

Conductance of interacting Aharonov-Bohm systems

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(Received 13 March 2003; revised manuscript received 12 May 2003; published 15 July 2003)

A simple formula for the zero-temperature linear response conductance of an interacting mesoscopic region, threaded by magnetic flux, and attached to noninteracting single-channel leads is presented. The formula is valid for a general interacting system exhibiting Fermi liquid properties. As an example of the efficiency of the formula the results for the conductance of a simple Aharonov-Bohm ring with Kondo-Fano resonance physics are presented and compared with numerical renormalization group results.

DOI: 10.1103/PhysRevB.68.033306

PACS number(s): 73.23.-b, 73.63.-b

The electron-electron interaction often plays a crucial role in transport through mesoscopic systems. The Kondo effect in quantum dots is, e.g., a prototype phenomenon, where correlations dominate the conductance.^{1,2} Another remarkable effect is the Fano resonance physics intertwined with Kondo physics.^{3,4} Recent advances in nanofabrication of Aharonov-Bohm (AB) devices made possible a realization and a systematic study of such phenomena.⁵

For systems where the interaction is absent, or very weak, transport properties may be determined using the Landauer-Büttiker formalism.⁶ On the other hand, if the interaction is important in the system being studied, the use of a more general approach is essential. An appropriate formalism, expressing the conductance in terms of nonequilibrium Green's functions, was developed by Meir and Wingreen.⁷ The formalism can in principle be used to treat systems at a finite temperature, finite source-drain voltage, and can even be extended to describe time-dependent transport phenomena.⁸ Another approach to describing the transport in interacting systems, applicable only to systems in the linear-response regime, is the Kubo formalism.⁹

Recently, a simple method for calculating the conductance through a region with electron-electron interaction (e.g., a molecule, a quantum dot, a quantum dot array or a similar "artificial molecule" system, . . .), connected to single-channel noninteracting leads, was presented in Ref. 10 (hereafter referred to as RR).¹¹ The conductance is determined solely from the ground-state energy of an auxiliary system, formed by connecting the ends of the leads of the original system into a ring and threaded by magnetic flux. The method is applicable to Fermi liquid systems at zero temperature and in the linear response regime. The validity is additionally restricted to the class of interacting systems obeying time reversal symmetry. Several conductance formulas, becoming exact in the limit of a very large ring, are derived, the most practical being the two-point formula

$$G = G_0 \sin^2 \left(\frac{\pi}{2} \frac{E(\pi) - E(0)}{\Delta} \right), \quad (1)$$

where $E(0)$ and $E(\pi)$ are the ground-state energies of the auxiliary interacting system with periodic and antiperiodic boundary conditions, respectively. The average level spacing at the Fermi energy $\Delta = [N\rho(\epsilon_F)]^{-1}$ is determined by the

density of states in an infinite lead $\rho(\epsilon)$ and the circumference of the ring N , and $G_0 = 2e^2/h$ is the conductance quantum. The corresponding ground-state wave function can be chosen real, which simplifies the determination of the ground-state energy by, for example, variational or density matrix renormalization group approaches.

In this paper we present a generalization of the conductance formula Eq. (1) to systems which explicitly exhibit time reversal asymmetry, such as, e.g., the AB type of system presented in Fig. 1(a). The formalism presented here is valid for general systems consisting of interconnected sites with

