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Transmission of electron through an Aharonov–Bohm interferometer with a quantum dot in Coulomb blockade regime*

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We calculate conductance of an Aharonov–Bohm (AB) interferometer for which a single-level quantum dot in the Coulomb blockade regime is embedded in one of its arms. Using the Schrödinger equations and taking into account the Coulomb interaction on the dot, we calculate conductance G as a function of flux ϕ threaded through the ring and as a function of gate voltage V applied to the dot. It is found that the AB oscillations of $G(\phi)$ depend on the particle occupation on the dot, controlled by V. If the system is closed, there is no loss of particles, $G(\phi)$ is periodic and $G(\phi) = G(-\phi)$, satisfying the Onsager relation. In this case $G(\phi)$ can reach its maximum value, $2e^2/h$, at the resonance. When the system is open, one has $G(\phi) \neq G(-\phi)$, $G(\phi)$ yields a phase shift which depends on the loss rate of electrons in this open system.

Keywords: Aharonov–Bohm interferometer, quantum dot, Coulomb blockade
PACC: 7320D, 7340G, 7340C, 7170G

1. Introduction

Recent lab measurements of transport properties through small semiconductor quantum dots have revealed interesting quantum-coherence phenomena ranging from Aharonov–Bohm (AB) oscillations of current through multiply connected geometries containing quantum dots,[1] to Fano-type line shapes in multichannel transport situations.[2] Theoretically, the transport of electrons through a quantum dot with Coulomb interaction has been investigated by perturbation theory and Green function method,[3–5] and the related transmission phases measured by closed or open AB interferometer have been discussed in Refs.[6] and [7] without considering the interaction on the dot. It is interesting to consider how the conductance of an AB interferometer is affected by the occupation and spin states of the embedded dot in the Coulomb blockade regime. In this paper, we solve the Schrödinger equation for the transmission of electrons through a closed or open AB interferometer with an embedded quantum dot in Coulomb blockade regime by using the equivalent single-electron network method.[8] For closed interferometers, we obtain the conductance G as a function of the flux ϕ threaded through the AB ring obeying the Onsager relation $G(\phi) = G(-\phi)$. So the initial phase of the first harmonic of $G(\phi)$ can only take values of 0 or π. We find that this phase and the magnitude of the conductance crucially depend on the occupation of the quantum dot. For the open AB interferometer, the system has no time-reversal symmetry. In this case the initial phase can take values other than 0 or π, depending on the states of the dot. The occupation of the quantum dot is controlled by the gate voltage V applied on the dot. In the presence of Coulomb interaction on the dot, there exists a finite range of V in which the dot is singly occupied. In this range the spin-flip scattering of the tunnelling electron is possible and the transport properties are much different from the situation of the empty dot.

The paper is organized as follows: in the next section we describe the model and basic formulae, in Section 3 the numerical results are presented and discussed, and the last section is a brief summary.

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2.Model and basic formulae

First we consider a closed model for a typical AB interferometer with one quantum dot inserted from which the transmission coefficient is calculated. The model of the system is shown in Fig.1.

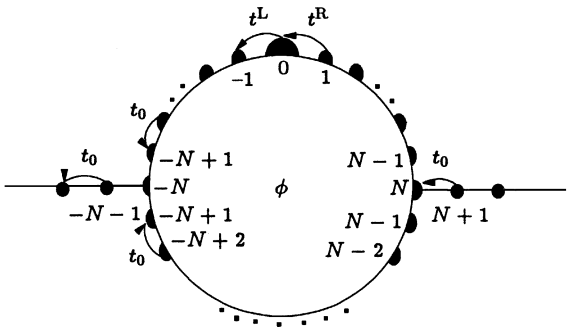


Fig.1. Structure of AB ring with a quantum dot.

The Hamiltonian of the system can be written as

$$H = H_1 + H_2,$$

where H_1 is the sub-Hamiltonian of the first arm, the leads and the quantum dot, and H_2 is sub-Hamiltonian of the second arm. In the tight-binding scheme they can be written as

$$\begin{aligned} H_1 =& \sum_{\sigma} \sum_{m\in[-N,N]} t_0(a^{\dagger}_{m\sigma}a_{m+1\sigma} + \mathrm{H.c.}) \\ &+ \sum_{m\neq 0}\sum_{\sigma} \varepsilon_0 a^{\dagger}_{m\sigma}a_{m\sigma} \\ &+ \sum_{\sigma} \sum_{m\in[-N,-1)\cup(+1,N]} t_0(a^{\dagger}_{m\sigma}a_{m+1\sigma} + \mathrm{H.c.}) \\ &+ \sum_{\sigma}[(t^{\mathrm{L}}a^{\dagger}_{-1\sigma}d_{\sigma} + t^{\mathrm{R}}\mathrm{e}^{\mathrm{i}\phi}a^{\dagger}_{1\sigma}d_{\sigma} + \mathrm{H.c.}) \\ &+ (\xi + V)d^{\dagger}_{\sigma}d_{\sigma}] + e^2\left(\sum_{\sigma} d^{\dagger}_{\sigma}d_{\sigma}\right)^2/2C, \end{aligned} \tag{1}$$

