Aharonov-Bohm Oscillations and Resonant Tunneling in Strongly Correlated Quantum Dots

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We investigate Aharonov-Bohm oscillations of the current through a strongly correlated quantum dot embedded in an arbitrary scattering geometry. Resonant-tunneling processes lead to a flux-dependent renormalization of the dot level. As a consequence, we obtain a fine structure of the current oscillations, which is controlled by quantum fluctuations. Strong Coulomb repulsion leads to a continuous bias voltage dependent phase shift and, in the nonlinear response regime, destroys the symmetry of the differential conductance under a sign change of the external flux.

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Phase-sensitive transport properties of interacting mesoscopic systems are important for several reasons. The small size of the samples gives rise to capacitances of order 10^{-15} F, which induce Coulomb blockade effects [1] and demand the necessity to generalize the Landauer-Büttiker formalism [2] to systems with strong interactions. Furthermore, the investigation of Aharonov-Bohm oscillations through quantum dots with strong Coulomb repulsion might give further experimental evidence for resonant tunneling and Kondo phenomena in nonequilibrium systems [3–5].

Interference effects in the Coulomb blockade regime have been measured by Yacoby *et al.* [6] by studying a quantum dot embedded in an Aharonov-Bohm ring. This experiment demonstrates that phase-coherent transport through quantum dots is possible in realistic experiments and is not destroyed by inelastic interactions. Recent theoretical work on Aharonov-Bohm oscillations in a mesoscopic ring with a quantum dot [7,8] uses a noninteracting model. Using the symmetry of the current under a sign change of the external flux in the linear response regime [9,10], it was shown in Ref. [7] that the phase of the Aharonov-Bohm oscillations can only take two possible values as a function of the gate voltage on the dot. However, the experiment of Yacoby *et al.* is performed in the Coulomb blockade regime where interaction effects are important. In this Letter we will take such correlations into account by setting up a complete and general theory for interference phenomena in strongly interacting quantum dots embedded in an arbitrary noninteracting multiprobe and multichannel scattering structure. As a consequence, we will show that the symmetry under sign change of the external flux is broken in the nonlinear response regime and that the phase can change continuously as a function of the bias voltage. Furthermore, we will analyze in detail the current oscillations as a function of the gate voltage caused by the flux-modulated renormalization of the local energy level of the dot.

To have a specific example, we will study the system shown in Fig. 1, although our formalism is valid for an arbitrary scattering geometry. For simplicity we start with the case of one-channel leads. The system without the quantum dot is described by scattering waves with zero boundary conditions at the tunneling barriers of the dot. Thus, in energy representation, this part of the Hamiltonian is given by $H_S = \sum_{\alpha\sigma} \int d\epsilon\, \epsilon a^\dagger_{\alpha\sigma}(\epsilon) a_{\alpha\sigma}(\epsilon)$, where $a^\dagger_{\alpha\sigma}(\epsilon)$ creates an incoming scattering wave in probe α with spin σ and total energy ϵ. The isolated dot is described by $H_D = \sum_\sigma \epsilon_\sigma d^\dagger_\sigma d_\sigma + U \sum_{\sigma<\sigma'} n_\sigma n_{\sigma'}$ with single particle energies ϵ_σ and on-site repulsion U. The position of the dot levels are controlled by an external gate voltage, and $U \sim 1-5$ K corresponds to the charging energy [11].

The tunneling of the electrons into or out of the dot is described by

$$H_T = \sum_{\alpha\sigma} \int d\epsilon \{t_\alpha(\epsilon) a^\dagger_{\alpha\sigma}(\epsilon) d_\sigma + \text{H.c.}\}. \qquad (1)$$

Here, $t_\alpha(\epsilon) = \sum_{i=L/R} t_i \langle \alpha\epsilon | x_i \rangle$ are the tunneling matrix elements in energy representation, where t_i are real quantities and $\langle x | \alpha\epsilon \rangle$ is the spin-independent scattering wave from reservoir α with energy ϵ at position x. By x_i, $i = L, R$, we denote an arbitrary point in the one-dimensional left or right lead that is connected to the dot [12]. Because of zero boundary conditions we have $\langle x_i | \alpha\epsilon \rangle = \rho(\epsilon)^{1/2} A^i_\alpha(\epsilon) \sin[k(\epsilon) x_i]$ with the one-dimensional density of states $\rho(\epsilon) = 1/\pi\hbar v(\epsilon)$ and energy $\epsilon = \hbar^2 k(\epsilon)^2/2m = \frac{1}{2} m v(\epsilon)^2$. The coefficients A^i_α

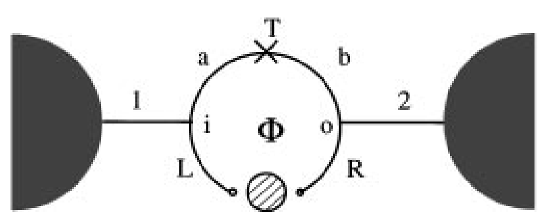

FIG. 1. Geometry of the model system studied here. Leads 1 and 2 connect to the left and right reservoirs (shaded). The ring is connected to a quantum dot via high tunneling barriers. Φ is the flux penetrating the ring.

