Tunneling and Nonhyperbolicity in Quantum Dots

Alessandro P. S. de Moura,[1] Ying-Cheng Lai,[1,2] Richard Akis,[2] Jonathan P. Bird,[2] and David K. Ferry[2]
[1]*Department of Mathematics and SSERC, Arizona State University, Tempe, Arizona 85287*
[2]*Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85287*
(Received 17 August 2001; published 28 May 2002)

We argue that many major features in electronic transport in realistic quantum dots are not explainable by the usual semiclassical approach, due to the contributions of the quantum-mechanical tunneling of the electrons through the Kolmogorov-Arnol'd-Moser islands. We show that dynamical tunneling gives rise to a set of resonances characterized by two quantum numbers, which leads to conductance oscillations and concentration of wave functions near *stable* and unstable periodic orbits. Experimental results agree very well with our theoretical predictions, indicating that tunneling has to be taken into account to understand the physics of transport in generic nanostructures.

DOI: 10.1103/PhysRevLett.88.236804 PACS numbers: 73.63.Kv, 05.45.–a, 05.60.Gg, 72.80.Ey

Electronic transport in semiconductor nanostructures is a frontier problem in condensed matter physics and nonlinear science. On submicron scales, quantum interference gives rise to such phenomena as conductance fluctuations and th eAharonov-Bohm effect [1,2]. The aim of this Letter is to report our finding concerning the fundamental role played by *dynamical tunneling* [3] in conductance fluctuations in realistic quantum dots. We present strong evidence that dynamical tunneling through regular phase-space structures, such as Kolmogorov-Arnold-Moser (KAM) islands, fundamentally determines the characteristics of conductance fluctuations in typical quantum dots. Theoretical analysis based on the tunneling mechanism gives *quantitative* predictions (the average frequency of the fluctuations) in excellent agreement with experimental measurements. To our knowledge, this is the first time that the major characteristics of *experimentally observable* conductance fluctuations in quantum dots are explained in a quantitative way, indicating the fundamental importance of dynamical tunneling in the transport dynamics of electrons in semiconductor nanostructures.

An important class of nanostructures is the two-dimensional electron gas (2DEG) quantum dots [1,2]. In these systems, electrons are restricted to a plane near the interface between two different semiconductors. Applying voltage to contact gates deposited above the junction allows for the construction of submicron-sized 2D cavities in which electrons are scattered ballistically. Furthermore, in 2DEGs the mean-free path and coherence lengths are typically much larger than the cavity length at milli-Kelvin temperatures. For low currents, the transport characteristics of the quantum dot are determined by the approximately ballistic and coherent motion of electrons in the cavity [1,2]. One can therefore expect that the classical electron dynamics (regular or chaotic) will play a major role in the transport. A popular approach is to assume that the underlying classical dynamics is completely chaotic (or *hyperbolic*), and then use the random matrix theory (RMT) [4] and similar approaches, which predict universal conductance fluctuations with a Lorentzian correlation function [5]. A fundamental difficulty with RMT-like approaches is that typical systems have a *nonhyperbolic* dynamics, with regions of chaotic scattering coexisting with nonescaping KAM islands surrounding stable orbits in phase space. Many experimental results have accumulated, suggesting that hyperbolicity is an unusual dynamical feature in 2DEG quantum dots [6–11]. Thus, for typical dots, the observed properties of the transport simply cannot be explained by RMT-like approaches. In these systems, the conductance shows strong *regular* fluctuations as the gate voltage (or the magnetic field) is varied, as opposed to the random behavior predicted by RMT-like theories [8,12]. An example of the measured fluctuations is shown in the lower-left inset of Fig. 1. These fluctuations have been found to be associated with high concentrations of wave functions ("scarring") around

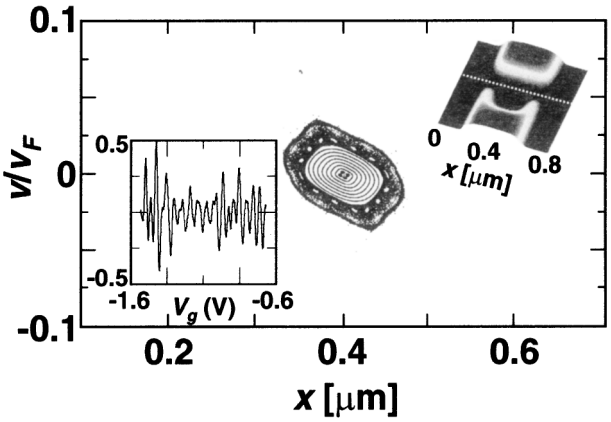

FIG. 1. Poincaré section for $V_g = -0.6$ V, with $E = E_F = 14.3$ mV. The section is taken along the dotted line. v is the x component of the velocity, and is given in units of the Fermi velocity. The "chaotic sea" surrounding the island is the plot of one single trajectory that stays a long time near the island before escaping. The phase-space area of the island is about $\hbar$. The upper-right inset shows the electrostatic potential profile (as a grey scale plot) of the dot for a gate voltage of -0.6 V. The lower-left inset shows the measured conductance fluctuations observed by varying the gate voltage. See Ref. [8] for further details.