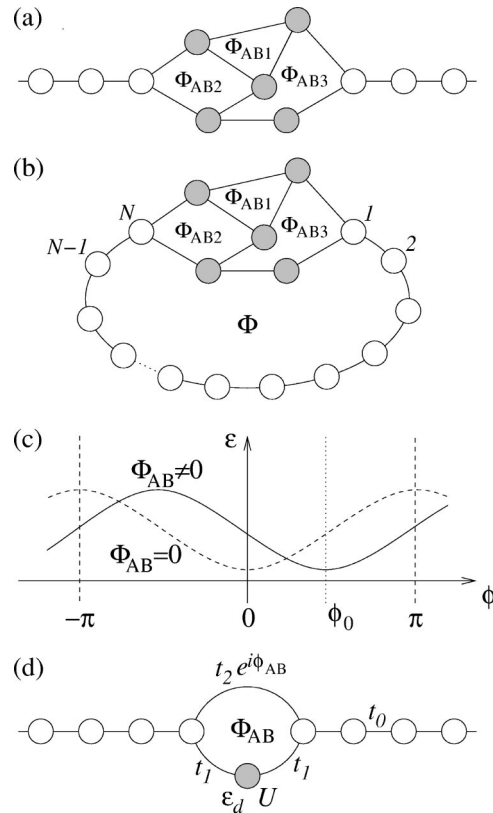


FIG. 1. (a) Interacting mesoscopic region (gray-shaded sites), threaded by magnetic flux and coupled to noninteracting leads. (b) Auxiliary ring system. (c) Behavior of energy levels as the flux threading the ring is varied. (d) System from Ref. 4 with a quantum dot embedded in an AB ring.

interaction, threaded with magnetic flux and connected to noninteracting leads.

First we consider the noninteracting case and single-electron states. The transmission amplitudes t_k and t'_k of an electron with a wave vector k and an energy ε_k describe the transmission from the left to the right lead and from the right to the left lead of the system presented in Fig. 1(a), respectively. They are related by an expression derived in RR,

$$t'_k e^{i\phi} + t_k e^{-i\phi} = e^{ikN} + \frac{t_k}{t_k^*} e^{-ikN}, \quad (2)$$

where $\Phi = (\hbar/e)\phi$ is the magnetic flux through the auxiliary system shown in Fig. 1(b). If there is no AB flux threading the mesoscopic region, the time reversal symmetry is restored, $t_k = t'_k$ and the energy is an even function of ϕ , as illustrated in Fig. 1(c). In the general case, the unitarity of the scattering matrix requires $|t_k| = |t'_k|$ and the transmission amplitudes are related as $t_k = \tilde{t}_k e^{i\phi_{0k}}$ and $t'_k = \tilde{t}'_k e^{-i\phi_{0k}}$. Expressing \tilde{t}_k in terms of its modulus $|t_k|$ and a phase shift φ_k , $\tilde{t}_k = |t_k| e^{i\varphi_k}$, the eigenenergy equation Eq. (2) reads

$$|t_k| \cos(\phi - \phi_{0k}) = \cos(kN - \varphi_k). \quad (3)$$

Algebraic manipulation equivalent to that in RR gives an implicit equation for $|t(\varepsilon_k)|$, exact to the leading order in $1/N$,

$$\frac{\partial \arccos\{\mp |t(\varepsilon_k)| \cos[\phi - \phi_0(\varepsilon_k)]\}}{\partial \cos \phi} = \pi N \rho(\varepsilon_k) \frac{\partial \varepsilon_k}{\partial \cos \phi}, \quad (4)$$

where the sign \mp depends on whether k belongs to a decreasing (+) or to increasing (−) branch of the cosine function in Eq. (3) and $\rho(\varepsilon) = (\pi \sqrt{4t_0^2 - \varepsilon^2})^{-1}$ with t_0 being the nearest neighbor hopping in the leads. By using the principle of mathematical induction, as in RR but generalized to a finite ϕ_0 , the transmission probability at the Fermi energy ε_F is expressed as

$$\frac{\partial \arccos^2\{\mp |t(\varepsilon_F)| \cos[\phi - \phi_0(\varepsilon_F)]\}}{\pi \partial \cos \phi} = \pi N \rho(\varepsilon_F) \frac{\partial E}{\partial \cos \phi}, \quad (5)$$

where E is the ground-state energy of a system containing an even number of electrons. Neglecting the variation of $t(\varepsilon_F)$ and $\rho(\varepsilon_F)$ with ϕ (the error made is of the order of $1/N$), Eq. (5) leads to a universal form of the ground-state energy of the auxiliary system¹²

$$E(\phi) = \frac{\Delta}{\pi^2} \arccos^2\{\mp |t(\varepsilon_F)| \cos[\phi - \phi_0(\varepsilon_F)]\} + \text{const.} \quad (6)$$

