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Electron Transport through Double Quantum Dot: from SU(4) Kondo to SU(2) Symmetry

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Electron transport across two capacitively coupled quantum dots in a parallel geometry is theoretically studied in the non-linear response regime with spin and orbital degrees of freedom taken into account and the Kondo effect induced by on-site and inter-dot Coulomb correlations is analyzed. For a system with each dot symmetrically coupled to a separate set of electrodes a well-defined spin and orbital contributions to zero-bias Kondo resonance are obtained. The Kondo peak splits if spin and/or orbital degeneracies are removed. A suppression of the orbital Kondo anomaly due to orbital asymmetry and channel mixing effects is discussed.

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1. Introduction

A nanoscopic system with N-degenerate ground state can exhibit, in a low temperature regime, a variety of the Kondo effects in dependence on the allowed transitions between degenerated states. Commonly, the spin Kondo phenomenon is observed which originates from spin fluctuations. An interplay between orbital and spin degrees of freedom can lead to the highly symmetric SU(4) Kondo effect. Such an anomaly was observed experimentally in vertical semiconductor quantum dots (QDs) [1] and carbon nanotubes [2] as well as it was studied theoretically with a variety of techniques [3, 4]. In the present work we consider such a problem in relation to a double quantum dot (DQD) and we investigate the electron transport through the system in a non-linear response regime with the use of the non-equilibrium Green function (GF) technique based on the equation of motion (EOM) method. The formalism, which allows us to describe the orbital (spinless) Kondo effect in a DQD system, was developed and presented in detail in our previous paper [5]. Here, we extend the approach taking into account spin degrees of freedom. We consider a system, presented schematically in Fig. 1, which con-

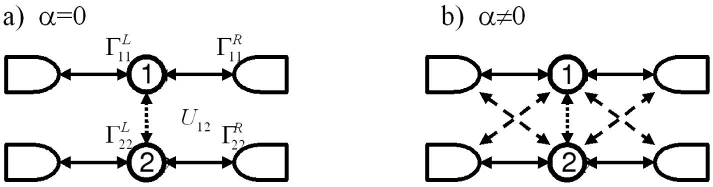

Fig. 1. The schematic diagram of the system.

sists of two capacitively coupled quantum dots in a parallel geometry with each dot connected to a separate set of left and right leads, so the transport can occur in two different channels corresponding to dot 1 and dot 2 (Fig. 1a). In such a situation the orbital quantum number (i = 1, 2) is conserved and the orbital (pseudo-spin) Kondo effect can appear if energy levels of the dots are aligned and the orbital degeneracy takes place [5]. With spin degrees of freedom included the system shows SU(4) symmetry and the SU(4) Kondo effect can be observed [4]. In the presence of channel mixing effects, schematically represented by dashed lines in Fig. 1b, electrons can tunnel coherently from one dot via reservoirs to another dot. The orbital asymmetry as well as channel mixing effects strongly influence the Kondo anomaly and differential conductance.

2. Model

Two single-level dots are described by the following Hamiltonian:

$$H_{\rm DQD} = \sum_{\sigma=\uparrow,\downarrow,i=1,2} E_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \sum_{i=1,2} U_i d^+_{i\uparrow} d_{i\uparrow} d^+_{i\downarrow} d_{i\downarrow} + U_{12} \sum_{\sigma,\sigma'} d^+_{1\sigma} d_{1\sigma} d^+_{2\sigma'} d_{2\sigma'},$$

