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Aharonov-Bohm oscillations in a mesoscopic ring with a quantum dot

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We present an analysis of the Aharonov-Bohm oscillations for a mesoscopic ring with a quantum dot inserted in one of its arms. It is shown that microreversibility demands that the phase of the Aharonov-Bohm oscillations changes abruptly when a resonant level crosses the Fermi energy. We use the Friedel sum rule to discuss the conservation of the parity of the oscillations at different conductance peaks. Our predictions are illustrated with the help of a simple one-channel model that permits the variation of the potential landscape along the ring.

A recent experiment by Yacoby et $al¹$ investigated the Aharonov-Bohm (AB) oscillations in a ring with a quantum dot (see Fig. 1). This experiment is of fundamental interest since it depends not only on the total transmission through the quantum dot but also on the phase accumulated by carriers traversing the dot. The experiment thus gives a direct demonstration that coherent resonant tunneling and sequential tunneling are not equivalent.²⁻⁴ Yacoby *et al.* emphasize two features of the Aharonov-Bohm oscillations: First, it was found that the phase of the AB oscillations changes abruptly whenever transmission through the quantum dot reaches a peak. Second, it was found that the AB oscillations at consecutive conductance peaks are in phase. Here we discuss these two observations, invoking only basic physical principles, and illustrate them with a simple model calculation.

First, consider the phase jump of π in the AB oscillations, which is observed each time a resonant condition is achieved. In a two-terminal conductance experiment the measured conductance is necessarily an even function of the AB flux through the ring,⁵⁻⁸ $G(\Phi) = G(-\Phi)$. In a Fourier representation of the conductance

$$
G(\Phi) = G_0 + \Delta \cos(2\pi \Phi/\Phi_0 + \delta) + \cdots, \qquad (1)
$$

this implies that the phase δ can only be either zero or π but nothing in between. In the experiment the phase δ is a function of gate voltage. If a phase change occurs as function of gate voltage it must, therefore, be a sharp jump of zero width. We call the two possibilities $\delta = 0$ and $\delta = \pi$ the parity of the AB oscillations. In contrast, Yacoby et aI. compare the sharp phase jump with an analysis that treats the AB effect as an interference of two partial waves. However, the AB effect in a conductor includes the partial waves generated by reflections. This simplified analysis leads Yacoby et al. to argue that a sharp phase jump is in contradiction with a noninteracting electron-transport picture. Early work on the transmission through one-channel loops does indeed show a symmetry-breaking term.⁹ Closer inspection of this result shows that the transmission probability is an even function of flux^{3,6} in a two-terminal geometry. Here we show that the abrupt phase change is a consequence of microreversibility only. It is a phenomena that occurs independently of whether interactions are significant or not. Moreover, the phase jump is abrupt even if there exists inelastic scattering. We conclude that any deviations from a sharp jump must be a consequence of fluctuations in the external control parameters.

We analyze the second feature, the conservation of parity of the AB oscillations at consecutive peaks, with the help of the Friedel sum rule, which remains valid in the presence of electron-electron interactions.^{10,11} The Friedel sum rule re-

FIG. 1. (a) Schematic representation of a mesoscopic ring threaded by a magnetic flux Φ with a quantum dot included in one of its arms. (b) Lattice model for this system.

FIG. 2. Transmission probability as a function of dot potential ϵ_D for fixed potential on the rest of the ring (fixed ϵ_0). The full and dotted lines indicate the regions of positive and negative parity, respectively (see text). The dashed line corresponds to the phase of the transmission amplitude.

lates the phase $\Delta \eta$ accumulated by a carrier traversing a region Ω to the electronic charge in this volume. The increment of phase and charge are related by

$$
\Delta Q = e \Delta \eta / \pi. \tag{2}
$$

If the volume Ω is chosen to include only the quantum dot then each addition of an electron to the dot requires an increase of η by π (see Fig. 2). Associated with this phase jump there is a parity change of the AB oscillations at each conductance peak. Consequently, the AB oscillations at consecutive conductance peaks would not be in phase. This is in contrast with the experimental observation of Ref. 1. However, what counts is not the phase of the quantum dot alone. The ring structure is connected to leads, which are in turn connected to reservoirs. As will be shown here, it is the phase accumulated in the entire coherence volume that counts. As a consequence, the relative parity on consecutive resonances might change if the addition of an electronic charge to the quantum dot is accompanied by the addition of a charge αe to the leads of the ring. Over large distances, the arms of the ring can be expected to remain in a charge neutral state. The additional charge is most likely accumulated at the barriers that separate the arms of the ring from the quantum dot. The physical reason is that the gate used to regulate the charge on the dot couples capacitively also to the gates used to form the barriers between dot and ring. A strict conservation of parity of the AB oscillations occurs if the total charge $(1+\alpha)e$ added is zero or an even multiple of 2e. Interestingly, because the phase observed in the transmission coefficient can only be 0 or π a "phase locking" occurs. Even if the additional charge α is not exactly an odd integer the parity of the AB oscillations at a number of consecutive conductance peaks will be the same. We expect that the parity of the AB oscillations is conserved only over a limited number of peaks and that this number depends on the geometry and electrostatic properties of the sample.