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depend on the detailed scattering problem under consideration. We have chosen the tunneling matrix elements t_i as real parameters, which means that we shift the complete flux dependence to the scattering Hamiltonian H_S via a standard gauge transformation.

Following Büttiker [13], we will use the following representation of the current operator in probe α:

$$\hat{I}_\alpha = \frac{e}{h} \int d\epsilon\, d\epsilon' \sum_\sigma [a^\dagger_{\alpha\sigma}(\epsilon) a_{\alpha\sigma}(\epsilon') - b^\dagger_{\alpha\sigma}(\epsilon) b_{\alpha\sigma}(\epsilon')], \tag{2}$$

where $b_{\alpha\sigma}(\epsilon) = \sum_\beta s_{\alpha\beta}(\epsilon) a_{\beta\sigma}(\epsilon)$ annihilates an outgoing carrier in probe α and s is the scattering matrix of the system without the dot. To calculate the average current $I_\alpha = \langle \hat{I}_\alpha \rangle$ in the stationary limit we need the stationary real-time Green's function $G^<(E) = \int dt\, e^{iEt} G^<(t)$ in Fourier space of two scattering field operators: $G^<_{\alpha\sigma,\alpha'\sigma'}(\epsilon, \epsilon'; t) = i\langle a^\dagger_{\alpha\sigma}(\epsilon, t) a_{\alpha'\sigma'}(\epsilon')\rangle$. Using the matrix notation

$$\hat{G} = \begin{pmatrix} G^R & G^< \\ 0 & G^A \end{pmatrix},$$

where G^R and G^A are the retarded and advanced Green's functions, and applying the Keldysh technique [14], we can express the Green's function $\hat{G}_{\alpha\sigma,\alpha'\sigma}$ exactly by the local Green's function $\hat{G}_\sigma$ of the dot, $\hat{G}_{\alpha\sigma,\alpha'\sigma}(\epsilon, \epsilon'; E) = \hat{g}_\alpha(\epsilon; E)\delta_{\alpha,\alpha'}\delta(\epsilon - \epsilon') + t_\alpha(\epsilon) t_{\alpha'}(\epsilon')^* \hat{g}_\alpha(\epsilon; E)\hat{G}_\sigma(E) \times \hat{g}_{\alpha'}(\epsilon'; E)$, where we have already used spin conservation. The Green's functions $\hat{g}_\alpha$ correspond to the Hamiltonian H_S and are given by $g^{R/A}_\alpha(\epsilon; E) = (E - \epsilon \pm i0^+)^{-1}$ and $g^<_\alpha(\epsilon; E) = 2\pi i f_\alpha(E)\delta(E - \epsilon)$ where f_α is the Fermi distribution function of reservoir α. Using this result in calculating the average current, inserting the form of the tunneling matrix elements, and performing the energy integrations [15], we obtain

$$I_\alpha = I^{(0)}_\alpha + \frac{e}{h} \mathrm{Re} \sum_\sigma \sum_{\beta\gamma} \int dE\, s^\dagger_{\alpha\beta} s_{\alpha\gamma} A_{\gamma\beta} \times \left(\frac{i}{2} G^<_\sigma + i f_\beta G^R_\sigma \right), \tag{3}$$

where $I^{(0)}_\alpha$ is the current without the dot (given by the usual Landauer-Büttiker formula) and $A_{\alpha\alpha'} = \sum_{ij} (\Gamma_i \Gamma_j)^{1/2} A^{i*}_\alpha A^j_{\alpha'}$ with $\Gamma_i(\epsilon) = 2\pi\rho(\epsilon) t_i^2$.