where $d^+_{i\sigma}$ creates an electron in the dot $i = 1, 2$ with spin σ. The dot energy is, in general, spin-dependent and equal to $E_{i\sigma} = E_i - \frac{1}{2}\hat{\sigma}\Delta$ and Δ corresponds to the spin-splitting in an external magnetic field. U_i, U_{12} are parameters which describe on-site and inter-dot Coulomb interaction. No tunnel processes between dots are assumed, so the dots are capacitively coupled. The DQD region is connected via tunneling barriers to the left (L) and right (R) electrodes treated as reservoirs of free electrons. When each dot is attached to a separate set of electrodes only diagonal terms $\Gamma^{L(R)}_{ii}$, which describe coupling strengths to the appropriate leads, represented by solid lines in Fig. 1, are different from zero. In a general case, channel mixing effects can be taken into account and cross-couplings are described by non-diagonal terms assumed in the form: $\Gamma^{L(R)}_{i-i} = \alpha\sqrt{\Gamma^{L(R)}_{11}\Gamma^{L(R)}_{22}}$. The mixing is characterized by the parameter α varied from 0 with no cross-coupling effects present in the system to 1, which corresponds to the situation with both dots coupled to common reservoirs when maximal mixing takes place. As electrodes are non-magnetic the coupling rates do not depend on spin index σ.

Electron transport is investigated in the Kondo regime using the non--equilibrium GF formalism and the relevant EOM. As the formalism was presented in detail in Ref. [5], here, we describe it very briefly, underlying mainly new elements related to spin. According to the formula derived by Meir et al. [6] the current I flowing through the system under the applied bias voltage V can be expressed by means of the retarded G^{r} (advanced G^{a}) and lesser $G^{<}$ Green functions. G^{r}, G^{a} with elements $G_{ij}^{\mathrm{r(a)}} = \langle\langle d_{i\sigma}, d_{j\sigma}^{+}\rangle\rangle_{\varepsilon}^{\mathrm{r(a)}}$ are calculated with the use of the EOM method and the appropriate decoupling procedure which allows one to study the Kondo phenomenon and can be considered as a generalization of the idea proposed by Meir et al. for the ordinary spin Kondo effect [6]. Spin and orbital degrees of freedom are taken into account, described with the use of $\sigma = \uparrow, \downarrow$ and $i = 1, 2$, respectively, so GFs are represented by matrices determined in a four--dimensional spin and pseudo-spin space and the system shows SU(4) symmetry (see also [4]). As the spin is conserved during tunneling processes the appropriate matrices are diagonal in the spin index and can be reduced to two spin-dependent non-diagonal matrices in a two-dimensional pseudo-spin space. After the decoupling procedure, the set of EOM is solved in the limit of strong correlations with $U_i \to \infty$, $U_{12} \to \infty$ and finally, expressed in the form of the Dyson equation $\hat{G}_\sigma(\varepsilon) = [\hat{g}_\sigma(\varepsilon)^{-1} - \hat{\Sigma}_\sigma(\varepsilon)]^{-1}$, where $g_{ii'\sigma}(\varepsilon) = \delta_{ii'}(\varepsilon - E_{i\sigma})^{-1}$ describes GF of the uncoupled DQD in the absence of any interaction, whereas $\hat{\Sigma}_\sigma(\varepsilon)$ denotes self--energy of the interacting system determined in the Kondo regime. The lesser GF is found from the Keldysh formula $\hat{G}_\sigma^{<} = \hat{G}_\sigma^{\mathrm{r}} \hat{\Sigma}_\sigma^{<} \hat{G}_\sigma^{\mathrm{a}}$ with $\hat{\Sigma}_\sigma^{<}$ calculated according to Ng and Lee ansatz [7]. Then, $I = \frac{e}{\hbar}\int \frac{\mathrm{d}\varepsilon}{2\pi} T(\varepsilon)(f_L - f_R)$, where $f_{L(R)}$ denotes the Fermi–Dirac distribution function in the lead and the transmission is expressed as $T(\varepsilon) = \frac{1}{2}\sum_\sigma \mathrm{Tr}(\hat{\Gamma}^L G_\sigma^{\mathrm{r}} \hat{\tilde{\Gamma}}_\sigma^R \hat{G}_\sigma^{\mathrm{a}} + \hat{\Gamma}^R G_\sigma^{\mathrm{r}} \hat{\tilde{\Gamma}}_\sigma^L \hat{G}_\sigma^{\mathrm{a}})$ with $\hat{\tilde{\Gamma}}_\sigma^{L(R)} = \hat{\Gamma}^{L(R)} \hat{\Gamma}^{-1} \hat{\Gamma}_\sigma^{\mathrm{ef}}$, $\hat{\Gamma} = \hat{\Gamma}^L + \hat{\Gamma}^R$ and $\hat{\Gamma}_\sigma^{\mathrm{ef}} = \mathrm{i}(\hat{\Sigma}_\sigma^{\mathrm{r}} - \hat{\Sigma}_\sigma^{\mathrm{a}})$ (for details see [5]). The presented scheme of calculations allows us to study electron transport in the non-linear response regime and to determine the differential conductance defined as $G_{\mathrm{diff}} = \mathrm{d}I/\mathrm{d}V$.

