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Orbital Kondo anomaly and channel mixing effects in a double quantum dot*

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A system consisting of two quantum dots connected to separate reservoirs is studied and electron transport properties are investigated in the Kondo regime with use of the non-equilibrium Green function technique based on the method of equation of motion. As the orbital quantum number is conserved during tunnelling processes when each dot is attached to its own leads, the orbital SU(2) Kondo effect is observed. It is shown that the mixing between the leads strongly modifies transport properties leading to a considerable suppression of the Kondo resonance.

Key words: *double quantum dot; Kondo effect*

1. Introduction

Electronic transport through quantum dot (QD) system has been intensely investigated during the last years. Fano-like features [1–3], Kondo resonance [4, 5] as well as interference effects [6] have been studied. It is well known that spin fluctuations can lead to the Kondo effect at a sufficiently low temperature. However, the Kondo resonance can also arise from the orbital degeneracy when a real spin degree of freedom is not taken into account [7–10]. The existence of the orbital or pseudo-spin Kondo resonance was first reported by Wilhelm et al. [7] in a double quantum dots (DQD) system with each dot connected to its own left and right electrodes. In this case, two degenerate states of DQD play the role of the pseudo-spin. The effect was also observed in a system with a parallel geometry in the presence of interdot coupling and anisotropy [8]. Quantum fluctuations between the orbital and spin degrees of freedom lead to SU(4) Kondo anomaly and the effect has been recently observed in a carbon nanotube quantum dot [9] as well as in vertical semiconductor QDs [10].The highly symmetric

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SU(4) Kondo was also studied theoretically with use of variety of techniques [11–17]. For example, in the work by Lim et al., the transition from the SU(4) symmetry to a SU(2)-Kondo was investigated in dependence on the mixing between channels and/or asymmetry [17].

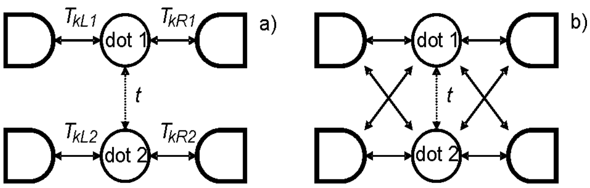

Fig. 1. Schematic diagram of the system: a) $\alpha = 0$, b) $\alpha \neq 0$

In this work, we study a DQD system consisting of two equivalent single-level dots, each coupled to left and right leads (Fig. 1). The electronic transport is theoretically studied by means of the non-equilibrium Green function and the equation of motion method. We focus on the orbital (pseudo-spin) Kondo effect. In contrast to the spin Kondo effect, two degenerate states of DQD play the role of the pseudo-spin. In this case the up and down pseudo-spins are related to an extra electron in the first (up) or second (down) dot. Tunnelling processes in which the orbital quantum number (pseudo-spin) is conserved can lead to the orbital Kondo effect (Fig. 1a). In the experiment, this conservation of the pseudo-spin quantum number is not obvious and some cross coupling may take place. The mixing between channels takes place when it is possible for electron to tunnel coherently from one dot via the reservoirs to another one (Fig. 1b). The maximal cross coupling is realized if quantum dots are attached to a single common lead.

2. Model

We model the system by the two-impurity Anderson Hamiltonian, which can be written as

$$H = H_L + H_R + H_{DQD} + H_T \tag{1}$$

Here

$$H_\beta = \sum_k \varepsilon_{k\beta} a_{k\beta}^{+} a_{k\beta}$$

with $\beta = L,R$ describes the non-interacting left ($\beta = L$) and right ($\beta = R$) reservoirs. $a_{k\beta}^{+}$ ($a_{k\beta}$) creates (annihilates) an electron in the state k with energy $\varepsilon_{k\beta}$ in lead β. The term H_{DQD} corresponds to the two-dot region and is written as

$$H_{DQD} = \sum_{i=1,2} E_i d_i^{+} d_i + t(d_1^{+} d_2 + d_2^{+} d_1) + U d_1^{+} d_1 d_2^{+} d_2 \tag{2}$$