Equation (3) is the first central result of this paper. It relates the current in probe α exactly to the local Green's functions of the dot and the scattering properties of the noninteracting medium surrounding the dot. This formula is a natural generalization of the Landauer-Büttiker formula to an interacting quantum dot. Furthermore, it generalizes current formulas through quantum dots connected to two leads without any possibility of a direct transition between the probes [16]. Here we are able to account for such transitions opening the possibility to study interference phenomena in the presence of locally interacting subsystems. The generalization of Eq. (3) to multichannel leads is straightforward. Again following Ref. [13] the field operators $a_{\alpha\sigma}$ in Eq. (2) have to be treated as vectors with a channel index n. Equivalently, the matrix elements $s_{\alpha\beta}$ and $A_{\alpha\beta}$ have to be treated like $Z_\alpha \times Z_\beta$ matrices where Z_α is the number of transverse channels in lead α. The final formula for the current is then exactly like Eq. (3) except that we have to take the trace of the matrix multiplication $s^\dagger_{\alpha\beta} s_{\alpha\gamma} A_{\gamma\beta}$.

The scattering matrices in Eq. (3) can be found by straightforward quantum-mechanical considerations depending on the specific geometry. For the Green's functions of the dot we will use a real-time technique developed in Ref. [17], which has been applied to a quantum dot in Ref. [4]. For a degenerate dot level (i.e., $\epsilon_\sigma = \epsilon_d$ independent of spin) and in the $U = \infty$ limit, one obtains $G^{</>}_\sigma(E) = 2\pi i \gamma^\pm(E)\, |E - \epsilon_d - \sigma(E)|^{-2}$. Here,

$$\sigma(E) = \int dE' \frac{M\gamma^+(E') + \gamma^-(E')}{E - E' + i0^+} \tag{4}$$

has the form of a self-energy that describes the renormalization and broadening of the dot level ϵ_d, $\gamma^\pm(E) = \sum_\alpha |t_\alpha(E)|^2 f^\pm_\alpha(E) = (1/4\pi)\sum_\alpha A_{\alpha\alpha}(E) f^\pm_\alpha(E)$ is the classical rate for a particle tunneling into or out of the dot, and $f^+_\alpha = f_\alpha$ while $f^-_\alpha = 1 - f_\alpha$. The retarded Green's function follows from $\mathrm{Im} G^R = (1/2i)(G^> - G^<)$, and the real part is obtained from the Kramers-Kronig relation.

The explicit result for the Green's functions together with the expression (3) for the current constitutes a complete theory of interference effects in mesoscopic scattering geometries with an interacting part given by a quantum dot with one degenerate level. Our result satisfies current conservation $\sum_\alpha I_\alpha = 0$, and all currents vanish in equilibrium. Furthermore, for the special case $M = 1$ where the Coulomb interaction does not play any role, our result is exact and can be shown to agree with the Landauer-Büttiker formalism.

The real part of the self-energy σ describes the renormalization of the dot level. If we neglect the energy dependence of $A_{\alpha\alpha}$ at the Fermi level, we obtain from Eq. (4) for a two-terminal system

$$\mathrm{Re}\sigma = \mathrm{Re}\sigma_1 + \frac{M-1}{8\pi} [(A_{11} + A_{22})(\chi_1 + \chi_2) + (A_{11} - A_{22})(\chi_1 - \chi_2)], \tag{5}$$

where σ_1 is the self-energy for $M = 1$ and $\chi_\alpha(E) = \mathrm{Re} \int dE' f_\alpha(E')/(E - E' + i0^+)$. Using a Lorentzian cutoff at D (which will be of the order of the Coulomb repulsion U), we obtain $\chi_\alpha(E) = \psi(\frac{1}{2} + D/2\pi T) - \mathrm{Re}\psi(\frac{1}{2} + i(E - \mu_\alpha)/2\pi T)$, where ψ is the digamma function and μ_α the chemical potential of reservoir α. σ_1 is always a symmetric function of the external flux Φ. Furthermore, for a spatially symmetric situation as in Fig. 1, $A_{11} \pm A_{22}$ is an even (odd) function of the phase $\varphi = 2\pi\Phi/\Phi_0$ (Φ_0 being the flux quantum). Because of $\mathrm{Re}\sigma_1$ the level position of the dot will oscillate with

φ with an amplitude of the order of Γ and phase 0 or π. For $M > 1$, there can be logarithmic corrections in temperature and bias voltage for the amplitude *and* phase of this oscillation due to the χ_α functions. The latter terms usually lead to Kondo-like correlations [3,4].

To exhibit the consequences of the oscillation of the renormalized dot level we will now apply our results to the specific scattering geometry of Fig. 1, which corresponds to the experimental setup of Ref. [6]. For simplicity we assume a one-dimensional structure, and we use the same scattering matrices $s^{i,o}$ for the incoming and outgoing junctions as in Ref. [9]. The scattering matrix of the upper arm (including the flux and the phases accumulated by free motion) is written in the form

$$s^T = p\begin{pmatrix} r & te^{-i\varphi} \\ te^{i\varphi} & r \end{pmatrix},$$

where $p = e^{ikl}$ is the phase acquired by free motion through the upper arm. Furthermore, we take the length of the leads connected to the quantum dot as $l_L = l_R = \frac{1}{2}l$, and we assume a symmetric quantum dot with $\Gamma_L = \Gamma_R = \Gamma$.

