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Two-level quantum dot in the Aharonov–Bohm ring. Towards understanding "phase lapse"*

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It is shown theoretically that indirect interaction between two quantum dot levels can generate an anomalous phase shift for a system of the dot placed in one of the arms of the Aharonov–Bohm ring. The interaction between levels arises from the non-conservation of the orbital quantum number during the hopping process of electrons between the levels and leads. Such an unusual "phase lapse" behavior is observed experimentally and still lacks of proper theoretical description.

Key words: *quantum dot; Aharonov–Bohm ring; phase shift; phase lapse*

1. Introduction

The "phase lapse" is a phenomenon which is characterized by a sudden decay of the phase shift [1,2] measured for the quantum dot (QD) in Aharonov–Bohm (A–B) geometry, when the gate voltage shifts the dot energy levels with respect to chemical potential of the leads. Several theoretical attempts have been made (see for example [3, 4]) to describe this unusual feature but none of them seems to be satisfactory. In the present work the evolution of the phase shift is investigated for a model of two-level quantum dot placed in one of the arms of Aharonov–Bohm ring. The levels have different hybridization strengths to the leads; one is well coupled to the leads and conducting, and the second is sharp in energy scale and inactive in transport. The orbital quantum number is not conserved while hopping process of electrons occurs between the dot and the leads. As a consequence, both the levels are coupled to each other via the leads. It causes a considerable deviation from the usual electron wave phase shift behaviour which rises from zero to π when QD level crosses effective Fermi energy. In particular, a lapse of the phase appears. It corresponds well to recent experimental observations of the phase evolution for the QD in Aharonov–

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Bohm geometry in the limit of small electron number in the dot [2], when the transport through the dot has just been initiated.

2. Hamiltonian of the system

We consider a system composed of a quantum dot placed in one of the arms of Aharonov–Bohm ring (see the inset to Fig. 3 for the schematic picture). The Hamiltonian describing the system has the form:

$$H = \sum_{k,\sigma,\alpha=L,R} \varepsilon_{k\alpha} c^{+}_{k\alpha,\sigma} c_{k\alpha,\sigma} + \sum_{\substack{\gamma=1,2\\ \sigma}} \varepsilon_{\gamma} d^{+}_{\gamma\sigma} d_{\gamma\sigma} + \sum_{\substack{k,\sigma,\alpha=L,R\\ \gamma=1,2}} \left[t_{\gamma\alpha} c^{+}_{k\alpha,\sigma} d_{\gamma\sigma} + h.c.\right] + \sum_{k,q,\sigma} \left[\tilde{t}_{LR}\, c^{+}_{qL,\sigma} c_{kR,\sigma} + h.c.\right] \tag{1}$$

The first term describes energy of the left and right lead. The next term represents quantum dot energy with two levels $\gamma = 1, 2$. The third term shows the hopping between the dot and electrodes. The last term describes tunneling through the direct Aharonov–Bohm channel and the track of the phase evolution of electron wave is kept by introduction of the phase dependence of the hopping matrix element between the leads, $\tilde{t}_{LR} = t_{LR} \mathrm{e}^{i\phi}$. The phase acquired by electron wave in the magnetic field perpendicular to the device plane is $\varphi = 2\pi\Phi/\Phi_0$, Φ being enclosed flux by the ring and $\Phi_0 = hc/e$ is a flux quantum.

3. Calculation of the conductance

The current is calculated starting from time evolution of non-equilibrium Green functions under assumption that the $\gamma = 1$ QD level is well coupled to the leads and active in electron transport, whereas $\gamma = 2$ level wave function has only a small, finite overlap with the states in the leads but does not directly participate in transport. It is indirectly coupled to the $\gamma = 1$ level via the leads, which has considerable effect on the phase evolution as will be shown below.

In the current calculation from the left lead we start from the time evolution of the particle number N_L: $J_L = ed\langle N_L \rangle/dt = (ie/\hbar)\langle [N_L, H]\rangle$, which gives the following expression:

$$J_L = \frac{ie}{\hbar} \sum_{\sigma,k} \left\{ t_{1L} \left\langle c^{+}_{kL,\sigma} d_{1\sigma} \right\rangle - t^{*}_{1L} \left\langle d^{+}_{1\sigma} c_{kL,\sigma} \right\rangle + \sum_{q} \left[\tilde{t}_{LR} \left\langle c^{+}_{qL,\sigma}\, c_{kR,\sigma} \right\rangle - \tilde{t}_{LR}{}^{*} \left\langle c^{+}_{kR,\sigma} c_{qL,\sigma} \right\rangle \right] \right\} \tag{2}$$

Eq. (2) is then written in terms of non-equilibrium "lesser" Green functions $G^{<}_{1,k\alpha}(t,t') = i\left\langle c^{+}_{k\alpha,\sigma}(t')d_{1\sigma}(t)\right\rangle$ and $G^{<}_{k\alpha',q\alpha}(t,t') = i\left\langle c^{+}_{q\alpha,\sigma}(t')c_{k\alpha',\sigma}(t)\right\rangle$ for $t = t'$. These functions describe electron propagation through QD placed in one of the arms of the Aharonov–Bohm ring and direct propagation through the second A–B arm, respectively.