d_i^+ (d_i) creates (annihilates) an electron in the dot i (i = 1, 2) with energy E_i and t describes the interdot hopping between dots. The interdot electron interactions are taken into account in a form of Hubbard-like term with the correlation parameter U. In this paper, we neglect on-site Coulomb repulsions and consider only empty or singly occupied states in each quantum dot. The last term in Hamiltonian (1):

$$H_T = \sum_{\substack{k,i=1,2\\ \beta=L,R}} (T_{k\beta i} a_{k\beta}^+ d_i + T_{k\beta i}^* d_i^+ a_{k\beta})$$

accounts for the tunnelling between the dots and reservoirs. $T_{k\beta i}$ are the tunnelling matrix elements which are related to the tunnelling rates by

$$\Gamma_{ii'}^{\beta} = 2\pi \sum_k T_{k\beta i} T_{k\beta i'}^* \delta(\varepsilon - \varepsilon_{k\beta})$$

In this work, $\Gamma_{ii'}$ are assumed to be independent of energy, constant within the electron band and zero otherwise. The exchange of electrons between the dots through the attached electrodes is determined by the parameter α, where $\alpha = \Gamma_{i-i}^{\beta} / \Gamma_{ii}^{\beta}$. The term Γ_{i-i}^{β} describes the tunnelling processes in which the orbital quantum number is not conserved. $\alpha = 0$ corresponds to the case of no mixing between two separated electrodes, whereas for $\alpha = 1$ quantum dots are coupled to a single common left and right reservoirs.

The non-equilibrium Green function formalism is introduced to describe transport properties of the system. The retarded G^r and advanced G^a Green functions are calculated with use of the equation of the motion method. In this work, we consider temperatures comparable to the Kondo temperature so high-order GFs are truncated using the decoupling procedure proposed by Meir [18]. Such an approximation is reasonable in the temperature range where the Kondo effect takes place. Finally, in the limit of infinite U ($U \to \infty$) GFs can be written in the following matrix which form corresponds to the Dyson equation

$$\hat{G}(\varepsilon) = [\hat{I} - \hat{g}(\varepsilon)\hat{\Sigma}(\varepsilon)]^{-1} \hat{g}(\varepsilon)$$

where $\hat{\Sigma}(\varepsilon)$ describes the self-energy of interacting system and is given by (for more details see Ref [19])

$$\hat{\Sigma}(\varepsilon) = \hat{g}(\varepsilon)^{-1} - \hat{\tilde{n}}^{-1} \hat{g}(\varepsilon)^{-1} + \hat{\tilde{n}}^{-1}(\hat{\Sigma}_0 + \hat{\tilde{\Sigma}}(\varepsilon) + \hat{T}) \tag{3}$$

with $T_{ii'} = \delta_{i-i'} t$, $\tilde{n}_{ii} = 1 - \langle d_{-i}^+ d_{-i} \rangle$, $\tilde{n}_{i-i} = \langle d_{-i}^+ d_i \rangle$. The term $g_{ii'} = \delta_{ii'}(\varepsilon - E_i)^{-1}$ describes GF of an uncoupled double quantum dot in the absence of any interaction and $\hat{\Sigma}_0$ is the self-energy of non-interacting system, whereas

$$\tilde{\Sigma}_{ii}(\varepsilon) = \sum_{k,\beta} \frac{|T_{k\beta-i}|^2}{\varepsilon - \varepsilon_{k\beta}} f_\beta(\varepsilon_{k\beta}) + \sum_{k,\beta} \frac{2t^2\left(|T_{k\beta i}|^2 + |T_{k\beta-i}|^2\right) f_\beta(\varepsilon_{k\beta})}{(\varepsilon - \varepsilon_{k\beta})\left[(\varepsilon - \varepsilon_{k\beta})^2 - 4t^2\right]} - \sum_{k,\beta} \frac{2t\, T_{k\beta i}^* T_{k\beta-i}}{(\varepsilon - \varepsilon_{k\beta})^2 - 4t^2} f_\beta(\varepsilon_{k\beta}) \tag{4}$$