We will look explicitly at two cases, viz., perfect transmission through the upper arm given by $r = 0$, $t = 1$, or weak transmission described by $r = -1$, $t = i|t|$. In the first case we obtain after a straightforward calculation $s_{11} = s_{22} = \frac{1}{2}p(p-1)$, $s_{12}(\varphi) = s_{21}(-\varphi) = \frac{1}{2}p(p+1)e^{i\varphi}$, $A_1^L = A_2^R = \frac{1}{2}i\sqrt{p}\,(2-p)$, and $A_1^L(\varphi) = A_2^R(-\varphi) = -\frac{1}{2}ip\sqrt{p}\,e^{i\varphi}$. In the second case one obtains $s_{11} = s_{22} = -p$, $s_{12}(\varphi) = s_{21}(-\varphi) = \frac{1}{2}ip|t|e^{i\varphi}$, $A_1^L = A_2^R = i\sqrt{p}$, and $A_1^L(\varphi) = A_2^R(-\varphi) = \frac{1}{2}[p\sqrt{p}/(1+p)]\,|t|e^{i\varphi}$. The phase p cannot be determined and will have some specific value in the experiment. We assume here always to be in the quantum region; i.e., the lengths associated with temperature, bias voltage, and Γ should exceed the system length, so that we can neglect the energy dependence of p. In the perfect transmission case we choose $p = i$ and get $\mathrm{Re}\sigma_1 = -\frac{1}{4}\Gamma(3+\cos\varphi)$, $A_{11} + A_{22} = \Gamma(3+\cos\varphi)$, and $A_{11} - A_{22} = -2\Gamma\sin\varphi$. For weak transmission we take $p = 1$ and obtain $\mathrm{Re}\sigma_1 = -\frac{1}{8}|t|\Gamma\cos\varphi$, $A_{11} + A_{22} = 2\Gamma$, and $A_{11} - A_{22} = -|t|\Gamma\sin\varphi$.

In Fig. 2 we show the linear conductance for perfect transmission and $T = \Gamma = 0.01$ (in units of the cutoff D) for various positions of the dot level. We have assumed $M = 2$, i.e., the interacting case. The linear conductance is symmetric under a sign change of the flux since the $\sin\varphi$ term is absent in Eq. (5) for $\chi_1 = \chi_2$. If the position of the dot level is below $\epsilon_d \approx -0.02$, the current has a maximum around $\varphi = 0$. For higher values of ϵ_d, the current has a minimum at $\varphi = 0$. Although this looks similar to the abrupt phase change of π described in Ref. [6], Fig. 2 shows that the response of the system cannot be described by the concept of a "phase shift." What happens instead is that the current (as a function of φ) changes its functional form. The scale of the transition is independent of temperature and is given by the intrinsic parameter Γ. For higher temperatures we find a smaller amplitude of the current oscillations, but the qualitative picture remains. For weak transmission, the results are similar, but the scale is given by $t\Gamma$.

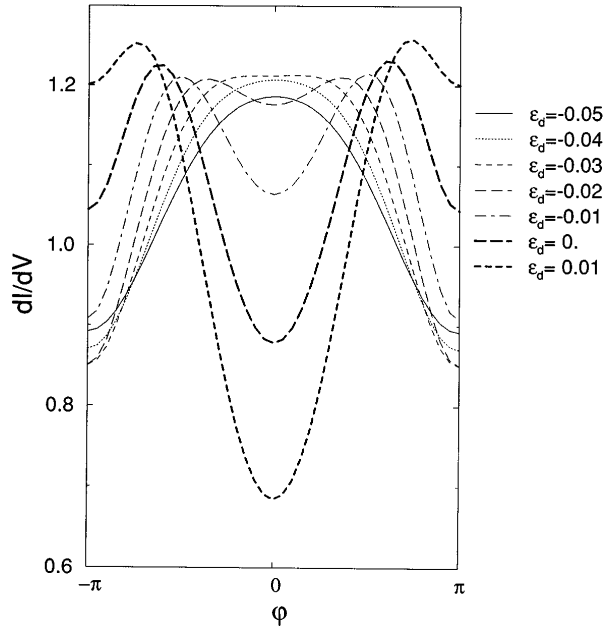

FIG. 2. Linear conductance (in units of e^2/h) as a function of magnetic flux for various positions of the level in the dot ($T = \Gamma = 0.01$, $M = 2$). We have assumed perfect transmission through the upper arm of the system as in the experiment by Yacoby *et al.* [6].