$$\begin{aligned} H_2 =& \sum_{\sigma} \sum_{m\in[-N+1,N-2]} t_0(b^{\dagger}_{m\sigma}b_{m+1\sigma} + \mathrm{H.c.}) \\ &+ \sum_{m\in[-N+1,N-1]} \sum_{\sigma} \varepsilon_0 b^{\dagger}_{m\sigma}b_{m\sigma} \\ &+ \sum_{\sigma} t_0(a^{\dagger}_{-N\sigma}b_{-N+1\sigma} + a^{\dagger}_{N\sigma}b_{N-1\sigma} + \mathrm{H.c.}), \end{aligned} \tag{2}$$

where $a_{m\sigma}$ ($b_{m\sigma}$) and d_{σ} are the annihilation operators of electrons on the mth site of the first (second) arm and at the dot, respectively, with spin σ, ε_0 is the site energy and t_0 the hopping integral in leads and arms, $t^{\mathrm{L(R)}}$ is the coupling between the dot state and the left (right) contact site of the first arm, ξ is the dot level energy, V is the dot potential induced by the plunger voltage, and C is the dot capacitance. When a magnetic flux φ is threaded through the AB ring, we adopt a gauge where the phase induced by the flux only occurs at one of the jumps, $t^{\mathrm{R}}\mathrm{e}^{\mathrm{i}\phi}$ ($\phi = e\varphi/\hbar c$), and the other jumps are unchanged according to the Lorentz invariability.

Because the interaction exists only on the quantum dot and the electrons are free in the leads and in other places of arms, we can consider many-body states on the dot and single-electron states in other places.[7] Thus, we are interested in a sub-Hilbert space where there is no restriction on the number of electrons on the dot, but there is at most one electron in other places. In this sub-Hilbert space one can construct the following set of basis functions:

$$\begin{aligned} \psi_{D,1,m,\sigma} &= a^{\dagger}_{m\sigma}\left|D\right\rangle, \\ \psi_{D,2,m,\sigma} &= b^{\dagger}_{m\sigma}\left|D\right\rangle, \\ \psi_{D,\sigma} &= d^{\dagger}_{\sigma}\left|D\right\rangle, \end{aligned} \tag{3}$$

where $|D\rangle$ is one of the dot states, $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$. In this basis a wavefunction can be expressed as a linear combination

$$\begin{aligned} \Psi = \sum_{D}\Bigg(& \sum_{\sigma}\sum_{m\neq 0} p_{D1m\sigma}\psi_{D,1,m,\sigma} \\ &+ \sum_{\sigma}\sum_{m} p_{D2m\sigma}\psi_{D,2,m,\sigma} + \sum_{\sigma} q_{D\sigma}\psi_{D,\sigma}\Bigg). \end{aligned} \tag{4}$$

By applying the Hamiltonian on the wavefunction, we obtain the Schrödinger equations for the coefficients:

$$\chi_D p_{D1m\sigma} + t_0(p_{D,1,m+1,\sigma} + p_{D,1,m-1,\sigma}) = Ep_{D1m\sigma} \quad \text{for} \quad m \neq 0, 1, -1, \tag{5}$$

$$\chi_D p_{D2m\sigma} + t_0(p_{D,2,m+1,\sigma} + p_{D,2,m-1,\sigma}) = Ep_{D2m\sigma} \quad \text{for} \quad m \in (-N, N), \tag{6}$$

$$\begin{aligned} &\chi_D p_{D,2,-N,\sigma} + t_0(p_{D,2,-N+1,\sigma} + p_{D,1,-N,\sigma}) \\ &= Ep_{D,2,-N,\sigma}, \end{aligned} \tag{7}$$

$$\chi_D p_{D,2,N,\sigma} + t_0(p_{D,2,N-1,\sigma} + p_{D,1,N,\sigma}) = Ep_{D,2,N,\sigma}, \tag{8}$$

$$\chi_D p_{D,1,-1,\sigma} + t_0 p_{D,1,-2,\sigma} + t^{\mathrm{L}}\mathrm{e}^{\mathrm{i}\phi}q_{D\sigma} = Ep_{D,1,-1,\sigma}, \tag{9}$$