After taking temporal Fourier transform the current takes the form:

$$J_L = \frac{e}{\hbar}\sum_{\sigma}\left\{\sum_{k}\int\frac{d\omega}{2\pi}2\Re\left[t_{1L}G^{<}_{1,kL}(\omega)\right] + \sum_{k,q}\int\frac{d\omega}{2\pi}2\Re\left[\tilde{t}_{LR}G^{<}_{qL,kR}(\omega)\right]\right\} \tag{3}$$

To obtain explicit expression for the current the "lesser" Green functions have to be known. They are calculated form the equation of motion (EOM) of the equivalent time-ordered Green functions and then Langreth continuation is performed to obtain lesser Green functions [5]. The calculated expression is exact, possible approximations are included only in the QD retarded Green function calculation (see Eq. (5) below).

Similar steps have been performed to obtain the current from the right lead, J_R. Symmetrization of the current and assumption on proportionate coupling to the leads gives the expression for the total current:

$$J = \frac{2e}{h}\sum_{\sigma}\int d\omega\left[f_L(\omega) - f_R(\omega)\right]T_{\sigma}(\omega) \tag{4}$$

where the transmission is expressed as:

$$\begin{aligned} T_{\sigma}(\omega) = T_b + \sqrt{\frac{4\Gamma_{1L}\Gamma_{1R}}{\left(\Gamma_{1L}+\Gamma_{1R}\right)^2}T_bR_b}\cos\varphi\frac{\Gamma_{1L}+\Gamma_{1R}}{1+\Gamma_{LR}}\Re G^{r}_{1\sigma}(\omega) \\ -\frac{1}{2}\left[\frac{4\Gamma_{1L}\Gamma_{1R}}{\left(\Gamma_{1L}+\Gamma_{1R}\right)^2}\left(1-T_b\cos^2\varphi\right) - T_b\right]\frac{\Gamma_{1L}+\Gamma_{1R}}{1+\Gamma_{LR}}\Im G^{r}_{1\sigma}(\omega) \end{aligned} \tag{5}$$

The transmission through direct arm is:

$$T_b = \frac{4\Gamma_{LR}}{\left(1+\Gamma_{LR}\right)^2} \quad \text{and} \quad \Gamma_{LR} = \pi^2\left|t_{LR}\right|^2\rho_L\rho_R, \quad \Gamma_{\gamma\alpha} = 2\pi\left|t_{\gamma\alpha}\right|^2\rho_{\alpha}$$

ρ_α being the spectral density of the lead α, constant and featureless and the spin index has been suppressed for brevity. The above general equation for the current through A–B ring with the QD has been obtained for the first time in [6].

Conductance through the system in a steady situation for the limit of zero bias voltage is of the form:

$$G = \frac{dJ}{d(eV)}_{eV\to 0} = \frac{2e^2}{h}\sum_{\sigma}\int d\omega\left(-\frac{df(\omega)}{d\omega}\right)T_{\sigma}(\omega) \tag{6}$$

4. Retarded quantum dot Green function

To calculate the conductance through the device, the retarded dot Green function is needed

$$G_{1\sigma}^{r}(t-t')=-i\theta(t-t')\langle\left[d_{1\sigma}(t),d_{1\sigma}^{+}(t')\right]_{+}\rangle$$

We emphasize that it has to be calculated in presence of the γ = 2 level and in presence of the direct channel. It is derived by the EOM approach and can be written in the form of Dyson equation (in energy domain) for one spin direction: $G_1^r(\omega)=G_1^{0r}(\omega)+\Sigma^r(\omega)G_1^r(\omega)$, where:

$$G_1^{0r}(\omega)=\left[\omega-\tilde{\varepsilon}_{1\sigma}+\frac{\sqrt{\Gamma_{LR}\Gamma_{1L}\Gamma_{1R}}\cos(\phi)}{1+\Gamma_{LR}}+\frac{\frac{i}{2}\left(\Gamma_{1L}+\Gamma_{1R}\right)}{1+\Gamma_{LR}}\right]^{-1} \tag{7a}$$