From this form, the transmission probability can be extracted, and the conductance is given by

$$G = G_0 \sin^2\left(\frac{\pi}{2} \frac{E(\phi_0 + \pi) - E(\phi_0)}{\Delta}\right), \quad (7)$$

where $\phi_0 \equiv \phi_0(\varepsilon_F)$ is determined by the position of the minimum (or maximum) in the energy vs flux ϕ curve, schematically shown in Fig. 1(c). The conductance can also be calculated from the more convenient four-point formula¹³

$$G = G_0 \left[\sin^2\left(\frac{\pi}{2} \frac{E(\pi) - E(0)}{\Delta}\right) + \sin^2\left(\frac{\pi}{2} \frac{E(\pi/2) - E(-\pi/2)}{\Delta}\right) \right] \quad (8)$$

and ϕ_0 can be determined from the expression

$$\phi_0 = -\arctan \frac{\sin\left(\frac{\pi}{2} \frac{E(\pi/2) - E(-\pi/2)}{\Delta}\right)}{\sin\left(\frac{\pi}{2} \frac{E(\pi) - E(0)}{\Delta}\right)}. \quad (9)$$

We now consider the interacting case. If no AB flux is present in the mesoscopic region and the ground state of the system exhibits Fermi liquid behavior, i.e., the perturbation theory in the interaction strength is valid, the imaginary part of the self-energy due to the interaction vanishes quadratically at the Fermi energy

$$\text{Im} \Sigma_{ij}(\omega + i\delta) \propto (\omega - \varepsilon_F)^2 \quad (10)$$

and a quasiparticle Hamiltonian can be constructed for each value of ε_F . As shown in RR the conductance calculated from the quasiparticle Hamiltonian reproduces the conductance of the interacting system, and is exactly given by Eq. (1) [or Eq. (8) since $E(\pi/2) = E(-\pi/2)$ in this case]. If the time reversal symmetry is broken due to AB flux, Eq. (10) is not valid and the proof has to be reconsidered. Repeating the steps as presented in detail in RR, the proof is restored and basically unchanged if the exact self-energy obeys the relation

$$\frac{1}{2i} [\Sigma_{ij}(\omega + i\delta) - \Sigma_{ij}(\omega - i\delta)] \propto (\omega - \varepsilon_F)^2. \quad (11)$$

It follows also that the linear response conductance of an interacting AB system at zero-temperature is given by the four-point formula (8). This condition is fulfilled if the system is a Fermi liquid.

In order to demonstrate the practical value of the method, we quantitatively analyze the conductance through an Aharonov-Bohm ring with a quantum dot placed in one of the arms as presented in Fig. 1(d).^{3,4} The quantum dot is described as an Anderson impurity with level position ε_d and a charging energy U , coupled to each of the leads with a tunneling matrix element t_1 . Electrons can also be transferred from one lead to the other directly through the upper arm of the AB ring. This process is described by a tunneling matrix element t_2 . The ring is threaded by an AB flux $\Phi_{AB} = (\hbar/e)\phi_{AB}$ in such a way that only the direct tunneling matrix element is affected, i.e., $t_2 \rightarrow t_2 e^{i\phi_{AB}}$. The Fermi energy is set at the middle of the band, thus $\Delta = 2\pi t_0/N$. We perform the finite-size analysis of the four-point formula Eq. (8), changing the circumference of the ring N . In order to be

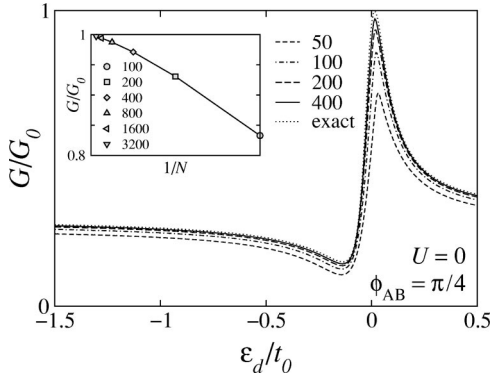


FIG. 2. The conductance of a noninteracting ($U=0$) AB ring at $\phi_{AB} = \pi/4$. The inset shows convergence of the conductance at the peak near $\varepsilon_d=0$. Parameters: $t_1=0.177t_0$, $t_2=0.298t_0$.

able to compare our results with those of the NRG method, we choose the same values of parameters as in Ref. 4.

In Fig. 2 the results for the conductance of a noninteracting ($U=0$) system with $\phi_{AB} = \pi/4$ are presented. Due to a nonzero AB flux, the ground-state energy must be determined at four ϕ points as required by Eq. (8). The conductance exhibits a typical Fano resonance with a dip and a sharp peak. Results calculated for various numbers of sites in the ring N are compared with the exact conductance curve. The inset shows a convergence test of the method at the peak near $\varepsilon_d=0$, where due to a strong energy dependence of the transmission amplitude the convergence is the most delicate.

