quad (4)$$

Here  $S_{\gamma}$  and  $M_{\gamma}$  are, respectively, the complex action and monodromy matrix of  $\gamma$ . ( $M_{\gamma}$  includes, if necessary, a factor representing linearization in the surface of the section of the symmetry operation  $g_{\gamma}$ .) We use a complex square root in the denominator, and the ambiguity in sign is determined by following the evolution of the square root in the complex plane—this mirrors the computation of Maslov indices for real orbits [11]. The factor 2 reflects a degeneracy in the direction of tunneling, and the dimensionless factor  $\beta_{\gamma}$ , explained below, is 1 for most orbits.

We explore this approximation for the two-dimensional potential

$$V(x, y) = (x^2 - 1)^4 + x^2 y^2. \quad (5)$$

When  $E < 1$ , the classical motion is confined to one of two symmetric wells, leading to splittings. There is a real periodic orbit confined to the  $x$  axis which has a bifurcation at  $E_c = 0.236$  such that it is elliptic for  $E < E_c$  and inverse hyperbolic for  $E > E_c$  (in which energy range phase space is predominantly chaotic). Tunneling in this system is dominated by a particular set of complex orbits that are similarly confined to the  $x$  axis. Their contributions are found by first considering the analogous one-dimensional orbits in the potential  $V(x, 0) = (x^2 - 1)^4$ . They are then dressed with the complex monodromy matrix obtained by embedding them in the other dimension. This is useful because a very careful analysis of such orbits is possible; the results of which can later be extended to more general orbits.

The simplest complex orbit starts on the  $x$  axis with negative kinetic energy and evolves after an imaginary time  $-i\tau$  to the symmetry-related point on the other side. It has real position and imaginary momentum, giving an imaginary action  $S = iK$ . The amplitude of this orbit is reduced by a factor of 2 on reflection from the inside of the barrier. This anomalous reflection coefficient derives from a calculation in which a Stokes constant is calculated on a Stokes line [10,12], and can be understood in simple terms by comparison with an exact calculation for the inverted harmonic oscillator [10]. As a result, the orbit contributes with a factor  $\beta_{\gamma} = 1/2$ . The monodromy matrix can be found by inverting the potential. The tunneling orbit then transforms to a real, unstable orbit running along the ridge  $y = 0$ , whose monodromy matrix  $M$  is readily calculated. Reverting to the upright potential, the monodromy matrix  $W$  is obtained from  $M$  by multiplying the off-diagonal elements by  $\pm i$ . This leaves eigenvalues unchanged. After including a phase factor from reflection inside the barrier, we obtain

$$f_0(E) = \frac{1}{\pi} \frac{e^{-K/\hbar}}{\sqrt{-\det(W - I)}}. \quad (6)$$

A final complication derives from the fact that we will consider separately states with even and odd  $y$  parity. The orbit lies on the corresponding symmetry axis and, as a result, contributes differently to the two parities. The amplitude must therefore be decomposed according to the prescription in [13].

For comparison with the theory, we also found the quantum eigenvalues corresponding to the potential (5) numerically. We used 100 harmonic oscillator basis states in both the  $x$  and  $y$  directions and diagonalized the resulting Hamiltonian. We worked to quadruple precision which allowed us to calculate splittings as small as about  $10^{-30}$ . All results shown are for  $\hbar = \sqrt{8}/100$ . We also used the appropriate bases to isolate the four symmetry classes. States even and odd with respect to  $x$  generate the splittings. The symmetry with respect to  $y$  is additional, and we refer to the corresponding parity classes as even and odd. For each of these classes, the Thomas-Fermi density of states  $\rho_0(E)$  is calculated following reduction to quadratures [10].

In Fig. 1 we show the exact splittings  $\Delta E_n$  weighted by  $\rho_0(E_n)$ . These are dimensionless numbers expressing the splittings in units of the mean level spacing. The solid curve is  $f_0(E)$  and provides a good description of the average behavior. In particular, the theory works for  $E < E_c$ , in which range the motion is mixed and the real one-dimensional orbit is stable. Therefore, the theory predicts the mean behavior whenever the tunneling is dominated by isolated orbits, regardless of the character of the classical motion in the wells.

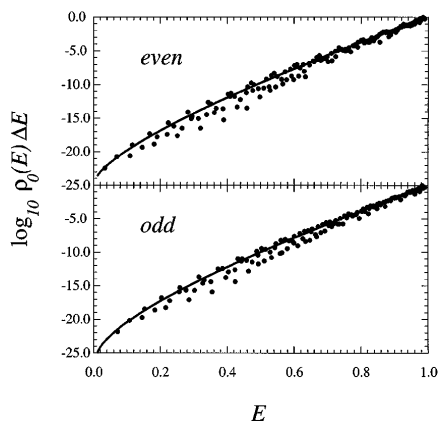


FIG. 1. The dots show the quantum splittings multiplied by the Thomas-Fermi density of states, and the solid curves show the results using  $f_0(E)$  of Eq. (6). “Even” and “odd” refer to the  $y$  parity.