$$\sum^{r}(\omega)=\left\{\frac{\left[\frac{1}{2}\sqrt{\Gamma_{LR}}\left(\sqrt{\Gamma_{1L}\Gamma_{2R}}+\sqrt{\Gamma_{2L}\Gamma_{1R}}\right)\cos(\phi)+\frac{i}{2}\left(\Gamma_{12L}+\Gamma_{12R}\right)\right]^2}{\left(1+\Gamma_{LR}\right)^2}+\frac{\left[\frac{1}{2}\sqrt{\Gamma_{LR}}\left(\sqrt{\Gamma_{1L}\Gamma_{2R}}-\sqrt{\Gamma_{2L}\Gamma_{1R}}\right)\sin(\phi)\right]^2}{\left(1+\Gamma_{LR}\right)^2}\right\}G_2^{0r}(\omega) \tag{7b}$$

and $G_2^{0r}(\omega)$ has the form similar to $G_1^{0r}(\omega)$, where index 1 has been replaced by 2, $\Gamma_{\gamma\gamma'\alpha}=2\pi t_{\gamma\alpha}t_{\gamma'\alpha}\rho_\alpha$, the dot levels are shifted uniformly by gate voltage V_g: $\tilde{\varepsilon}_{\gamma\sigma}=\varepsilon_{\gamma\sigma}-V_g$.

5. Calculation of the phase shift

The phase shift of the electron wave propagating through the device is calculated from the generalized Friedel sum rule [7] which describes the relation between phase shift of the electron wave scattered by an impurity and the particle number present at the impurity site. For one spin direction, it has the form of:

$$\delta=\pi n_{\mathrm{imp}}=\pi\int_{-\infty}^{\varepsilon_F}d\omega\rho_{\mathrm{imp}}(\omega) \tag{8}$$

where the integration is taken up to the Fermi level ε_F assumed to be zero, and the spectral density $\rho_{imp}(\omega) = -(1/\pi)\Im G^r_{1\sigma}(\omega)$ of the impurity (in the considered case QD level $\varepsilon_{1\sigma}$) is calculated in the presence of the direct channel and the $\varepsilon_{2\sigma}$ dot level.

6. Numerical results

The evolution of the phase shift for various values of the level splitting defined by Δ is shown in Fig. 1, $\Delta > 0$ means that ε_2 is situated above ε_1 in the energy scale. When the gate voltage increases, both the dot levels are shifted uniformly towards the resultant chemical potential defined in the leads. For a single ε_1 dot level which crosses chemical potential, the phase shift changes from 0 to π as expected for a resonant level model (see inset of Fig. 1).

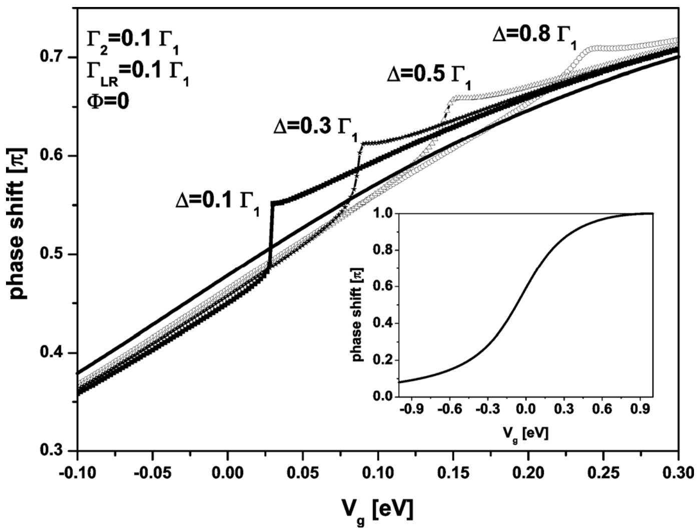

Fig. 1. Evolution of the phase shift of the electron wave traversing the device with respect to gate voltage for various spacings between QD levels ε_1 and $\varepsilon_2 = \varepsilon_1+\Delta$; ε_2 is above ε_1 in energy scale. The values of Δ are indicated in the figure. The bold solid line (and the inset) shows a phase shift for a single ε_1 active dot level. The calculation has been made for the Aharonov–Bohm phase $\Phi = 0$

The situation changes when the influence of the ε_2 level is also considered. When ε_2 approaches the Fermi level, an increase of the phase shift appears which is followed by a dip. The increase of the phase is due to a temporal increase of the particle number of ε_1 level when ε_2 (interacting with ε_1 via electrodes) crosses chemical potential and is being filled by electrons. The anomaly then vanishes when ε_2 is further shifted below the Fermi level, becoming fully occupied, and its influence on ε_1 level starts to be screened and negligible. The anomaly gets smoother shape when the splitting between the levels increases.