certain periodic orbits within the dot. In this Letter, we argue that, to explain these results, it is necessary to take into account the quantum-mechanical tunneling of electrons through the KAM islands (dynamical tunneling), which corresponds to classically forbidden trajectories that are not taken into account in the usual semiclassical approach. We show that resonant features in the conductance correspond to the values of the external parameter (the gate voltage) for which the semiclassical quantization condition is satisfied for periodic orbits with low period, including stable orbits within the KAM islands. These features correspond to tunneling resonances neglected by usual semiclassical approaches. We compare the predictions of our theory to the results of a recent experiment [8], in which a gate-voltage variation was used to generate oscillations in the conductance of GaAs/AlGaAs quantum dots. In a fully quantum-mechanical analysis of this behavior, the conductance oscillations were found to be correlated to the excitation of specific wave function concentrations in transport. In this Letter, we provide a semiclassical description of this effect, and show that the periods of the experimentally measured conductance oscillations agree extremely well with those predicted by our theory.

Although our theory can be applied to any 2DEG quantum dots, we focus on a specific system for which experimental data are available [8]. The self-consistently computed profile of this dot is shown in the upper-right inset of Fig. 1 (for more details on this, see [8]). For the range of voltages we have studied, the shape remains basically the one shown in the inset of Fig. 1. For higher voltages (in modulus), the potential is more confining, and the two openings become smaller as $|V|$ increases. The low-temperature electron mobility and density of this dot are 4×10^{15} m^{-2} and 70 m^2/V s [8], respectively, with a corresponding Fermi energy of 14.3 meV. Each gate voltage corresponds to a different shape of the electrostatic potential. This potential is computed self-consistently on a grid using a Poisson solver for several gate voltages; for points not on the grid, it is calculated using cubic spline interpolation [13]. The transmission of a conducting electron can be described as a scattering process: The electron enters the dot by one lead, bounces around for a while, and then leaves. To study the classical dynamics of the scattering, we simulate the motion of the electron on the previously calculated potentials, with the electron at the Fermi energy. We use a Poincaré section to visualize the dynamics. For hyperbolic dynamics, all orbits are unstable, and all initial conditions escape the dot in a finite time (except for a set of null measure). The Poincaré section of almost every initial condition consists then of a finite number of points, and there are no stable orbits or KAM islands in phase space. From the results shown in Fig. 1, however, we see that the dynamics is clearly nonhyperbolic, with a large KAM island dominating the phase space. This island is centered on a period-1 orbit that bounces back and forth vertically at the center of the dot, called the *bouncing-ball orbit*. Clearly, RMT cannot be applied to this system. The features of Fig. 1 appear to be typical for most quantum dots.

There are some important theoretical works on the semiclassics of nonhyperbolic systems [9–11,14], but they also predict stochastic conductance fluctuations (with different statistical properties than in the hyperbolic case), and fail to predict the regular fluctuations seen in experiments. This is because the usual semiclassical theory considers only interference between classically allowed trajectories, and, hence, ignores the possibility of electron tunneling into the KAM island (corresponding to diffraction in optics). This effect is negligible only if the electron de Broglie wavelength λ_e is much smaller than the cavity size. For dots with a typical size of 1 μm, λ_e is typically one-tenth of the cavity length, and therefore tunneling *cannot* be neglected, as we will show. On the other hand, λ_e is small enough so that some important semiclassical concepts such as the Bohr-Sommerfeld quantization of periodic orbits can still be applied. Conductance measurements reveal that these regular oscillations have only a few main frequencies; this is shown by the Fourier analysis of the fluctuations, which exhibits a few well-defined peaks [8]. We can now argue that these peaks are due to dynamical tunneling [15]: There is a probability that an incoming electron tunnels inside the KAM island. If the electron energy and the system parameters are such that the semiclassical quantization condition (see below) is satisfied for a low-period stable periodic orbit within the island, there is a resonance with a sharp decrease in the transmission. As the system's parameters change, these resonances occur with a period given by the position of the peaks in the Fourier transform. These arguments are made quantitative below. We note that dynamical tunneling is of great importance in many fields, in particular in cold-atom physics [3]. Recent studies have demonstrated a mixed phase space in the atomic optical billiard [16], so the results of our study may be important for such systems.