In addition to the mean behavior, there is an oscillatory structure in the splittings. To explain this, we consider orbits obtained by attaching, to the basic tunneling orbit above, real periodic orbits in the wells on either side—always with  $y = 0$ . We denote by  $S_0$  and  $T_0$  the action and period of the real primitive orbit segment. Restricting the sum to orbits which tunnel only once, we allow any number of iterations of the real orbit in the first well before tunneling and in the second well after tunneling. Orbits going from left to right with a total action  $rS_0 + iK$  occur with a degeneracy  $r$ . On doing the trace integral in the wells, we get a contribution to  $g_+(E) - g_-(E)$  with an amplitude factor  $rT_0/i\hbar$ . Summation over these contributions is sufficient in one-dimensional calculations to identify poles in  $g_{\pm}(E)$  and obtain individual splittings [4,5]. For a consistent approximation of  $f(E)$ , however, it is also necessary to add a term with amplitude  $-i\tau/i\hbar$  that arises from integration across the forbidden region—a contribution which was not included (or needed) in the one-dimensional calculations. The integration in energy leading to the staircase functions leaves a denominator  $\partial(rS_0 + iK)/\partial E$  which cancels this combination of periods. Including a factor 2 to account for the choice of starting well, the result is (4) with  $\beta_{\gamma} = 1$ . This argument can be made precise by considering the problem of an infinite square well with a finite square barrier in the middle [10]. The equivalent calculations are exact and free from the ambiguities inherent in comparing exponentially small quantities in WKB calculations.

The monodromy matrix for an orbit with  $r$  real handles is conjugate to  $M_r = WM_0^r$ , where  $M_0$  is the real monodromy matrix of a primitive real orbit segment.  $M_r$  has complex entries. Collectively, these orbits contribute

$$f_{\text{osc}}(E) = \frac{2}{\pi} \text{Im} \sum_{r=1}^{\infty} \frac{e^{(riS_0 - K)/\hbar}}{\sqrt{-\det(WM_0^r - I)}} \quad (7)$$

to  $f(E)$ . To determine the branch of the square root, we write  $\sqrt{-\det(M - I)} = \sqrt{\lambda(1 - \lambda^{-2})}$ , where  $M$  is a surface-of-section matrix with the leading eigenvalue  $\lambda$ , defined at each point along the orbit. Initially,  $\lambda = 1$ , and it then grows along the real axis if we start with the tunneling segment. With subsequent evolution in real time,  $\lambda$  moves into the complex plane. When the real segment is unstable, it executes a counterclockwise rotation of approximately  $\pi$  with each period  $T_0$ , this becoming more exact with every iteration. To this evolution should be added a counterclockwise rotation of  $\pi$  at each turning point. Asymptotically, each iteration then leads in the unstable case to a phase factor  $(-i)^3$  in the amplitude, reflecting the Maslov index  $\sigma = 3$  of the real orbit [11].

Adding  $f_{\text{osc}}(E)$  to  $f_0(E)$  is similar to adding periodic orbit contributions to the Thomas-Fermi density of states. It introduces oscillatory structure to the monotonically increasing background. To make a comparison with exact results, it is useful to divide out this background (shown in Fig. 1)—the result should be a fluctuating function with mean value 1. We compare in Fig. 2 the Thomas-Fermi density-weighted splittings  $\rho_0(E_n)\Delta E_n/f_0(E_n)$  (filled circles) with the function  $1 + f_{\text{osc}}(E)/f_0(E)$  (lower solid curve) obtained by summing over the first ten repetitions  $r$ .

Let us first discuss the energy regime  $E < E_c$ , where the real orbit is stable. Here, summation over  $r$  results explicitly in delta functions—apparent as the first narrow peaks in Fig. 2. (In order that the quantum data not be obscured, sidebands around the peaks have been graphically removed.) The positions give the mean energies of states localized near the orbit in the surrounding island, analogous to a quantization of stable orbits obtained in the usual trace formula [15]. The peaks have weights of

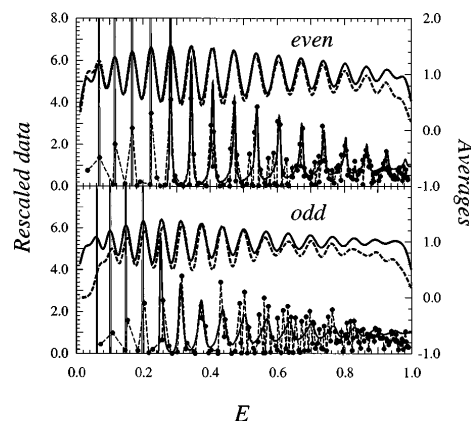


FIG. 2. The same as Fig. 1 but with the mean  $f_0(E)$  scaled out. The dots are the quantum data with dashed lines connecting them. The lower solid curve is  $1 + f_{\text{osc}}(E)/f_0(E)$ . The upper dashed and solid curves are the corresponding results averaged with a Gaussian of variance 0.015. Their scale should be read from the right axis.