3. Results and discussion

A spectral function of the DQD system and differential conductance are calculated for situations with each dot connected to a separate set of electrodes ($\alpha = 0$) as well as with channel mixing effects included and described by various values of the parameter α (Fig. 1). In a general case, asymmetry of the couplings to both dots is taken into account and the following form is assumed: $\Gamma_{ii}^{L(R)} = 0.5\Gamma_0[1 - (-1)^i \beta]$ with Γ_0 being constant within the electron band of the width D and zero otherwise. It describes the lead-dot tunneling rate and is taken here as an energy unit. Numerical calculations have been performed for $D = 500\Gamma_0$. The parameter β varies between 0 and 1 and is a measure of the asymmetry. If $\beta = 0$ both dots are equally coupled to their electrodes. With β increasing the dot 1 is strongly connected to its left and right electrodes and $\Gamma_{11}^{L(R)} = 0.5\Gamma_0(1 + \beta)$, whereas $\Gamma_{22}^{L(R)} = 0.5\Gamma_0(1 - \beta)$ and the dot 2 becomes gradually disconnected.

First, we assume that each dot is connected to a separate set of electrodes, so we put $\alpha = 0$ and analyze an influence of the coupling rate asymmetry, described by the parameter β, on transport properties. The spectral function (density of states, DOS) of the dot 1 determined by the formula $(i/2)\sum_\sigma(G^{\mathrm{r}}_{11\sigma} - G^{\mathrm{a}}_{11\sigma})$ as well as the transmission $T(\varepsilon)$ calculated for $\alpha = 0$ and different values of β are depicted in Fig. 2a (left and right parts, respectively). It is assumed that energy levels of both dots are degenerated and equal to $E_1 = E_2 = E_0$. Then, the orbital splitting defined as $\Delta_{\mathrm{orb}} = E_2 - E_1$ and the spin splitting Δ are equal to zero. If both dots are equally connected to separate electrodes ($\beta = 0$) the system shows SU(4) symmetry and a well-defined SU(4) Kondo anomaly can be observed. The resonance appears for energies higher than $E_{\mathrm{F}} = 0$ and is much wider than the Kondo peak corresponding to the ordinary spin Kondo phenomenon [4]. When $\beta \neq 0$ the orbital asymmetry appears. Coupling strengths for two dots are different and the orbital Kondo effect is gradually diminished which strongly influences DOS of each dot. As β increases the dot 1 becomes strongly connected to electrodes, in such a situation the resonance gradually shifts approaching E_{F} for higher values of β and the SU(2) spin-Kondo effect can be observed (Fig. 2a, left part). The second dot becomes disconnected and the corresponding DOS shows no Kondo anomaly when β tends to 1. The transmission is also strongly influenced by the orbital asymmetry which is demonstrated in Fig. 2a (right part). The main peak which appears for $\beta = 0$ just above E_{F} starts to split into two components and a well-defined spin Kondo resonance, pinned to the Fermi level, develops for higher values of β. Intensity of the peak is rather low, so in this energy region ($E_0 = -5.5\Gamma_0$) the spin contribution to the total Kondo anomaly is relatively small. The second component is shifted towards higher energies, considerably greater than E_{F}, and therefore, it does not contribute to the conductance in the presence of strong orbital asymmetry.

