Classical and Quantum Mechanical Transport Simulations in Open Quantum Dots

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In order to apply quantum dots as electronic devices in the near future, a quantitative understanding of the details of electron transport in the dots is required. *Open* quantum dots [1], considered here, consist of small cavities connected to two-dimensional regions of electron gas (2DEG) by narrow constrictions which allow several modes to propagate. An interesting aspect of open quantum dots is the interplay of regular, quasi-regular and chaotic behavior of the electron transport, where one is concerned with the correspondence of classical and quantum mechanical behavior [2].
In this work we focus on the transport in open quantum-dot arrays regarding the correspondence of classical and quantum-mechanical treatments. We analyze, in particular, a prominent peak that was recently reported in the low-field magneto-resistance, MR, of a single dot and arrays with different numbers of dots [3,4]. Certain details of the behavior of this MR peak can be interpreted in the classical treatment only by additionally assuming phase-space tunneling. In the quantum-mechanical interpretation an important result is the opening of gaps in the (complex) band structure and the decay of the wave function along the dot array and its dependence on the energetic position in the gap.
The quantum-mechanical calculation is performed by discretizing the Schrödinger equation onto a finite-difference mesh and using it in its discrete form to set up a numerically stabilized variant of the transfer matrix [5,6] approach. By imposing an electron flux from the left, one obtains the transmission coefficient that enters the Landauer-Buttiker formular to give the conductance. For obtaining the band structure periodic boundary conditions are assumed at the ends of a single dot. The confinement is modeled by a smooth potential.
In the classical treatment this is approximated by a parabolic potential. It allows us solving the equation of motion analytically. Choosing certain initial conditions (position and velocity) the further path of the electron can be calculated in closed form; reflected (backscattered to the entrance constriction) and transmitted trajectories can be distinguished. The weighting of the direction of the initial velocity v_0 is chosen to be Lambert like, i.e. it depends as $\cos\alpha$ on the entrance angle.
Electrons are counted as transmitted if they hit the part of the boundary corresponding to the exit constriction. They are counted as backscattered if they hit the entrance constriction.
Finally, the conductance is obtained as

$$G(B) = \left\langle G(B,\alpha)\cos\alpha \right\rangle_{\alpha} = \frac{\int_{-\pi/2}^{\pi/2} G(B,\alpha)\cos\alpha d\alpha}{\int_{-\pi/2}^{\pi/2} \cos\alpha d\alpha} \qquad (1)$$

In order to visualize the electron dynamics in the phase space of the array we also compute Poincaré sections.
The Poincaré sections provide a useful numerical tool for testing the phase space for different magnetic fields. We get a mixed phase space for the open dot array. At the MR peak the phase space consists of periodic and chaotic orbits whereas by moving the magnetic field away from the peak position the phase space shows quasi-periodic and chaotic orbits. Quasi periodic and periodic orbits emerge due certain initial conditions within the dot and are classically inaccessible. In the literature these closed orbits are referred to as Kalmogorov-Arnol'd-Moser (KAM) islands [2].
The quantum-mechanically computed band structure shows, in contrast to the zero field case, band gaps at the MR peak. For an energy situated within the gap the probability density, $|\psi(x,y)|^2$, (Fig.1), shows a fast exponential decay which indicates tunneling through the array. The $|\psi(x,y)|^2$ in the first dot corresponds in shape to the backscattered trajectory of the classical calculation. When positioning the considered energy near the bottom of the gap we reveal a probability density which is peaked in the 3rd dot (Fig.2). The decay of $|\psi(x,y)|^2$ is now weaker than in Fig.1. Again the $|\psi(x,y)|^2$ in the 3rd dot can be described by a combination of two classically calculated trajectory with starting angle α_1=227° (red) and α_2=47° (green). Identifying the orbits as closed we argue that the transmission through the array is based on tunneling between these closed orbits. In order to

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describe the transmission through the dot the classically inaccessible regions existing in the mixed phased space have to be taken into account. This is only possible by assuming phase space tunneling introduced above.

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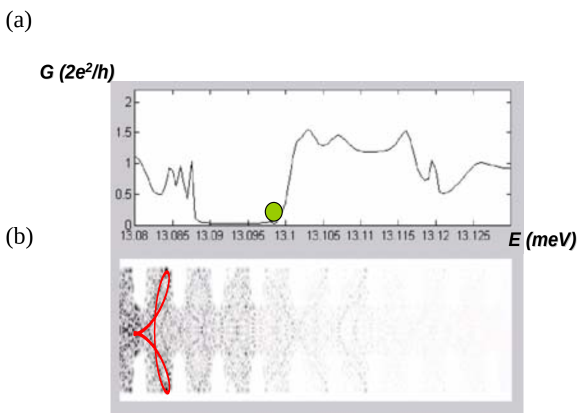

Fig. 1. (a) The calculated conductance as a function of energy at the magnetic field position of the MR peak. The Green point indicates the energy position for the calculated $|\psi(x,y)|^2$. (b) $|\psi(x,y)|^2$ looks like an ***open, backscattered*** trajectory of the classical calculation (superimposed in red in the 1st dot).

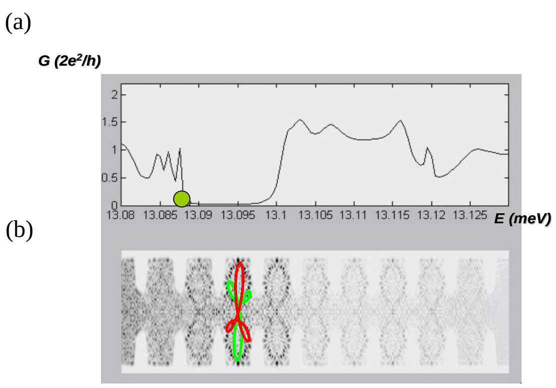

Fig. 2 (a) The calculated conductance as a function of energy at the magnetic field position above the MR peak. The green point indicates the energy position for the calculated $|\psi(x,y)|^2$. (b) The $|\psi(x,y)|^2$ in the 3rd resembles two ***closed*** trajectories (red and green) that are classically inaccessible from the outside, indicating that conductance is only possible by assuming phase-space tunnelling.

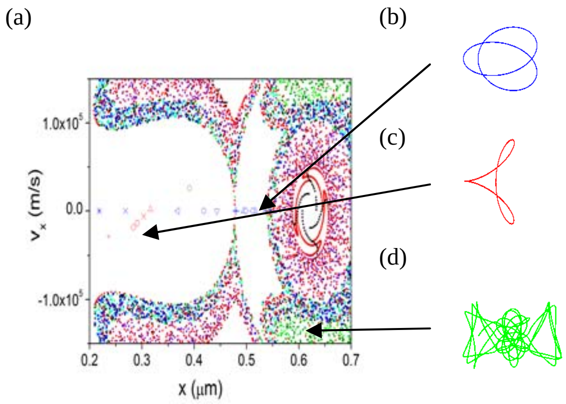

Fig. 3. (a) Poincaré section at the MR peak. (b) A periodic orbit (blue open symbols), (c) backscattered trajectory (red open symbols) (d) chaotic trajectory (green points). The arrows mark points representing v_x and x at y=0 on the trajectories shown.