$$\tilde{\Sigma}_{i-i}(\varepsilon) = -\sum_{k,\beta} \frac{T^*_{k\beta i} T_{k\beta -i}}{\varepsilon - \varepsilon_{k\beta}} f_\beta(\varepsilon_{k\beta}) + \sum_{k,\beta} \frac{t\left(\left|T_{k\beta i}\right|^2 + \left|T_{k\beta -i}\right|^2\right)}{\left(\varepsilon - \varepsilon_{k\beta}\right)^2 - 4t^2} f_\beta(\varepsilon_{k\beta}) - \sum_{k,\beta} \frac{4t^2 T^*_{k\beta i} T_{k\beta -i} f_\beta(\varepsilon_{k\beta})}{\left(\varepsilon - \varepsilon_{k\beta}\right)\left[\left(\varepsilon - \varepsilon_{k\beta}\right)^2 - 4t^2\right]} \tag{5}$$

The mean values $< d_i^+ d_{i'} >= -i\int \frac{d\varepsilon}{2\pi} G^<_{i'i}$ are calculated self-consistently. To do this, we obtain the lesser GF $G^<$ with use of Keldysh equation $\hat{G}^< = \hat{G}^r \hat{\Sigma}^< \hat{G}^a$ with the self-energy $\hat{\Sigma}^<$ determined from the Ng ansatz [20] with $\hat{\Sigma}^< = \hat{\Sigma}_0^< (\hat{\Sigma}_0^r - \hat{\Sigma}_0^a)^{-1} (\hat{\Sigma}^r - \hat{\Sigma}^a)$ and $\Sigma_0^< = i(\hat{\Gamma}^L f_L + \hat{\Gamma}^R f_R)$, where $f(\varepsilon)$ is the Fermi–Dirac distribution function for the lead β. Finally, the current flowing from the lead β can be calculated according to the formula derived by Meir[18]

$$I^\beta = i\frac{2e}{\hbar} Tr\int \frac{dE}{2\pi} \hat{\Gamma}^\beta(\varepsilon)\left\{\hat{G}^<(\varepsilon) + f_\beta(\varepsilon)\left[\hat{G}^r(\varepsilon) - \hat{G}^a(\varepsilon)\right]\right\} \tag{6}$$

3. Results and discussion

We analyze the symmetric system with

$$\Gamma^L_{11} = \Gamma^L_{22} = \Gamma^R_{11} = \Gamma^R_{22}$$

Moreover, in order to normalize the total tunnelling rate, we assume

$$\hat{\Gamma}^L = \hat{\Gamma}^R = \frac{\Gamma}{1+\alpha}\begin{pmatrix} 1 & \alpha \\ \alpha & 1 \end{pmatrix}$$

where Γ represents the tunnelling coupling and is treated here as the energy unit. Calculations are performed for $kT = 0.01\Gamma$, $U \to \infty$, equal level positions $E_1 = E_2 = E_0$ and square electron band of width $D = 500\Gamma$.

First, we consider the system with dots coupled capacitively, so there is no direct tunnelling between dots and $t = 0$ is assumed. Figure 2 shows the density of states (DOS) and the transmission in the Kondo regime ($E_0 = -4\Gamma$) calculated for several values of α. When $\alpha = 0$, we can see a well defined Kondo peak in DOS pinned at the Fermi energy of the leads (the peak is well presented in the inset). With increase of mixing between channels, the peak becomes strongly asymmetric and DOS is considerably suppressed for energies higher than E_F.