In order to understand the behavior of the AB oscillations in a device like that of Fig. $1(a)$ we start by analyzing a single-channel noninteracting model. Our aim is to investigate both the inhuence of inelastic scattering within the dot and of the effective potential landscape along the ring. We use a tight-binding representation of the electron states [the corresponding lattice model is represented in Fig. 1(b)], which allows for a qualitative description of any potential profile. The effect of the magnetic flux Φ is taken into account by a phase factor affecting the hopping matrix elements $V_{i,j}$. We denote by L, R, D, and F the left and right leads, the arm with the dot, and the free arm. The effective electrostatic potential on the dot arm is parametrized by the quantities ϵ_D (dot potential), ϵ_B (barrier heights), and ϵ_0 (potential outside the dot) which are schematically represented in Fig. 1(b). Inelastic scattering is simulated by a third lead g. 1(b). Inelastic scattering is simulated by a third $(2-14)$ (denoted by *I*) coupled to the dot arm by a hopping element V_I .

The transmission properties of this model can be easily obtained in terms of Green functions. $13-15$ In the absence of inelastic scattering $(V_I=0)$, the two-terminal conductance is proportional to the transmission coefficient T_{LR} , which can be written in terms of the retarded Green functions as¹⁶

$$
T_{LR} = 4V_L^2 V_R^2 |G_{0,N+1}(E_F)|^2 \text{Im} g_L(E_F) \text{Im} g_R(E_F), \quad (3)
$$

where $g_{L,R}(E_F)$ denote the local Green functions on the uncoupled leads at the Fermi energy and $V_{L,R}$ are the hopping elements connecting the ring to the leads. One can establish a correspondence between $2V_L V_R \sqrt{\text{Im}g_L(E_F) \text{Im}g_R(E_F) G_{0,N+1}(E_F)}$ and the elastic transmission amplitude t for this single-channel case. The phase η of t is, therefore, equal to that of $G_{0,N+1}(E_F)$.

Taking the case where $V_L = V_R = 0$ as the unperturbed case (for which the isolated ring Green functions are denoted by $g_{i,j}$) and using standard Green functions techniques, 13 $G_{0,N+1}$ can be written as

 $G_{0,N+1}$

$$
=\frac{g_{0,N+1}}{(1-g_{0,0}\Sigma_L)(1-g_{N+1,N+1}\Sigma_R)-g_{0,N+1}\Sigma_Rg_{N+1,0}\Sigma_L},\tag{4}
$$

where $\Sigma_{\alpha} = V_{\alpha}^2 g_{\alpha}$; $\alpha = L, R$. For a ring without inelastic scattering the functions $g_{i,j}$ behave as $exp[i\phi(i-j)]/N$ +1)] $f_{i,j}(\phi)$, where $2\phi = \pi \Phi/\Phi_0$ is the phase associated with the magnetic flux and $f_{i,j}$ is a real even function of ϕ . The transmission coefficient, therefore, satisfies the symmetry relation $T_{LR}(\Phi) = T_{LR}(-\Phi)$, which implies that $\partial T_{LR}/\partial \Phi$ _{$|\Phi=0$} = 0 in this limit.

In the presence of inelastic scattering the isolated ring Green functions $g_{i,j}$ get an extra phase that depends on the distance $|i-j|$ and $\frac{\partial T_{LR}}{\partial \Phi}|_{\Phi=0} = 0$ no longer holds. Noice, however, that time-reversal symmetry always implies
hat $T_{LR}(\Phi) = T_{RL}(-\Phi)$.⁵ We can analyze the flux dependence of the two-terminal conductance in this case by coupling the ring to the third lead. The condition of no net current flow through this lead yields a two-terminal conductance proportional to the total transmission probability, given by²

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$$
T_{\text{total}} = T_{LR} + \frac{T_{LI}T_{IR}}{1 - R_{II}},\tag{5}
$$

where R_{II} is the reflection probability on the third lead. Taking into account the property $\Sigma_i T_{ij} = 1 - R_{ii}$ one can easily show that

$$
T_{\text{total}} = 1 - R_{LL} + \frac{T_{LI} T_{IL}}{1 - R_{II}},\tag{6}
$$

and therefore $T_{\alpha\beta}(\Phi) = T_{\beta\alpha}(-\Phi)$ implies that T_{total} is an even function of the magnetic flux. This simple calculation shows that even in the presence of inelastic scattering the only possible phases for the AB oscillations are 0 and π and thus the transition from one to the other should always be abrupt. The only effect of inelastic scattering is to reduce the amplitude of the AB oscillations by decreasing the direct elastic transmission T_{LR} .