Because KAM separatrices are classically impenetrable, the classical dynamics restricted to the island shown in Fig. 1 is that of a closed system. For closed systems, it is well known from the expansion of the Gutzwiller trace formula that each *stable* orbit generates a series of delta functions in the density of states, at energies for which the resonance condition holds [17,18]:

$$S_{\text{eff}} = S + \frac{\omega}{2\pi}\left(m + \frac{1}{2}\right) + \frac{\lambda}{4\pi} = n\,, \qquad (1)$$

where $S = \frac{1}{h}\int \mathbf{p}\cdot d\mathbf{q}$ is the action along the periodic orbit in units of Planck's quantum, ω is the stability angle of the orbit, and λ is the Maslov index [4,17]; $m, n = 0, 1, 2, \ldots$. Our system is open, however. Just as an incoming electron can tunnel in, an electron within the island is in a *metastable* state, and may "decay" by escaping. This causes the peaks in the density of states to broaden, and

their width is inversely proportional to the average time it takes for an electron to tunnel out of the island. If this time is not too short, the peaks will be sharp enough to be resolved, and their positions are given by Eq. (1).

Consider first the case $m = 0$. Note that n is the *longitudinal quantum number,* and counts the number of nodes in the "eigenfunction" along the orbit (of course this is not a true eigenfunction, since the system is metastable). Within the island of Fig. 1, there are infinitely many periodic orbits, but only the lowest-period ones are expected to be resolved (high-period orbits generate peaks that are too closely spaced to be resolved, even more so with the broadening of the levels caused by the quantum metastability of the system). The most important orbit in the island is the period-1 bouncing-ball orbit corresponding to the fixed point in the center of the island in Fig. 1. We calculate numerically S_{eff} in Eq. (1) as a function of the gate voltage for this island, and compare to the experimental results. The result is shown in Fig. 2, and we see that the points fall reasonably well on a straight line, which corresponds to a periodic recurrence of the resonance. Since a resonance happens each time S_{eff} goes through an integer, the (absolute value of) the slope of the straight line gives the semiclassical prediction for the frequency of the conductance oscillations. We find this frequency to be 16.4 V^{-1}, in remarkable agreement with the measured value of 15 V^{-1} [8]. This shows that this peak corresponds to recurring tunneling resonances, and cannot be explained by the usual

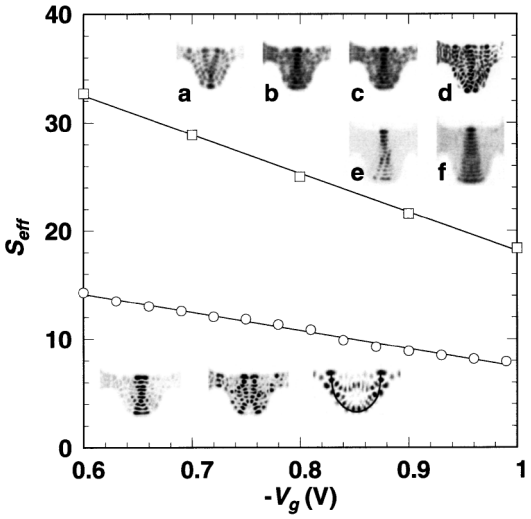

FIG. 2. Effective action versus the gate voltage, for the stable (circles) and the unstable (squares) orbits. The lower inset shows a pair of closely spaced concentrated wave functions corresponding to the stable bouncing-ball orbit (left and center images), and a scar due to the unstable orbit (right image) along with its corresponding classical orbit, obtained by a full quantum-mechanical simulation of the open system. A sequence of concentrations of wave functions around some classical periodic orbits, as the gate voltage changes, is also shown, where (a)–(f) correspond to $V_g = -0.928$ V, $V_g = -0.862$ V, $V_g = -0.807$ V, $V_g = -0.755$ V, $V_g = -0.700$ V, and $V_g = -0.640$ V, respectively.

semiclassical theory, where tunneling is ignored. This is further reinforced by a fully quantum mechanical simulation of the *open* system [8]. Figure 2 shows a sequence of concentrations of wave functions (the top six insets), computed from the results of the simulation following the technique shown in [19], each corresponding to a different value of the gate voltage. The recurrence frequency of the concentrated wave function was determined to be 16 V^{-1}, in agreement with our semiclassical prediction and with the experimental result. Since this orbit is classically inaccessible from the outside, this figure gives us more direct evidence of dynamical tunneling.