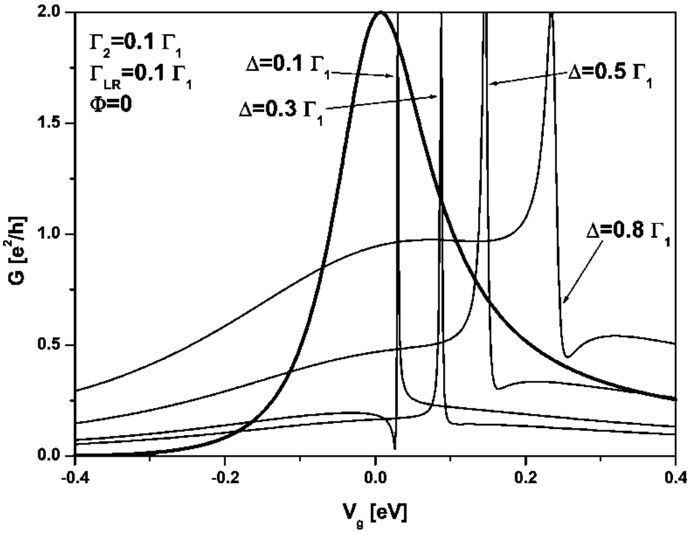

Fig. 2. Conductance through the device calculated for the same parameters as in Fig. 1. The bold solid line shows the conductance for a single QD level ε_1 only

The results of conductance calculations for the same parameters as in Fig. 1 are depicted in Fig. 2. Although ε_2 does not participate directly in electron transport through the device, it has considerable influence on the conductance shape. The bold continuous curve shows the conductance for ε_1 only level. The asymmetry of the conductance peak

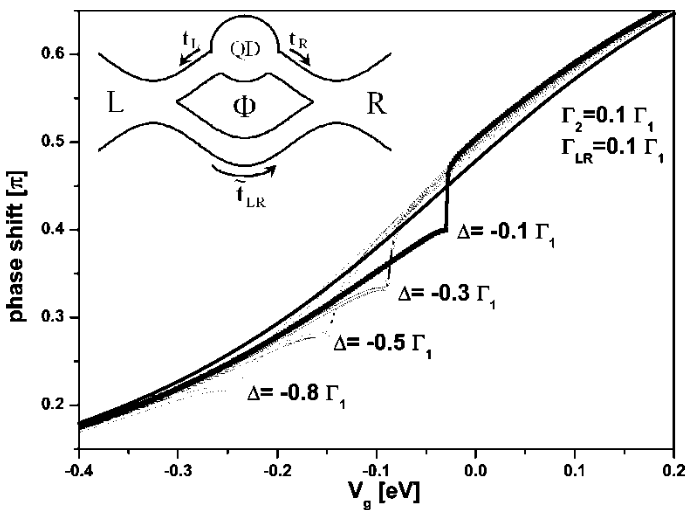

Fig. 3. Evolution of the phase shift with respect to gate voltage of the electron wave traversing the device for various spacings between QD levels ε_1 and $\varepsilon_2 = \varepsilon_1+\Delta$; ε_2 is below ε_1 in energy scale. The values of Δ are indicated in the figure. The inset shows the scheme of the device under consideration

arises from the Fano effect [8] which develops itself due to the presence in transport of the direct channel apart from resonant dot level. Inclusion of the ε_2 level, which is coupled indirectly to conducting ε_1, causes the appearance of sharp Fano resonances, whose shapes depend on the QD level splitting. A similar feature (not shown) appears for $\Delta < 0$, with Fano resonance shapes being mirror reflected. It shows that the position of ε_2 with respect to the Fermi level determines the shape of the Fano conductance peaks through ε_1 and Fano parameter $q \propto -\Gamma_2/\varepsilon_2$. A similar situation has been encountered in the case of a large dot with strongly variable hybridization of the levels to the leads [9].

Results in Figure 3 are calculated for the case when the ε_2 level lies below ε_1 in the energy scale ($\Delta < 0$). When the gate voltage decreases, ε_1 crosses the Fermi energy as the first, is followed by ε_2 crossing. It results in a temporal decrease of particle number of ε_1; a part of charge from ε_1 can be absorbed into ε_2 which becomes unoccupied when approaching the Fermi level. It results in the appearance of the minimum of the phase shift, also observed experimentally [2]. The inset of Fig. 3 shows the scheme of the device under consideration. The calculated anomalies are very weakly sensitive to the external Aharonov–Bohm phase (not shown).

In conclusion, we have shown that indirect coupling between the QD energy levels and large difference of their coupling strength to the leads causes an anomaly of the phase shift, as observed experimentally for the Aharonov–Bohm geometry. The shape of the anomaly depends on the QD level arrangement in energy scale.

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