Notice that this result is also true at finite temperatures: thermal averaging can degrade the amplitude of the AB oscillations but cannot introduce additional phases between 0 and π . The only possible sources of phase smearing in the experiments should be traced to fiuctuations in the gate voltages.

We can thus study the parity of the AB oscillations by computing $\Delta_2 = \frac{\partial^2 T_{LR}}{\partial \Phi^2}\Big|_{\Phi=0}$, which tells us whether δ =0 (Δ_2 <0) or $\delta = \pi$ (Δ_2 >0). We now show how the parity change in the AB effect is related to the parity effect of the isolated ring. It is well known¹⁷ that, for the case of spinless electrons, the ring with an odd number of particles has a diamagnetic response, whereas for an even number the response is paramagnetic. In a noninteracting model the parity is determined mainly by the uppermost occupied state. Near a resonant level, we can approximate $G_{0,N+1}$ as

$$
G_{0,N+1} \sim \frac{\psi_{n_0} \psi_{n_{N+1}}^*}{(E_F - \epsilon_n - \Delta_n) + i\Gamma_n},\tag{7}
$$

where ϵ_n is the isolated ring eigenvalue closest to E_F , ψ_{n_i} denote the components of the corresponding wave function, and Δ_n and Γ_n are the real and imaginary parts of the electron self-energy due to coupling with the leads $(\Delta_n + i\Gamma_n = |\psi_{n_0}|^2 V_{LSL}^2 + |\psi_{n_{N+1}}|^2 V_{RSR}^2)$. The only flux sensitive quantities in this expression are ϵ_n and ψ_{n_j} . In particular, $\psi_{n}(\phi) = \exp[i\phi j/(N+1)]\psi_{n}(0)$, and one has

$$
\frac{\partial G_{0,N+1}}{\partial \phi} \lrcorner_{\phi=0} \sim -iG_{0,N+1},
$$
\n
$$
\frac{\partial^2 G_{0,N+1}}{\partial \phi^2} \lrcorner_{\phi=0} \sim G_{0,N+1} \left[-1 + \frac{1}{(E_F - \epsilon_n - \Delta_n) + i\Gamma_n} \right]
$$
\n
$$
\times \left(\frac{\partial^2 \epsilon_n}{\partial \phi^2} \lrcorner_{\phi=0} \right) \bigg],
$$
\n(8)

where we have used $\epsilon_n(\phi) = \epsilon_n(-\phi)$. The behavior of Δ_2 . near a resonance is thus given by

$$
\Delta_2 \sim T_{LR} \frac{E_F - \epsilon_n - \Delta_n}{(E_F - \epsilon_n - \Delta_n)^2 + \Gamma_n^2} \left(\frac{\partial^2 \epsilon_n}{\partial \phi^2} \lrcorner_{\phi = 0} \right). \tag{9}
$$

We see that when the resonance corresponds to a paramagnetic state of the isolated ring (i.e., $\partial^2 \epsilon_n / \partial \phi^2 |_{\phi=0} < 0$) Δ_2 changes from positive to negative as the state crosses the Fermi energy, while the opposite behavior is found when $\partial^2 \epsilon_n / \partial \phi^2 |_{\phi=0} > 0.$

Next, let us investigate why the phase of the AB oscillations on consecutive dot resonances appears to be the same. Within the spinless electron model and assuming that the effect of the dot gate is to modify the value of ϵ_D alone, Eq. (9) predicts that the AB oscillations on consecutive resonances should be out of phase. This is illustrated in Fig. 2, where $T_{LR}(\Phi=0)$ is plotted as a function of ϵ_D . The full and dotted lines indicate the regions where Δ_2 is positive or negative, respectively. We also show the phase of the transmission amplitude, which, as mentioned above, is proportional to the electronic charge accumulated within the sample as $\epsilon_0 - \epsilon_D$ increases. As can be observed, this rigid model for the potential landscape variation leads to an increase in the charge of one electron each time a resonance is crossed.