If dot levels are not aligned ($\Delta_{\mathrm{orb}} \neq 0$) the orbital degeneracy is removed which for $\beta = 0$ leads to the orbital splitting of the Kondo resonance and the appropriate components appear below and above E_{F} (see inset in Fig. 2a, where the total DOS of both dots is presented in the case of $\beta = 0$). As $\Delta = 0$ the spin--dependent states are degenerated and a well-defined peak, pinned to the Fermi energy, can be observed which corresponds to the spin Kondo effect (thick solid line in the inset). An additional splitting of each of the components is obtained in the presence of magnetic field which removes the spin degeneracy ($\Delta \neq 0$). The splitting increases with Δ which is well demonstrated in the inset.

An influence of the orbital asymmetry, described by β, on the differential conductance is depicted in Fig. 2b for two cases: (1) $\Delta_{\mathrm{orb}} \neq 0$ and $\Delta = 0$ (left part), (2) $\Delta_{\mathrm{orb}} \neq 0$ and $\Delta \neq 0$ (right part). Let us discuss the first case. For small values of β three well-defined resonance peaks can be seen (Fig. 2b, left part). As for $\Delta_{\mathrm{orb}} \neq 0$ the orbital degeneracy is removed, the orbital Kondo anomaly is split and two components appear at en-