We now consider the general case, when m is any positive integer. The second term in S_{eff} (1) represents the quantization of the component of the motion transversal to the periodic orbit. This means that for each n there is actually a (theoretically infinite) set of resonances, labeled by m, similar to a vibrational band in a molecule. Assuming that S_{eff} changes linearly with the gate voltage V_g (which, as Fig. 2 shows, is a good approximation), we can estimate the separation ΔV_g between two resonances with consecutive transversal quantum numbers: $\Delta V_g \approx \frac{\omega}{2\pi |dS_{\text{eff}}/dV_g|}$, where it is assumed that ω does not change much between the two resonances. Although ω depends on n, its values are found (numerically) to lie in the range between 1 and 2 rad. Using the value of $|dS_{\text{eff}}/dV_g|$ derived from Fig. 2, we obtain that ΔV_g is between 1×10^{-2} V and 2×10^{-2} V. Just as n counts the number of nodes along the orbit, m counts the number of nodes across it, so we expect from all this that, for each n, there is a set of concentrated wave functions having $0, 1, 2, \ldots$ transversal nodes, separated by a gate voltage interval of ΔV_g. Such recurring pairs of concentrated wave functions were observed in the quantum-mechanical simulation for the bouncing-ball orbit, separated by a gate voltage difference of about 2×10^{-2} V, which agrees well with our prediction. One pair is shown in Fig. 2 (the lower-left and middle insets), and we see that they correspond to $m = 0$ and $m = 1$. They are also found for the other values of n, and they recur at the *same* period, as predicted. We stress that this phenomenon cannot be explained without tunneling, since it requires electrons to access the stable orbit, which is classically (and also semiclassically) forbidden. The concentrated wave function corresponding to higher values of m ($m = 2, 3, \ldots$) are not resolved by the simulation, presumably because they have a short lifetime; from Fig. 2, we see that the $m = 1$ wave function is quite "fat," and as m increases it becomes even more so, since the number of nodes increases. For $m > 1$, we expect the wave function to have a large overlap with that outside of the island, which corresponds to orbits that escape quickly, thus making these resonances very short lived, and so unresolved.

Although we focused on the stable orbits, unstable orbits are also present in the system and contribute to the density of states. The concentrated wave function (scar)

corresponding to the main unstable orbit is displayed in the lower-right inset of Fig. 2. A classical trajectory analysis suggests the orbit giving rise to this whispering-gallery scar is guided by the soft walls around the perimeter of the lower section of the dot, bouncing from the upper wall at two points, located close to the two lead openings. This classical orbit is depicted in the same inset. The resonant condition for unstable periodic orbits is given by Eq. (1) without the ω term [17]. This means that unstable orbits do not give rise to the subband of resonances associated with m. In the Fourier transform of the conductance oscillations, a peak is observed at $V_g \approx 37$ V, corresponding to an unstable periodic orbit of period 1. Figure 2 shows a plot of S_{eff} versus V_g for this orbit, and from the slope we get a recurrence frequency of 36.3 V^{-1}, again in very good agreement with the experimental result. The concentrated wave functions related to these resonances are seen in the quantum-mechanical simulation, but no subband is seen, confirming our predictions. The other main periodicities found in the conductance correspond to harmonics of the main stable and unstable resonances studied above. Note that, in [11], isolated resonances are predicted to arise from the chaotic part of the phase space outside the islands (see Fig. 1), but these can be detected for smaller values of $\hbar$ only, i.e., larger quantum dots [20].

In summary, we argue that the usual semiclassical approach is not enough to explain the transport characteristics of typical semiconductor nanostructures, and the quantum-mechanical tunneling of the electron through KAM islands has to be taken into account. Tunneling resonances caused by low-period stable and unstable periodic orbits within the KAM islands cause regular oscillations of the conductance. Such oscillations have been observed experimentally, and they are very well predicted by our theory. These results are expected to hold for any mesoscopic system. Our general standpoint is that tunneling plays a fundamental role in mesoscopic transport [21]. While periodic oscillations dominate the conductance of the small dot that we study here, in other experimental work we have shown that the periodic nature of the fluctuations becomes steadily obscured as the dot size is increased [22]. Experimental studies of such larger dots have therefore typically focused on a discussion of the statistical properties of the fluctuations, emphasizing the characteristics of their nonperiodic components.

