Aharonov-Bohm oscillations and resonant tunneling in strongly correlated quantum dots

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(March 23, 2022)

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.

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 and demand the necessity to generalize the Landauer-Büttiker formalism 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.

Interference effects in the Coulomb blockade regime have been measured by Yacoby et al. 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 uses a noninteracting model. Using the symmetry of the current under sign change of the external flux in the linear response regime, it was shown in Ref. that the phase of the Aharonov-Bohm oscillations can only take two possible values as 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 multi-probe and multi-channel 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. 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

$$H_S = \sum_{\alpha} \int d\epsilon \, \epsilon a_{\alpha \sigma}^\dagger a_{\alpha \sigma}(\epsilon) ,$$

where $a_{\alpha \sigma}(\epsilon)$ creates an incoming scattering wave in probe $\alpha$ with spin $\sigma$ and total energy $\epsilon$. The isolated dot is described by $H_D = \sum_\sigma \epsilon_\sigma d_\sigma^\dagger d_\sigma + U \sum_{\sigma < \sigma'} n_{\sigma} n_{\sigma'}$ with single particle energies $\epsilon_\sigma$ and on-site repulsion $U$. The position of the dot levels are controlled by an external gate voltage and $U \sim 1 - 5K$ corresponds to the charging energy.

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

$$H_T = \sum_{\alpha \sigma} \int d\epsilon \{ t_{\alpha}(\epsilon) a_{\alpha \sigma}^\dagger d_\sigma + h.c. \} .$$

(1)

Here, $t_{\alpha}(\epsilon) = \sum_i \langle x_i | \alpha \rangle t_i$ are the tunneling matrix elements in energy representation, where $t_i$ are real quantities and $\langle x_i | \alpha \rangle$ is the spin-independent scattering wave from reservoir $\alpha$ with energy $\epsilon$ at position $x_i$. By $x_i$, $i = L, R$, we denote an arbitrary point in the one-dimensional left or right lead which is connected to the dot. Due to zero boundary conditions we have $\langle x_i | \alpha \rangle = \rho(\epsilon)^{1/2} \tilde{A}_\alpha(\epsilon) \sin(k(\epsilon)x_i)$ with the one-dimensional density of states $\rho(\epsilon) = 1/(\pi \hbar v(\epsilon))$ and energy $\epsilon = \hbar^2 k^2(\epsilon)/2m = \frac{1}{2} m v(\epsilon)^2$. The coefficients $\tilde{A}_\alpha$ 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, we will use the following representation of the current operator in probe $\alpha$

$$\hat{I}_\alpha = \frac{e}{h} \int d\epsilon d\epsilon' \sum_\sigma [ a_{\alpha \sigma}(\epsilon) a_{\alpha \sigma}(\epsilon') - b_{\alpha \sigma}^\dagger(\epsilon) b_{\alpha \sigma}(\epsilon') ] .$$

(2)
where \( b_{a\sigma}(\epsilon) = \sum_\beta s_{a\beta}(\epsilon)a_{\beta\sigma}(\epsilon) \) annihilates an outgoing carrier in probe \( \alpha \) and \( s \) is the scattering matrix of the system without the dot. To calculate the average current \( I_\alpha = \langle \mathcal{I}_\alpha \rangle \) in the stationary limit we need the stationary real-time Green’s function \( G^<(\epsilon) = \int dt e^{i\epsilon t} G^<(t) \) in Fourier space of two scattering field operators: \( G^<_{a\sigma, \alpha'\sigma'}(\epsilon, \epsilon'; t) = i\langle a_{\alpha\sigma}(\epsilon, t) a_{\alpha'\sigma'}(\epsilon') \rangle \). Using the matrix notation \( \hat{G} = \begin{pmatrix} G^R & G^\Lambda \\ G^\Lambda & G^A \end{pmatrix} \), where \( G^R \) and \( G^A \) are the retarded and advanced Green’s functions and \( G^\Lambda \) is the number of transverse channels in lead \( \alpha \) treated as vectors with a channel index \( \alpha \).