$$\chi_D p_{D,1,1,\sigma} + t_0 p_{D,1,2,\sigma} + t^{\mathrm{R}}q_{D\sigma} = Ep_{D,1,1,\sigma}, \tag{10}$$

$$\chi_{D\sigma} q_{D\sigma} + t^{\mathrm{L}^*}\mathrm{e}^{-\mathrm{i}\phi}p_{D,1,-1,\sigma} + t^{\mathrm{R}^*}p_{D,1,1,\sigma} = Eq_{D\sigma}, \tag{11}$$

where E is the total energy of the electron system, and χ_D ($\chi_{D\sigma}$) is ε_0, $\varepsilon_0 + V + \xi + e^2/2C$, and $\varepsilon_0 + 2V + 2\xi + 2e^2/C$, if the dot state $|D\rangle$ ($d_\sigma^\dagger |D\rangle$) is empty ($|0\rangle$), singly occupied ($|\uparrow\rangle$ or $|\downarrow\rangle$), and doubly occupied ($|\uparrow\downarrow\rangle$), respectively. In the above equations the terms with $q_{D\sigma}$ are zero if $d_\sigma^\dagger |D\rangle$ is not allowed according to the Pauli exclusion principle.

When an electron with spin σ is incident from the left lead and the dot state is in $|D\rangle$, it can be partly reflected and partly transmitted, and the coefficients in the leads can be expressed as

$$p_{D,1,m,\sigma'} = \begin{cases} \delta_{\sigma\sigma'} \mathrm{e}^{ikm} + r_{D;\sigma\sigma'} \mathrm{e}^{-ikm} & \text{for } m < -N, \\ t_{D;\sigma\sigma'} \mathrm{e}^{ikm} & \text{for } m > N, \end{cases}$$

where $r_{D;\sigma\sigma'}$ and $t_{D;\sigma\sigma'}$ are reflection and transmission amplitudes, respectively, with dot state being $|D\rangle$ and spin from σ to σ', and k is the momentum satisfying $E - \chi_D = 2t_0 \cos(k)$. From the above equations we can solve $r_{D;\sigma\sigma'}$ and $t_{D;\sigma\sigma'}$. At zero temperature, the conductance can be calculated with the Landauer formula:

$$G(\varphi) = \frac{e^2}{h} \sum_D P_D(\varepsilon_\mathrm{F}, V) \sum_{\sigma,\sigma'} |t_{D;\sigma\sigma'}(\varepsilon_\mathrm{F})|^2,$$

where ε_F is the Fermi level in the leads, and $P_D(\varepsilon_\mathrm{F}, V)$ is statistical factor of dot state $|D\rangle$ at given gate voltage V and Fermi level ε_F. At zero temperature, one has

$$\begin{aligned} P_0(\varepsilon_\mathrm{F}, V) =& \theta\left(V + \xi + \frac{e^2}{2C} - \varepsilon_\mathrm{F}\right), \\ P_\uparrow(\varepsilon_\mathrm{F}, V) =& P_\downarrow(\varepsilon_\mathrm{F}, V) \\ =& \frac{1}{2}\theta\left(V + \xi + \frac{3e^2}{2C} - \varepsilon_\mathrm{F}\right) \\ & \times \theta\left(\varepsilon_\mathrm{F} - V - \xi - \frac{e^2}{2C}\right), \\ P_{\uparrow\downarrow}(\varepsilon_\mathrm{F}, V) =& \theta\left(\varepsilon_\mathrm{F} - V - \xi - \frac{3e^2}{2C}\right), \end{aligned}$$

where $\theta(x)$ is the step function. From these expressions it can be seen that by varying the gate voltage, the dot state can be changed from empty, single occupation, to double occupation. In the next section we will present numerical results of $G(\varphi)$ for different dot sates.

3. Numerical results

In this section we present numerical results for the conductance as a function of the magnetic flux. For simplicity we use t_0 as unit of energy ($t_0 = 1$), and assume that t^L is equal to t^R and they are real numbers. For given Fermi energy ε_F and given spin of the incident electron, both reflection and transmission coefficients, as well as the coefficients in arms and on the dot, are unknown. They can be uniquely solved from the Schrödinger equation. For a closed system we obtain an even function of $G(\varphi)$, i.e. $G(\varphi) = G(-\varphi)$.[9]