A. P. S. M. and Y. C. L. were supported by AFOSR under Grant No. F49620-98-1-0400. R. A., J. B., and D. K. F. acknowledge support from ONR.

[1] D. K. Ferry and S. M. Goodnick, *Transport in Nanostructures* (Cambridge University Press, Cambridge, England, 1997).

[2] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, England, 1995).

[3] Some recent works on dynamical tunneling in atomic physics include the following: W. K. Hensinger *et al.,* Nature (London) **412**, 52 (2001); D. A. Steck, W. H. Oskay, and M. G. Raizen, Science **293**, 274 (2001). For a recent review on tunneling and chaos, see S. Tomsovic, Phys. Scr. **T90**, 162 (2001). The novelty of our work lies in, however, the finding of the role played by dynamical tunneling in quantum-dot transport.

[4] H.-J. Stockmann, *Quantum Chaos: An Introduction* (Cambridge University Press, Cambridge, England, 1999).

[5] R. Blümel and U. Smilansky, Phys. Rev. Lett. **60**, 477 (1988); R. A. Jalabert, H. U. Baranger, and D. A. Stone, Phys. Rev. Lett. **65**, 2442 (1990).

[6] J. P. Bird *et al.,* Europhys. Lett. **35**, 529 (1996); R. Akis, D. K. Ferry, J. P. Bird, and D. Vasileska, Phys. Rev. B **60**, 2680 (1999); Y. Takagaki *et al.,* Phys. Rev. B **62**, 10 255 (2000); R. Akis, J. P. Bird, D. K. Ferry, and D. Vasileska, Physica (Amsterdam) **7E**, 745 (2000).

[7] A. P. Micolich *et al.,* J. Phys. Condens. Matter **10**, 1339 (1998); R. P. Taylor *et al.,* Phys. Rev. B **58**, 11 107 (1998); A. P. Micolich *et al.,* Phys. Rev. Lett. **87**, 036802 (2001).

[8] J. P. Bird, R. Akis, D. K. Ferry, D. Vasileska, J. Cooper, Y. Aoyagi, and T. Sugano, Phys. Rev. Lett. **82**, 4691 (1999).

[9] R. Ketzmerick, Phys. Rev. B **54**, 10 841 (1996); A. S. Sachrajda *et al.,* Phys. Rev. Lett. **80**, 1948.

[10] B. Huckestein, R. Ketzmerick, and C. H. Lewenkopf, Phys. Rev. Lett. **84**, 5504 (2000); T. Geisel, R. Ketzmerick, and O. Schedletzky, Phys. Rev. Lett. **69**, 1680 (1992); Y. Takagaki and K. H. Ploog, Phys. Rev. E **62**, 4804 (2000).

[11] L. Hufnagel, R. Ketzmerick, and M. Weiss, Europhys. Lett. **54**, 703 (2001).

[12] J. P. Bird, R. Akis, and D. K. Ferry, Phys. Rev. B **60**, 13 676 (1999).

[13] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C* (Cambridge University Press, Cambridge, England, 1997).

[14] Y.-C. Lai *et al.,* Phys. Rev. Lett. **68**, 3491 (1992).

[15] P. Seba, Phys. Rev. E **47**, 3870 (1993).

[16] A. Kaplan, N. Friedman, M. Andersen, and N. Davidson, Phys. Rev. Lett. **87**, 274101 (2001).

[17] M. C. Gutzwiller, J. Math. Phys. (N.Y.) **12**, 343 (1971); M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990).

[18] W. H. Miller, J. Chem. Phys. **63**, 996 (1975).

[19] T. Usuki, M. Saito, M. Takatsu, R. A. Kiehl, and N. Yokoyama, Phys. Rev. B **52**, 8244 (1995).

[20] In contrast to Ref. [11], $\hbar$ is the size of the island and therefore the hierarchical part of phase space surrounding the island is not resolved quantum mechanically. That is the reason why the resonances due to the hierarchical states are not observed. Note, however, that these are always *broader* than the ones due to the stable island.

[21] Signature of periodic orbits in transmission through an open resonator has been studied experimentally by Katine *et al.* [Phys. Rev. Lett. **79**, 4806 (1997)] and subsequently theoretically by Hersch *et al.* [Phys. Rev. Lett. **83**, 5342 (1999)] which emphasizes the significance of diffracting effects in mesoscopic structures. However, the issue of dynamical tunneling is not discussed in these papers.

[22] J. P. Bird, R. Akis, D. K. Ferry, Y. Aoyagi, and T. Sugano, J. Phys. Condens. Matter **9**, 5935 (1997).