where \( G_\alpha^{\Lambda R}(\epsilon) = \sum_{\alpha'} g_\alpha^{\Lambda R}(\epsilon; E) g_{\alpha'}^{\Lambda R}(\epsilon; E) \) where we have already used spin conservation. The Green’s functions \( \hat{g}_\alpha \) correspond to the Hamiltonian \( H_S \) and are given by \( g_\alpha^{\Lambda R}(\epsilon; E) = (E - \epsilon \pm i0^+)^{-1} \) and \( g_\alpha^{\Lambda A}(\epsilon; E) = 2\pi f_\alpha(E) \delta(E - \epsilon) \) where \( f_\alpha \) is the Fermi distribution function of reservoir \( \alpha \). Using this result in calculating the average current, inserting the form of the tunneling matrix \( G^\Lambda \) is the number of transverse channels in lead \( \alpha \) treated as vectors with a channel index \( \alpha \). Equally, the matrix elements \( s_{\alpha\beta} \) and \( A_{\alpha\beta} \) have to be treated like \( Z_\alpha \times Z_\beta \) matrices where \( Z_\alpha \) is the number of transverse channels in lead \( \alpha \). The final formula for the current is then exactly like Eq. (3) except that we have to take the trace of the matrix multiplication \( s_{\alpha\beta}^\dagger s_{a\gamma} A_{\beta\gamma} \).

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., \( \epsilon_\alpha = \epsilon_d \) independent of spin) and in the \( U = \infty \) limit, one obtains \( G^{\pm \pm}(E) = 2\pi i \frac{\gamma^\pm(E)}{E - \epsilon_d - \sigma(E)} \). Here,

\[
\sigma(E) = \int dE' \frac{M\gamma^+(E') + \gamma^-(E')}{E - E' + i\delta} \tag{4}
\]

has the form of a self-energy which describes the renormalization and broadening of the dot level \( \epsilon_d \). \( \gamma^\pm(E) = \sum_\alpha f_\alpha(E) f_{\alpha}(E) \) is the classical rate for a particle tunneling in or out of the dot, and \( f_\alpha = \frac{1}{2} - f_\alpha \). The retarded Green’s function follows from \( \text{Im} G^R = 1/(2\pi)(G^> - G^<) \) 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 \( \sigma \) 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

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

where \( \sigma_1 \) is the self-energy for \( M = 1 \) and \( \chi_\alpha(E) = Re \int dE' f_\alpha(E')/(E - E' + i\delta) \). Using a Lorentzian cutoff at \( D \) (which will be of the order of the Coulomb repulsion \( U \)), we obtain \( \chi_\alpha(E) = \psi(1 + \frac{E - E_0}{\delta}) \) where \( \psi \) is the digamma function and \( \mu_0 \) the chemical potential of reservoir \( \alpha \). \( \sigma_1 \) is always a symmetric function of the external flux \( \Phi \). Furthermore, for a spatially symmetric situation as in Fig. 1, \( A_{11} \pm A_{22} \) is an even (odd) function of the phase \( \varphi = 2\pi \Phi/\Phi_0 \) \( (\Phi_0 \) being the flux quantum). Due to \( Re \sigma_1 \) the level position of the dot will oscillate with \( \varphi \) with an amplitude of the order of \( \Gamma \) and phase \( \varphi \). For \( M > 1 \), there can be logarithmic corrections in temperature and bias voltage for the amplitude and phase of this oscillation due to the \( \chi_\alpha \) functions. The latter terms usually lead to Kondo-like correlations [13].

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 \( s_{\alpha\beta} \) 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
\[ s^r = p \left( \frac{r}{t e^{i \varphi}} \right), \]
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
\[ s_{11} = s_{22} = \frac{1}{2} p (p - 1), \]
we get for the differential conductance as function of the bias voltage which again is absent for \( M = 1 \). It is determined by the last term in Eq. (3) as well as by \( \sin \varphi \) terms occurring explicitly in the current formula (3) via the \( A_{ik}^s \) matrices. Note that the temperature is one order of magnitude larger than \( \Gamma \) in this figure, i.e., an interference experiment of this type might yield information about correlation effects at temperatures which are accessible in experiments [8].

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 function of the gate voltage. In a noninteracting model two adjacent peaks correspond to transport through two different energy levels of the dot which 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 \( \pi \). 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 which 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 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 \( \frac{d \varphi}{d t} (\varphi) \) 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.

ACKNOWLEDGMENTS

It is a pleasure to thank G. Hackenbroich for initiating this work and for stimulating discussions. We would also like to acknowledge helpful discussions with M. Büttiker, Y. Imry, J. König, and A. Yacoby. This work was supported by the Deutsche Forschungsgemeinschaft through
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