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Tunneling transport through multi-electrons states in coupled quantum dots with Coulomb correlations

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ABSTRACT

We investigated the peculiarities of non-equilibrium charge configurations in the system of two strongly coupled quantum dots (QDs) weakly connected to the reservoirs in the presence of Coulomb correlations. We revealed that total electron occupation demonstrates in some cases significant decreasing with increasing of applied bias – contrary to the situation when Coulomb correlations are absent and found well pronounced ranges of system parameters where negative tunneling conductivity appears due to the Coulomb correlations.

1. Introduction

Electron tunneling through the system of coupled QDs in the presence of strong Coulomb correlations is one of the most interesting problems in the solid state physics. The present day experimental technique gives possibility to produce single QDs with a given set of parameters and to create coupled QDs with a different spatial geometry [1–3]. Thereby the main effort in the physics of QDs is devoted to the investigation of non-equilibrium charge states and different charge configurations due to the electrons tunneling [4–8] through the system of coupled QDs in the presence of strong Coulomb interaction.

One of the most intensively studied problems in this field is tunneling through the single QD [10,11] and interacting QDs [4,5,12,13] in the Kondo regime, which reveals rich physics for small bias voltage compared to the tunneling rates. It was demonstrated [12] that Coulomb correlations in QDs lead to bistable behavior in the Kondo regime at zero bias voltage. Charge redistribution between different spin configurations in the system of two interacting QDs in the Kondo regime was regarded in [4]. The authors considered the situation when the detuning between the energy levels in the QDs exceeds the dots coupling and on-site Coulomb repulsion is present only in a single dot.

A great attention is also paid to the double QDs as attractive systems for spin-dependent transport [14–16]. In [14] authors studied transport through double QD both in sequential tunneling and co-tunneling regimes by means of master equation for density matrix in the basis of exact eigenfunctions and eigenvalues. Unfortunately only transitions between the empty states and states with one and two electrons were considered. Results obtained in [15,16] deal with the investigation of transport in the double QD system weakly coupled to spin-polarized leads. The method of charge and spin transport analysis presented in [15] is based on the Liouville equation for the reduced density matrix in lowest order in the tunneling transitions. Authors analyzed tunneling conductivity and $I-V$ characteristics as functions of magnetic leads polarization and gate voltage. The system where only one or two electrons can be localized simultaneously due to the specific features of the ferromagnetic leads was investigated in [16].

In the present paper we consider electron tunneling through the coupled QDs in the regime when applied bias can be tuned in a wide range and the on-site Coulomb repulsion can be comparable to the other system parameters. We analyze different charge configurations in the system of two strongly coupled quantum dots (QDs) weakly connected to the reservoirs in the presence of Coulomb correlations in a wide range of applied bias in terms of pseudo-operators with constraint [17–19,8]. For large values of applied bias Kondo effect is not essential so we neglect any correlations between

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electron states in the QDs and in the leads. This approximation allows us to describe correctly non-equilibrium occupation of any single- and multi-electron state due to the tunneling processes. We revealed the presence of negative tunneling conductivity in certain ranges of the applied bias voltage and revealed that total electron occupation demonstrates in some cases significant decreasing with increasing of applied bias – contrary to the situation when Coulomb correlations are absent.

2. The theoretical model

We consider a system of coupled QDs with the single particle levels $\tilde{\varepsilon}_1$ and $\tilde{\varepsilon}_2$ connected to the two leads. We assume that the single-particle level spacing in the dots is larger than energy levels width, so that one electron spin-degenerate levels of QDs spectrum are well resolved. Moreover for reasonable values of applied bias in STM/STS experiments only one single electron energy level contributes significantly to the tunneling current [9]. The Hamiltonian can be written as

$$\hat{H}=\sum_{\sigma}c_{1\sigma}^{+}c_{1\sigma}\tilde{\varepsilon}_1+\sum_{\sigma}c_{2\sigma}^{+}c_{2\sigma}\tilde{\varepsilon}_2+U_1\hat{n}_{1\sigma}\hat{n}_{1-\sigma}+U_2\hat{n}_{2\sigma}\hat{n}_{2-\sigma}+\sum_{\sigma}T(c_{1\sigma}^{+}c_{2\sigma}+c_{2\sigma}^{+}c_{1\sigma}) \tag{1}$$

where operator $c_{l\sigma}$ creates an electron in the dot l with spin σ, $\tilde{\varepsilon}_l$ is the energy of the single electron level in the dot l and T is the inter-dot tunneling coupling, $n_{l\sigma}=c_{l\sigma}^{+}c_{l\sigma}$ and $U_{1(2)}$ is the on-site Coulomb repulsion of localized electrons. When the coupling between QDs exceeds the value of interaction with the leads, one has to use the basis of exact eigenfunctions and eigenvalues of coupled QDs without the interaction with the leads. In this case all energies of single- and multi-electron states are well known:

One electron in the system: two single electron states with the wave function

$$\psi_i^{\sigma}=\mu_i\cdot|0\uparrow\rangle|00\rangle+\nu_i\cdot|00\rangle|0\uparrow\rangle \tag{2}$$