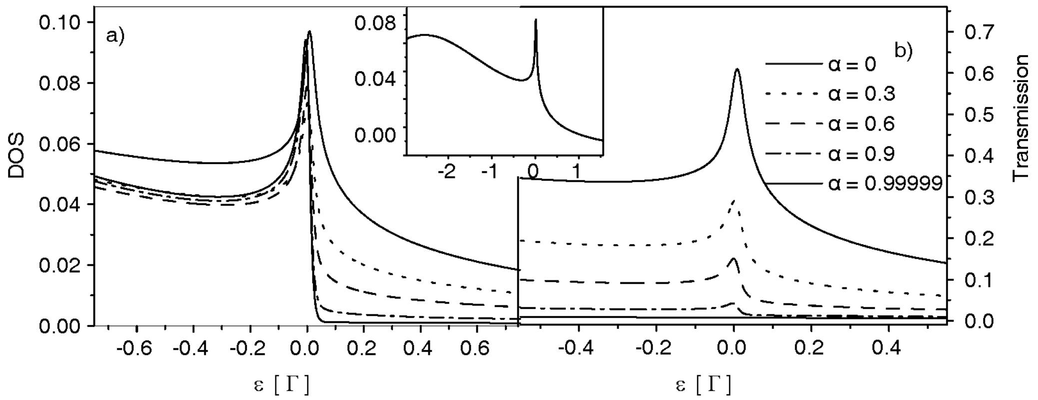

Fig. 2. Density of states and transmission for various cross-coupling parameters α and $E_0 = 4\Gamma$, $t = 0$

Next, the influence of mixing between leads on the transmission is investigated. We can see that the peak in transmission is the highest when no mixing between channels is taken into account. The peak intensity decreases with increasing cross-coupling (α). In such a situation, transport of electrons between the dots through the reservoirs is possible, what breaks the conservation of the pseudo-spin. The peak completely disappears when α approaches unity, $\alpha \approx 1$ (single common electrode for both quantum dots). Tunnelling electrons lose information about their pseudo-spin orientation and the orbital Kondo effect is destroyed. It is important to emphasize that the orbital Kondo vanishes only for the totally symmetric coupling of each leads to both dots.

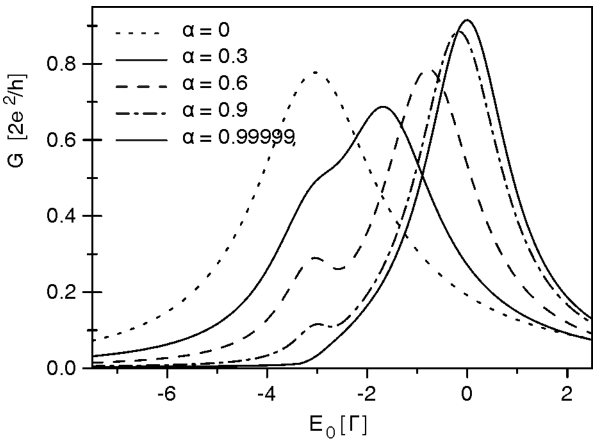

Fig. 3. The linear conductance in function of the dot level position E_0 for indicated values of α and $t = 0$

An influence of mixing on the linear conductance G is presented in Fig. 3 in which spectra calculated for various values of α are plotted. Results presented in Fig. 3 well confirm the conclusion that channel mixing effects suppress the orbital Kondo resonance. With no cross-coupling between leads taken into account ($\alpha = 0$), the conductance is maximal in the Kondo regime, as expected. For $\alpha \neq 0$, the conductance shows a small cusp apart from the main peak. With increase of channel mixing parameter α, the position of the cusp remains constant and corresponds to the Kondo regime, while the maximum moves towards higher energies. First, we focus on the Kondo regime. The mixing violates the conservation of the pseudo-spin and Kondo effect is destroyed gradually. Indeed, with increase of α the side peak becomes narrower and its intensity decreases considerably. At the same time, the right maximum becomes higher and is shifted toward the Fermi energy of electrodes $E_F = 0$. For $\alpha \approx 1$ there is only one maximum and the shape of the conductance curve resembles very well the one obtained with use of standard Hartree–Fock approximation where no Kondo effect is expected.