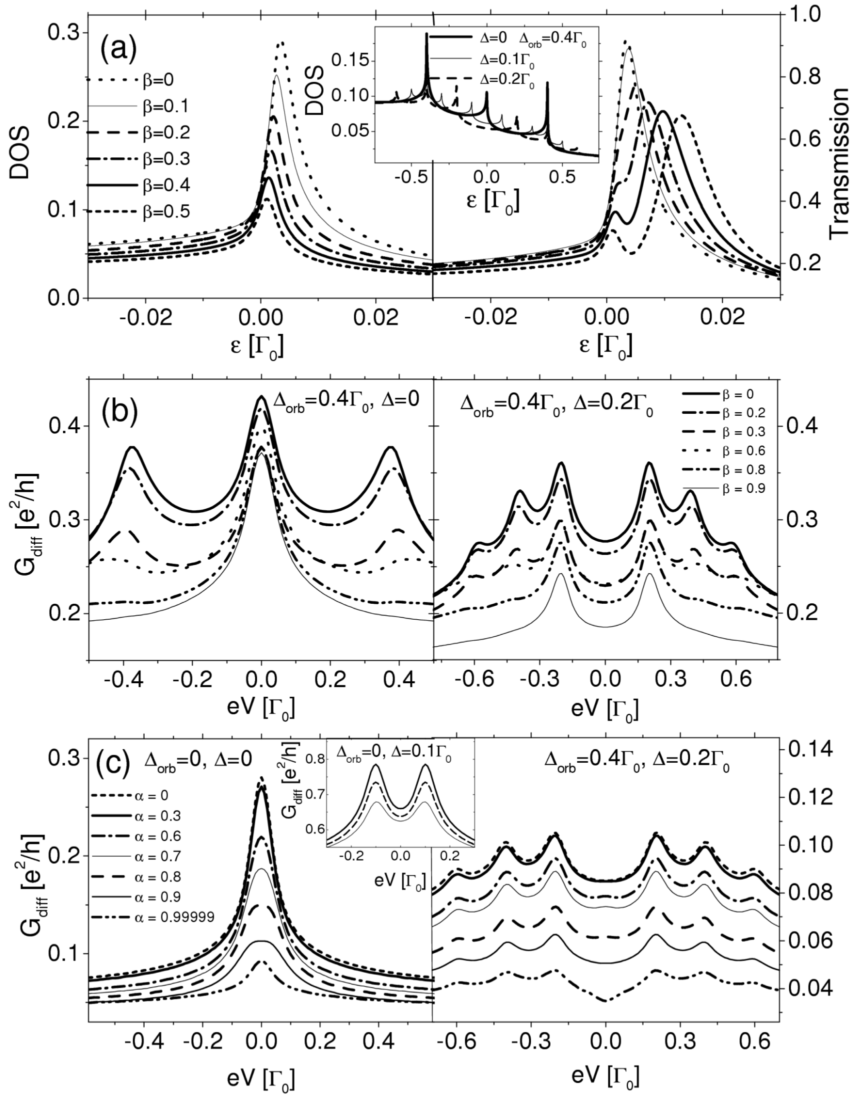

Fig. 2. (a) Local density of states of dot 1 (left part) and transmission (right part) for $\alpha = 0$ and different values of β, $E_0 = -5.5\Gamma_0$, $kT = 0.001\Gamma_0$, $\Delta = 0$, $\Delta_{\rm orb} = 0$. Inset shows DOS for $\beta = 0$, $\Delta_{\rm orb} = 0.4\Gamma_0$ and indicated values of Δ. (b) Bias dependence of differential conductance $G_{\rm diff}$ for $\alpha = 0$ and indicated values of β. $E_0 = -4\Gamma_0$, $kT = 0.01\Gamma_0$. (c) Differential conductance calculated for $\beta = 0$ and different values of α, $E_0 = -5.5\Gamma_0$, $kT = 0.01\Gamma_0$. Inset shows bias dependence of $G_{\rm diff}$ for $\beta = 0$ and different values of α, $U_{12} = 0$, $E_0 = -2\Gamma_0$, $kT = 0.01\Gamma_0$.

ergies $eV = \pm\Delta_{\rm orb}$. With an increase in β intensities of both the components are considerably suppressed and the resonances disappear in the presence of the strong orbital asymmetry (β close to 1), so the orbital Kondo anomaly is destroyed. At the same time, for different values of β a well-defined zero--bias anomaly can be seen when energy levels of both dots are spin degenerated and $\Delta = 0$ (Fig. 2b, left part). Therefore, the peak can be treated as corresponding to the spin Kondo effect of SU(2) symmetry which in this energy region ($E_0 = -4\Gamma_0$) is quite well pronounced and its contribution to the total anomaly is considerable. If additionally, as in the second case, the spin degeneracy is removed and $\Delta \neq 0$, the zero-bias resonance splits into two components located at $eV = \pm\Delta$ (Fig. 2b, right part). The behavior is typical of the spin Kondo phenomenon for which the peak splits in the presence of the magnetic field removing the degeneracy. In the case under investigation the components, which correspond to the orbital Kondo effect, are also split which is well demonstrated for small β in Fig. 2b (right part). However, they are strongly suppressed for higher values of β.

Now, we analyze the influence of channel mixing effects on the differential conductance (Fig. 2c). For simplicity we consider only the system with symmetric couplings for both dots and put $\beta = 0$. The cross-couplings are described by the parameter α which is varied from 0 with no mixing effects included to 1 when both dots are equally coupled to common left and right reservoirs. If energy levels are degenerated ($\Delta_{\rm orb} = 0$ and $\Delta = 0$) the zero-bias Kondo anomaly can be seen (Fig. 2c, left part). The peak intensity strongly depends on α. With increase in α the intensity drops as the orbital number is not conserved due to channel mixing effects and the orbital Kondo anomaly is destroyed. The results show that in the presented energy region ($E_0 = -5.5\Gamma_0$) the spin Kondo anomaly is not much pronounced and for $\alpha = 0$ the main contribution to the differential conductance comes from the orbital Kondo phenomenon, which disappears gradually with α increasing. It is also well demonstrated in the right part of Fig. 2c, where the appropriate curves are presented for $\Delta_{\rm orb} \neq 0$ and $\Delta \neq 0$. The components, which appear due to the splitting of the main peak as spin and orbital degeneracies are removed, can be well seen in the differential conductance for $\alpha = 0$. With an increase in α the peaks are influenced by channel mixing effects and their intensities drop. Resonances located at $eV = \pm\Delta$ include spin and orbital contributions due to overlapping the appropriate components when both types of degeneracy are removed, and therefore, their intensities diminish with α increasing. On the other hand, in a system with inter-dot Coulomb interaction turned off ($U_{12} = 0$), only the spin Kondo effect, induced by on-site correlations, develops which, as presented in the inset in Fig. 2c, is not substantially influenced by the channel mixing effects.

In summary, it can be stated that the orbital asymmetry and channel mixing effects considerably influence the spectral function and differential conductance and substantially suppress the orbital Kondo phenomenon. In the presence of strong asymmetry a transition to spin Kondo effect can be observed.

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