the form  $(2\hbar A/T_0)e^{-K/\hbar}$  [10], where  $A$  is a function of  $W$  and  $M_0$ . These weights approximate the splittings and are similar to the one-dimensional case (for which  $A = 1$ ). In Table I the positions of the peaks and their semiclassical weights are compared with the quantum-mechanical mean levels and splittings, respectively. Agreement is reasonable. There are also states which do not correspond to peaks in the theoretical curve. We presume that these are associated with regions of phase space removed from the orbit. It should be noted that, in the limit  $E \rightarrow 0$ , the real orbit suffers an infinite cascade of bifurcations. Unfortunately, the lowest even state has an energy near the first such bifurcation, so the theory cannot be trusted and we do not plot the theoretical curve in this range.

At energies above  $E_c$ , the real orbit is unstable, and phase space is dominated by chaos. The theory has smooth oscillations, and there are no longer any individual states associated with these orbits. However, the theory does reproduce with some detail a marked periodicity in the splittings. Such oscillations have recently been observed experimentally by Wilkinson *et al.* [16] in quantum wells and interpreted by them as corresponding to enhanced tunneling in states “scarred” by a real orbit. In our formalism, we obtain an explicit quantitative prediction, but for averaged tunneling properties and not (in the chaotic regime) for individual states. For a quantitative comparison, we also compare in Fig. 2 the results of convolving quantum-mechanical and semiclassical rescaled quantities with a Gaussian. The mean theory overestimates the splittings near  $E = 1$  because the matrix  $W$  becomes marginal; this can, in principle, be corrected by existing theories for bifurcations [14]. Also, the cascade of bifurcations at small energies means that the theory is not to be trusted in this range either. Other than these effects, there is detailed agreement of period, amplitude, and phase. [For the odd states,  $f_0(E)$  is smaller and corrections become more apparent after rescaling.] Notice also that, as far as averaged quantities are concerned, there is no qualitative difference between the regimes in which the orbit is stable or unstable.

The problem studied here made use of a class of orbits which are essentially one dimensional—their two-

dimensional character being carried exclusively through the monodromy matrix. This is an artifact of the reflection symmetry about the  $y$  axis, and it will be interesting to follow these orbits, as the symmetry is broken, by adding another term to the potential and including a magnetic field. This would be the first step in understanding how to combine the contributions of many complex orbits so as to get individual splittings in the chaotic case. Another necessary ingredient is some form of symbolic dynamics of the complex orbits so that we have a systematic way of searching for orbits; without this, it is an extremely difficult task to find long orbits. A distinct problem is to determine whether the statistics of the splittings conform to any universal distributions.

The form of analysis developed here may help in understanding mesoscopic systems such as Coulomb blockade peaks in which electrons tunnel into a quantum dot, and on which, to date, only statistical analyzes have been brought to bear [17]. For this purpose, we note that a very natural extension of the theory developed here would allow us to find the width-weighted density of resonances for unbounded problems. The formalism might also be used to investigate leakage from or between billiards with small holes. If the holes are small enough, the contribution of leaking orbits will be suppressed diffractively so that the widths or splittings will decay algebraically with wavelength, as opposed to the exponential decay found in tunneling.

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TABLE I. Semiclassical energies and splittings predicted by the stable orbit are compared with exact results.

$y$ parity	$E_{qm}$	$E_{sc}$	$\Delta E_{qm}$	$\Delta E_{sc}$
+	0.0694	0.0679	$0.548 \times 10^{-22}$	$0.522 \times 10^{-22}$
+	0.1158	0.1147	$0.227 \times 10^{-20}$	$0.222 \times 10^{-20}$
+	0.1677	0.1667	$0.881 \times 10^{-19}$	$0.841 \times 10^{-19}$
+	0.2237	0.2222	$0.304 \times 10^{-17}$	$0.261 \times 10^{-17}$
−	0.0718	0.0608	$0.655 \times 10^{-23}$	$0.477 \times 10^{-23}$
−	0.1076	0.1013	$0.210 \times 10^{-21}$	$0.194 \times 10^{-21}$
−	0.1531	0.1480	$0.754 \times 10^{-20}$	$0.724 \times 10^{-20}$
−	0.2038	0.1988	$0.275 \times 10^{-18}$	$0.225 \times 10^{-18}$

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