In the interacting case, we determined the required ground-state energies using an approach similar to the variational method of Gunnarsson and Schönhammer^{10,14} for the Anderson model. The variational basis set is generated from the ground state $|\bar{0}\rangle$ of an auxiliary noninteracting Hamiltonian in which the energy level of the dot ε_d and the hopping matrix element t_1 between the dot and the leads are renormalized in such a way to minimize the ground-state energy. Apart from the Hartree-Fock case where this is the only variational wave function, we form two additional basis sets. The first has three variational wave functions $P_0|\bar{0}\rangle$, $P_1|\bar{0}\rangle$, and $P_2|\bar{0}\rangle$, where P_0 , P_1 , and P_2 are projectors onto unoccupied, singly occupied, and doubly occupied dot site. In the second basis set we add four additional wave functions $P_0VP_1|\bar{0}\rangle$, $P_2VP_1|\bar{0}\rangle$, $P_1VP_0|\bar{0}\rangle$, and $P_1VP_2|\bar{0}\rangle$, where V is the operator describing hopping between the leads and the dot. In all the three cases, the noninteracting limit is correctly reproduced. Furthermore, except in the Hartree-Fock case, the method is also exact in the limit where the dot is decoupled from the rest of the system.

An interacting AB ring with $U \neq 0$ serves as a good nontrivial test of the method. We choose a strong coupling regime as in Ref. 4, with $U=8\Gamma$, where $\Gamma=4\pi t_1^2\rho(\varepsilon_F)$ is the linewidth of the dot level in the absence of the upper arm of the AB ring. The results are presented in Fig. 3 and compared with results obtained using the NRG method,⁴ together with the corresponding Hartree-Fock (HF) curve. It should be noted that with the parameter set chosen, the underlying physics is in the strong correlation regime, where, e.g., the

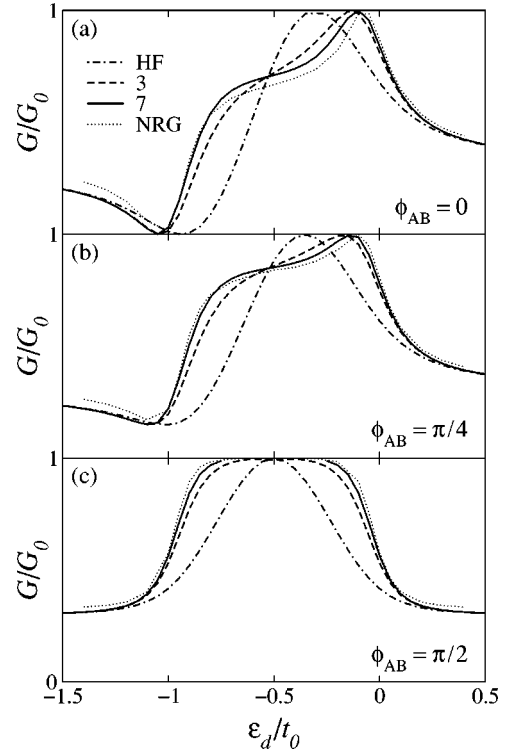


FIG. 3. Zero-temperature linear response conductance as a function of level position ε_d for various values of the AB flux. Labels “3” and “7” correspond to variational wave functions with three and seven terms, respectively. The dash-dotted line is the result obtained using the HF approximation and the dotted line is the NRG result from Ref. 4. Parameters: $t_1=0.177t_0$ ($\Gamma=0.125t_0$), $t_2=0.298t_0$, $U=t_0=8\Gamma$.

width of the Kondo peak is of the order $10^{-4}U$. The HF method therefore fails to reproduce NRG results, while the variational results are very close to the NRG curve. By extending the variational space from 3 to 7 terms, the agreement with NRG improves even further and the small remaining discrepancy would most probably be additionally reduced if an even richer variational wave function is used. Interestingly, we find the largest deviation in the “empty orbital” regime $\varepsilon_d \lesssim -U$. The results of the variational and the HF methods here agree, both deviating from the NRG result, while asymptotically all the curves reach the correct limit $G=0.3G_0$.⁴ We have also checked the result in this regime using the second order perturbation theory approach¹⁵ which gives a conductance in agreement with variational and HF methods (not shown).