We will now turn to the nonlinear conductance. Figure 3 depicts the differential conductance for weak transmission as a function of φ for different voltages and level positions ($T = 10\Gamma = 0.1$). For $V = 0$, the differential conductance is symmetric around $\varphi = 0$, in the nonlinear response case, this symmetry is absent due to the last term in Eq. (5). The behavior of the differential conductance at the origin changes from a minimum to a maximum as a function of the level position ϵ_d, this time rather abruptly (energy scale $t\Gamma$). The asymmetry of the conductance curves for finite voltages is a genuine interaction effect; it disappears for $M = 1$. Furthermore, we observe a continuous phase shift of the current oscillations as a function of the bias voltage, which again is absent for $M = 1$. It is determined by the last term in Eq. (5) as well as by $\sin\varphi$ terms occurring explicitly in the current formula (3) via the $A_{\gamma\beta}$ matrices. Note that the temperature is 1 order of magnitude larger than Γ in this figure; i.e., an interference experiment of this type might yield information about correlation effects at temperatures that are accessible in experiments [18].

Finally we want to comment on the influence of interactions on the relative phase of the Aharonov-Bohm oscillations at successive peaks in the linear conductance as a function of the gate voltage. In a noninteracting model two adjacent peaks correspond to transport through

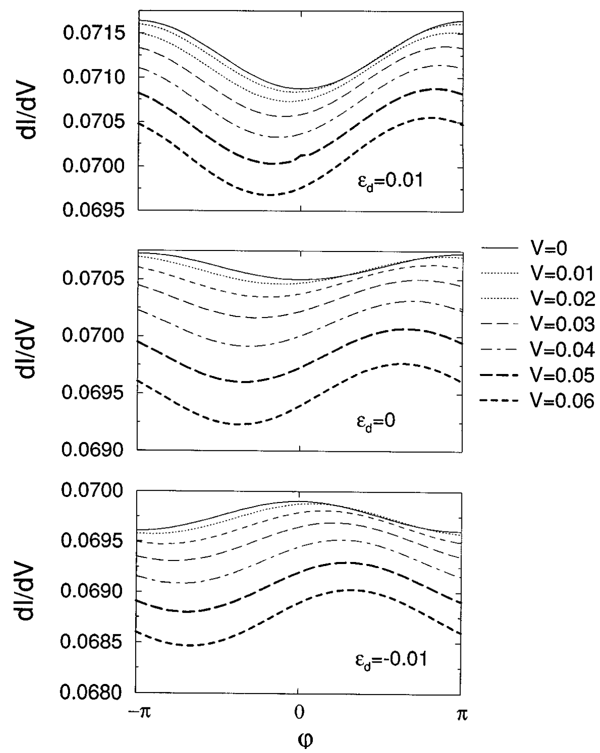

FIG. 3. Differential conductance (in units of e^2/h) for the case of weak transmission ($t = 0.1$) as a function of magnetic flux for various voltages and positions of the level in the dot ($T = 10\Gamma = 0.1$, $M = 2$). Note that the linear conductance ($V = 0$) is symmetric around $\varphi = 0$, whereas there is no such symmetry in the nonlinear response case.

two different energy levels of the dot that have different parity. Thus the relative sign of t_L and t_R would change from one level to the next, and consequently one expects a phase shift of π. However, in the experiment of Yacoby *et al.* no phase shift was measured. In addition to the discussion of Ref. [7], a strong Coulomb repulsion on the quantum dot could be an explanation for this observation. If there are N states on the dot that lie close together in energy but with the same parity in longitudinal direction (e.g., spin degenerate states or states differing in the transverse channel number), there would be N adjacent Coulomb peaks with the same phase of the Aharonov-Bohm oscillations. The distance of these Coulomb peaks is given by the charging energy U, whereas in the noninteracting case all these peaks would fall together into one single peak. Therefore we conclude that in the presence of interactions the parity of the energy levels contributing to the transport at adjacent Coulomb peaks can be the same, which provides an explanation for Yacoby's experiment.

In conclusion, we have presented a complete theory for interference phenomena in strongly correlated quantum dots embedded in a scattering geometry. On one hand, we have found that the functional form of $dI(\varphi)/dV$ is changing with the gate voltage on the scale of temperature-independent intrinsic parameters. In linear response this change cannot be interpreted as a phase shift. On the other hand, we have shown that in the nonlinear response regime correlation effects break the symmetry under sign change of the external flux and lead to a real continuous phase shift as a function of the bias voltage.

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