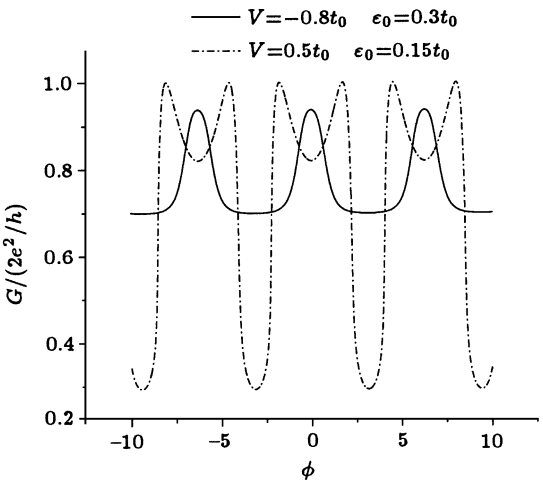


Fig.2. Conductance as a function of the magnetic flux in a closed AB ring with a quantum dot embedded in one of the arms. The parameters for the quantum dot are: $t^\mathrm{L} = t^\mathrm{R} = 0.5t_0$, $e^2/C = 1.5t_0$, $N = 38$, and $\xi = 0.2t_0$. The solid line corresponds to the case of single occupation, and the dash-dotted line corresponds to the empty case.

In Fig.2 we show the conductance as a function of the flux for both the empty and singly occupied cases. Here the Fermi level of the leads is set to be the energy zero, $\varepsilon_\mathrm{F} = 0$. It can be seen that the AB oscillations deviated from the standard harmonic form, and complete destructive interference [$G(\varphi) = 0$] cannot be reached. This is due to the scattering of the quantum dot which alters the direction and paths of the electron propagation. In particular, the shapes of curves are drastically different for the singly occupied and empty cases. This is because in the former there exists spin-flip scattering that changes spin direction of the incident electron, making the spin of the quantum dot also altered, while in the latter two spin channels are completely separated. Apart from the spin-flip processes, the transmission through the quantum dot is governed by the level position, the interaction, and the hopping strength between the arm and the dot. Maximum transmission through the dot is achieved at the resonance where the energy of the incident electron coincides with the energy of the intermediate state in which the tunnelling electron is

located on the dot. Thus, the maximum of the conductance through the whole system is determined not only by the interference effect of the arms, but also by the resonance through the dot. In one period there are two maxima in the empty case, and there is only one maximum in the single occupation case, reflecting substantial difference in the transmission of quantum dot between the two cases. In both cases the Onsager relation, $G(\varphi) = G(-\varphi)$, is satisfied. We do not show the curves for the double occupation case, because in this case the arm with the quantum dot is completely blocked and there is no AB oscillation.

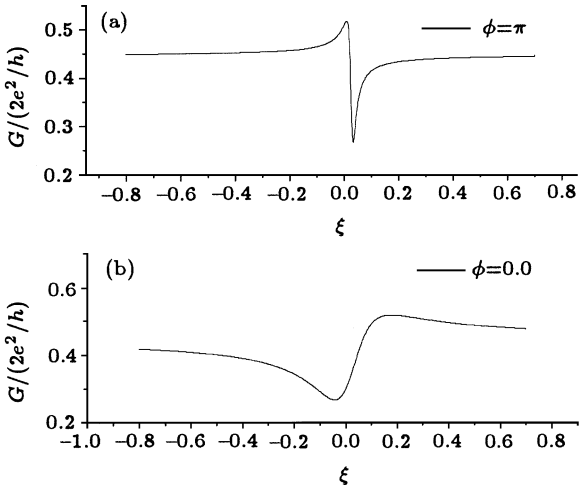


Fig.3. Conductance in a closed AB ring as a function of energy level of the quantum dot. The parameters are $V = -0.8t_0$, $e^2/C = 1.5t_0$, $\varepsilon_0 = 0.08t_0$, $N = 38$, and $t^{\mathrm{R}} = t^{\mathrm{L}} = 0.1t_0$. The parameters correspond to the single occupation region. For $\phi = 0$, the valley occurs at $\xi = -0.036t_0$, while for $\phi = \pi$, the valley is at $\xi = 0.33t_0$. The appearance order of peak and valley is also altered by changing ϕ.

In order to investigate the resonance of the quantum dot in such a structure, in Fig.3 we plot the conductance of the closed AB ring as a function of the energy level of the quantum dot. The peak position corresponds to the resonant transmission through the quantum dot, while the valley indicates the effect of the destructive interference of the AB ring. The curves show asymmetric Fano line shape [10] due to the existence of two paths, one with the embedded dot and another without it. With varying ξ the Fermi level crosses over the resonant level of the dot, changing the phase of the transmission through the dot by π. This results in changing the interference of the two arms from constructive to destructive, corresponding to the adjacent peak-valley structure in the curves. It can be seen that this peak-valley structure can be easily controlled by changing the flux, implying the sensitivity of the Fano effect to the phase induced by the flux.