In Fig. 4 a convergence test of the method for the result from Fig. 3(b) is shown. The convergence with N is fast in the empty orbital regime and becomes progressively slower as ε_d shifts toward the Kondo regime. The reason can clearly be attributed to a very strong coupling regime resulting in an extremely narrow Kondo peak. A very fine energy resolution is therefore required to resolve the peak and to obtain a converged conductance curve.

Broken time reversal symmetry in AB systems is signaled by $\phi_0 \neq 0$. In Fig. 5 the phase shift ϕ_0 corresponding to Figs. 2 and 3(b) as determined from Eq. (9) is shown. In contrast

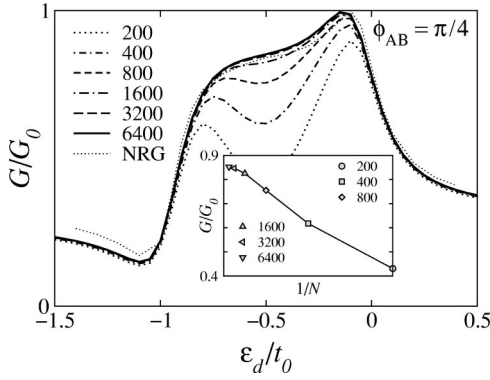


FIG. 4. The same as in Fig. 3(b), but calculated for different numbers of sites in the auxiliary ring N . The inset shows convergence of the conductance at $\epsilon_d = -U/2$.

to the smooth noninteracting result, the phase shift in the interacting case exhibits a well developed plateau, corresponding to the Fano-suppressed Kondo plateau in the conductance. The ϕ_0 curve, which clearly cannot be correctly reproduced in the HF approximation, can be explained as follows: In the empty orbital regime, the current mainly flows through the upper arm of the ring and therefore, electrons acquire an additional phase shift $\phi_0 \sim \phi_{AB}$ (note that ϕ_0 and $\phi_0 - \pi$ are physically equivalent). On the other hand, in the Kondo regime almost all the current passes through the quantum dot and no additional phase shift is present, $\phi_0 \sim 0$.

In summary, we have derived a formula for zero-temperature linear response conductance of an interacting electron region coupled to single-channel leads where the electron-electron interaction is absent. The interacting part of the system can be a general Aharonov-Bohm type of interferometer with broken time reversal symmetry [Fig. 1(a)]. The conductance of such an *open* system is exactly deter-

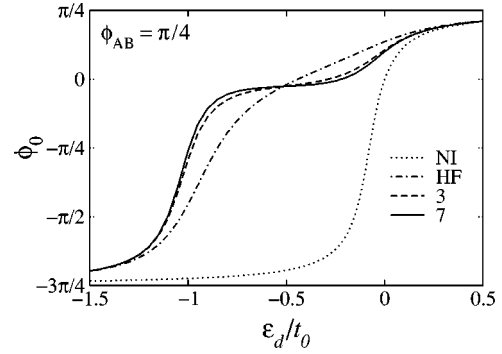


FIG. 5. Phase shift ϕ_0 as a function of ϵ_d/t_0 for the noninteracting AB ring of Fig. 2 (NI) and for various ground-state energy methods applied to the interacting AB ring of Fig. 3(b).

mined from an auxiliary *closed* system [Fig. 1(b)], where the leads of the original system are connected to form a ring of N noninteracting sites threaded by an auxiliary magnetic flux. Eq. (8), which follows from the universal form of the ground-state energy of the auxiliary system for a large but finite N , expresses the conductance in terms of the ground-state energy evaluated at four different values of the auxiliary flux. The proof of validity of the formula for interacting systems relies on the mapping of the system onto an effective quasiparticle problem and is therefore valid for systems exhibiting Fermi liquid properties. We have demonstrated the usefulness of the formula by applying it to a prototype system exhibiting Kondo-Fano behavior. Results based on the four-point formula and variational ground-state energies confirm results of the numerical renormalization group method.

The authors wish to acknowledge P. Prelovšek and X. Zotos for helpful discussions and W. Hofstetter for useful correspondence regarding his results. We acknowledge J. H. Jefferson for useful remarks and the financial support of QinetiQ.

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