In a real situation one expects the potential in the regions close to the QD (not only within the dot) to vary as the gate voltage is modified. This effect can be included in our model by allowing ϵ_0 to vary together with ϵ_D . Let us assume that this variation can be described by $\delta \epsilon_0 = a \delta \epsilon_D / (\rho_0 \Delta E)$, where ρ_0 is the mean density of states for the ring regions where the potential equals ϵ_0 and ΔE is the mean separation between dot resonances. The actual relationship between ϵ_0 and ϵ_D should depend on the mutual capacitances between the ring and the gate electrodes. The effect of this selfconsistency condition is simply to add a fractional charge $\alpha e \sim a e$ to the ring between two resonances. Note that α and a are in general not equal, since the charge added depends on the actual density of states and not the average density of states ρ_0 .

Figure 3 illustrates the effect of increasing the parameter a. Notice that the calculated transmission exhibits now a varying background in addition to the dot resonances, which reflects the level structure of the ring.¹⁸ In case (a) the extra charge added to the system is $\alpha e \sim 0.30e$ per cycle. It can be observed that an additional phase jump appears close to the third resonance. Notice that the second and third resonances exhibit now the same parity. For increasing a new phase jumps appear between resonances. In this way, when α ~1 $[Fig. 3(b)]$ several peaks with the same parity may be found.

Since the phase δ of the AB oscillations can only be 0 or π it is not necessary to add exactly a multiple of 2e to find the same phase at consecutive peaks. Instead, the parity of the AB oscillations at the n th resonance will be determined by the integer multiple of charge en_{eff} where n_{eff} is the integer that is closest to the charge $n(1+\alpha)$ added after n cycles. For $-1 \le \alpha \le -0.5$ (if the ring and dot remain approximately charge neutral), this will create a sequence of effective charge states en_{eff} with $n_{\text{eff}} = 0$ for a number of cycles k . The parity will change after the first k cycles, which add half an electronic charge and cause the effective charge state to jump to $en_{\text{eff}}=e$. Hence for this case the number of parity conserving cycles is $k(1+\alpha)=1/2$ or $k=(1/2)(1+\alpha)^{-1}$. For $0.5 \le \alpha \le 1$ (if we add nearly two electrons) we will still obtain an effective charge sequence $e n_{\text{eff}}$ with $e n_{\text{eff}}$ equal to an even multiple of e but only for a finite sequence of cycles. The parity will change after k

FIG. 3. Same as in Fig. 2 but allowing ϵ_0 to vary together with ϵ_D . Case (a) corresponds to parameter $a \sim 0.3$ and case (b) to $a \sim 1$.

cycles, for which a deficit of half an electronic charge occurs. For this case the number of parity conserving cycles is $k(|\alpha - 1|) = 1/2$ or $k = (1/2)(|\alpha - 1|)^{-1}$. If α is in the interval $-0.5<\alpha<0.5$, then the parity will change at every peak except, occasionally, when the effective charge state jumps

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by 2e. For α in this interval we can at most observe two consecutive peaks which are in phase. Thus we find that it is possible to observe many consecutive conductance peaks at which the parity of the AB oscillations is conserved if α - 1 or if α - 1. The question of which of the two cases, the approximate preservation of overall charge neutrality or the addition of nearly two electrons (or another even multiple) per cycle, is realized in the experiment cannot be answered without a detailed determination of the relevant capacitance matrix for the structure.

Our discussion applies similarly to the case of a backgated sample,⁸ where a changing Fermi level affects both the phase of the dot and of the arms of the ring. The ideas presented here can be tested in an experiment in which the charge of either the dot or of the arms of the ring is controlled independently. If instead of the third lead of Fig. 1(b) an additional gate is brought into proximity with the lower arm of the ring, a change in the voltage of this gate should permit a change in the charge and the phase of the ring. As a function of this voltage we predict that an inversion of the AB-effect parity from one peak to the next could be observed.

We therefore conclude that within the spinless electron model the conservation of parity of the AB phase on consecutive resonances is indicating that either zero or an even number of electrons are added to the system per cycle. We expect that the inclusion of spin degrees of freedom does not change our conclusions: The charging energy of the dot will ensure that in each cycle at most one electronic charge can be added to the dot. The important conclusion of our analysis is that the phase of AB oscillations is not related to the dot charge alone but to the total charge of the system. It is the charge of the ring and the dot that counts.

Note added in proof. Closely related works by Bruder, Fazio, and Shoeller¹⁹ and by Yacoby, Heiblum, Mahalu, and Shtrikman²⁰ have come to our attention.

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