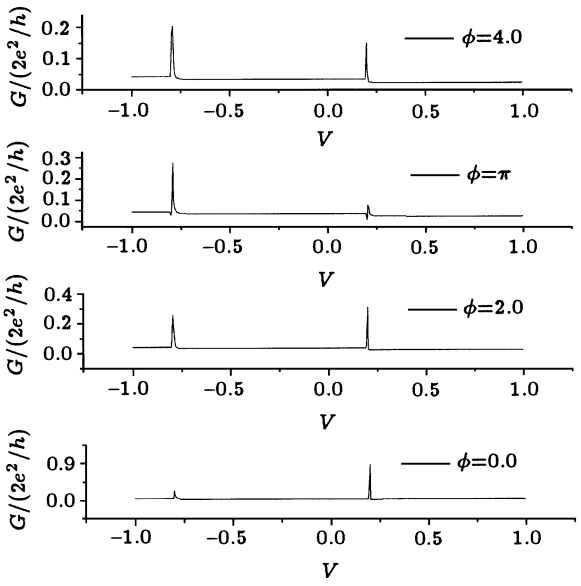


Fig.4. Conductance in a closed AB ring as a function of the gate voltage. The parameters are $e^2/C = 1.0t_0$, $\varepsilon_0 = 0.07t_0$, $N = 38$, $\xi = -0.26t_0$, and $t^{\mathrm{R}} = t^{\mathrm{L}} = 0.1t_0$. The double occupation, single occupation, and empty regions correspond to $V < -0.8t_0$, $0.2t_0 > V > -0.8t_0$, and $V > 0.2t_0$, respectively.

In order to study the effect of Coulomb blockade on the conductance, in Fig. 4 we display the conductance as a function of the gate voltage. Due to the Coulomb interaction on the dot, there are two resonance peaks in varying the gate voltage, although there is only one level on the dot. One resonance peak ($V = 0.2t_0$) corresponds to the change from the empty state to the single occupation state, and the other ($V = -0.8t_0$) to the change from single to double occupation. The spacing between these two peaks is just the strength of the Coulomb interaction. Physically this spacing is the energy cost for an electron to overcome the Coulomb blockade on the quantum dot. In varying the flux, both peaks oscillate, but with different phases. This reflects the different quantum interference for these resonances due to different transmission phases through the dot.

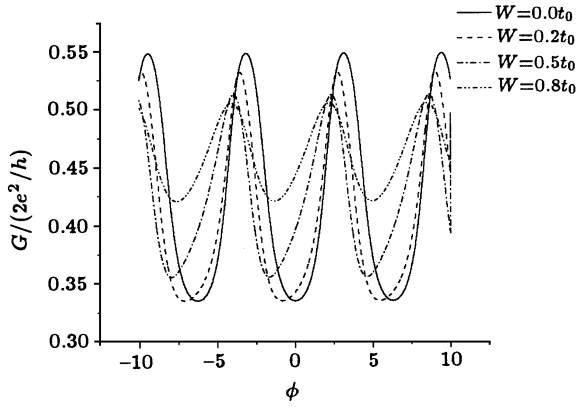


Fig.5. Conductance in an open AB ring as a function of the flux. The parameters are $e^2/C = 1.0t_0$, $\varepsilon_0 = 0.1t_0$, $N = 38$, $V = -0.6t_0$, $\xi = -0.2t_0$, and $t^{\mathrm{R}} = t^{\mathrm{L}} = 0.1t_0$. W is the hopping strength from the dot to an additional lead.

In experiments [11−14] an open system, in which there is electron leakage, is adopted. The experimental results show additional phase shift β in the AB oscillations. In Fig.5, we show the calculated results for the conductance of an open system as a function of the flux. The open system is realized by adding an additional lead to the quantum dot. It can be seen that in this case the Onsager relation is violated, and the additional phase shift is increased by increasing the hopping strength between the dot and the additional lead.

4. Summary

In summary, we have investigated the transport properties of a dot in the Coulomb blockade regime embedded in an arm of the AB ring in both the closed and open cases. The calculated results show different interference behaviour if the occupation of the quantum dot is different. The resonances exhibit Fano line shape, and the Coulomb blockade causes splitting of the resonance peak due to the charging energy. In an open system an additional phase shift in the AB oscillations appears, and the Onsager relation is violated due to the breaking of the conservation of the particle number.

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