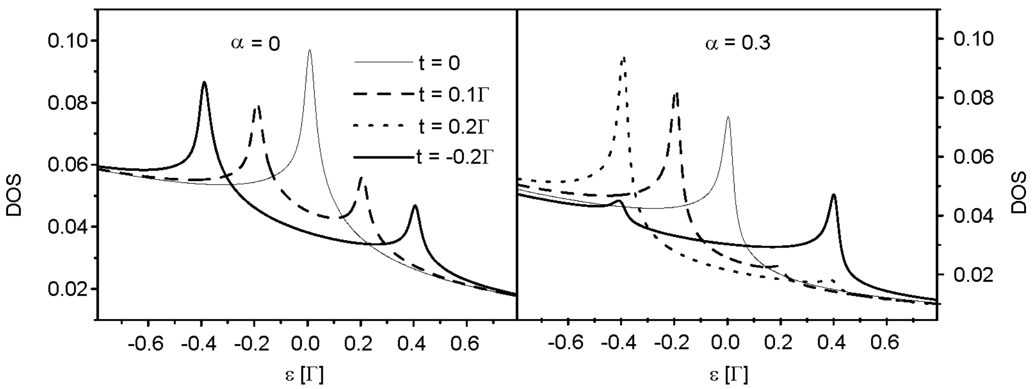

Fig. 4. Densities of states (DOS) in the Kondo regime ($E_0 = -4\Gamma$) calculated for indicated values of α and tunnelling rate t

Next, the influence of tunnelling coupling between dots on the Kondo anomaly is analyzed. Densities of states are plotted in Fig. 4 for indicated values of tunnelling rate t and the parameter α. When interdot coupling is taken into account, the Kondo peak becomes split into two components centred at $\varepsilon = \pm 2t$, what also leads to the suppression of the effect. It is worth mentioning that the interdot tunnelling t affects the orbital Kondo resonance in similar way as a magnetic field does for the spin Kondo. For $\alpha \neq 0$, no peaks practically appear at $\varepsilon = 2t$ and the curves have an asymmetric shape. Only for $\alpha = 0$ results are identical for negative and positive values of the interdot coupling ($t = 0.2\Gamma$ and $t = -0.2\Gamma$).

The differential conductance ($G_{\text{diff}} = dI/dV$) calculated for several values of interdot tunnelling t and α is presented in Fig. 5. For the system with energy levels of both dots aligned, the results are fully symmetric with respect to the bias reversal. For $t = 0$ there is a pronounced zero-bias maximum which intensity strongly decreases when mixing effects become important (compare results presented for $\alpha = 0$ and $\alpha = 0.3$). When interdot tunnelling effects are included, the peak splits into two components centred at $eV = \pm 2t$. This result is in good qualitative agreement with experimental data [8]. With increase of cross-coupling α the differential conductance drops, peak intensity is lower but their positions remain unchanged.

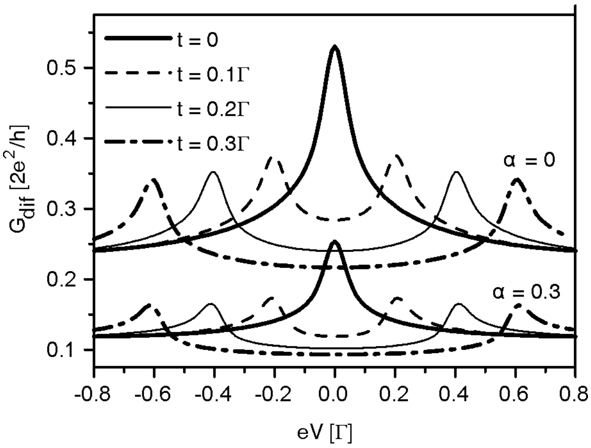

Fig. 5. Bias dependence of differential conductance for indicated values of t, $E_0 = -4\Gamma$, $\alpha = 0$ (upper curves) and $\alpha = 0.3$ (lower curves)

4. Conclusions

We have analyzed the electron transport though the system in the Kondo regime in a presence of channel mixing effects. The orbital Kondo phenomenon has been studied when α changes from 0 with no mixing to 1 with maximum mixing what corresponds to both dots coupled to common left and right reservoirs. The zero-bias Kondo anomaly in the differential conductance is obtained for $t = 0$. With increase of α, the Kondo effect is gradually destroyed and intensity of the Kondo peak is lowered. A strong suppression of the linear conductance G in the Kondo regime due to channel mixing effects is also obtained. For maximum mixing, the system corresponds to DQDs in parallel configuration with orbital Kondo effect destroyed. Therefore, the linear conductance shows only a peak in a the vicinity of the Fermi level in the leads. A presence of the tunnelling coupling between dots leads to a splitting of the Kondo anomaly and to additional suppression of the effect.

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