Single electron energies and coefficients μ_i and ν_i can be found as eigenvalues and eigenvectors of matrix:

$$\begin{pmatrix}\varepsilon_1 & -T\\ -T & \varepsilon_2\end{pmatrix} \tag{3}$$

Two electrons in the system: two states with the same spin $\sigma\sigma$ and $-\sigma-\sigma$ and four two-electron states with the opposite spins $\sigma-\sigma$ with the wave function:

$$\psi_j^{\sigma-\sigma}=\alpha_j\cdot|\uparrow\downarrow\rangle|00\rangle+\beta_j\cdot|\uparrow0\rangle|0\downarrow\rangle+\gamma_j\cdot|0\downarrow\rangle|\uparrow0\rangle+\delta_j\cdot|00\rangle|\uparrow\downarrow\rangle \tag{4}$$

Two electron energies and coefficients α_j, β_j, γ_j and δ_j are the eigenvalues and eigenvectors of matrix:

$$\begin{pmatrix}2\varepsilon_1+U_1 & -T & -T & 0\\ -T & \varepsilon_1+\varepsilon_2 & 0 & -T\\ -T & 0 & \varepsilon_1+\varepsilon_2 & 0\\ 0 & -T & -T & 2\varepsilon_2+U_2\end{pmatrix} \tag{5}$$

Three electrons in the system: two three-electron states with the wave function

$$\psi_m^{\sigma\sigma-\sigma}=p_m|\uparrow\downarrow\rangle|\uparrow\rangle+q_m|\uparrow\rangle|\uparrow\downarrow\rangle \qquad m=s,a \tag{6}$$

Three electron energies and coefficients p_m and Q_m can be found as eigenvalues and eigenvectors of matrix:

$$\begin{pmatrix}2\varepsilon_1+\varepsilon_2+U_1 & -T\\ -T & 2\varepsilon_2+\varepsilon_1+U_2\end{pmatrix} \tag{7}$$

Four electrons in the system: one four-electron state with energy $E_{IV}=2\varepsilon_1+2\varepsilon_2+U_1+U_2$ and wave function

$$\psi=|\uparrow\downarrow\rangle|\uparrow\downarrow\rangle \tag{8}$$

If coupled QDs are connected with the leads of the tunneling contact the number of electrons in the dots changes due to the tunneling processes. Transitions between the states with a different number of electrons in the two interacting QDs can be analyzed in terms of pseudo-particle operators with constraint on the physical states (the number of pseudo-particles). Consequently, the electron operator $c_{\sigma l}^{+}$ $(l=1,2)$ can be written in terms of pseudo-particle operators as

$$c_{\sigma l}^{+}=\sum_i X_i^{\sigma l}f_{\sigma i}^{+}b+\sum_{j,i}Y_{ji}^{\sigma-\sigma l}d_j^{+\sigma-\sigma}f_{i-\sigma}+\sum_i Y_i^{\sigma\sigma l}d^{+\sigma\sigma}f_{i\sigma}+\sum_{m,j}Z_{mj}^{\sigma\sigma-\sigma l}\psi_{m-\sigma}^{+}d_j^{\sigma-\sigma}+\sum_m Z_m^{\sigma-\sigma-\sigma l}\psi_{m\sigma}^{+}d^{-\sigma-\sigma}+\sum_m W_m^{\sigma-\sigma-\sigma l}\varphi^{+}\psi_{m\sigma} \tag{9}$$

where $f_{\sigma}^{+}(f_{\sigma})$ and $\psi_{\sigma}^{+}(\psi_{\sigma})$—are pseudo-fermion creation (annihilation) operators for the electronic states with one and three electrons correspondingly. $b^{+}(b)$, $d_{\sigma}^{+}(d_{\sigma})$ and $\varphi^{+}(\varphi)$—are slave boson operators, which correspond to the states without any electrons, with two electrons or four electrons. Operators $\psi_{m-\sigma}^{+}$— describe system configuration with two spin up electrons σ and one spin down electron $-\sigma$ in the symmetric and asymmetric states.

Matrix elements $X_i^{\sigma l}$, $Y_{ji}^{\sigma-\sigma l}$, $Y_{ji}^{\sigma\sigma l}$, $Z_{mj}^{\sigma\sigma-\sigma l}$, $Z_{mj}^{\sigma-\sigma-\sigma l}$ and $W_m^{\sigma-\sigma-\sigma l}$ can be evaluated as

$$\begin{aligned}
X_i^{\sigma l}&=\langle\psi_i^{\sigma}|c_{\sigma l}^{+}|0\rangle\\
Y_{ji}^{\sigma-\sigma l}&=\langle\psi_j^{\sigma-\sigma}|c_{\sigma l}^{+}|\psi_i^{-\sigma}\rangle\\
Y_{ji}^{\sigma\sigma l}&=\langle\psi_j^{\sigma\sigma}|c_{\sigma l}^{+}|\psi_i^{\sigma}\rangle\\
Z_{mj}^{\sigma\sigma-\sigma l}&=\langle\psi_m^{\sigma\sigma-\sigma}|c_{\sigma l}^{+}|\psi_j^{\sigma-\sigma}\rangle\\
Z_m^{\sigma-\sigma-\sigma l}&=\langle\psi_m^{\sigma-\sigma-\sigma}|c_{\sigma l}^{+}|\psi_j^{-\sigma-\sigma}\rangle\\
W_m^{\sigma-\sigma-\sigma l}&=\langle\psi^{\sigma\sigma-\sigma-\sigma}|c_{\sigma l}^{+}|\psi_m^{\sigma-\sigma-\sigma}\rangle
\end{aligned} \tag{10}$$

Finally one can easily express matrix elements through the matrixes (3), (5), (7) eigenvectors elements:

$$\begin{aligned}
&X_i^{\sigma1}=\mu_i;\quad X_i^{\sigma2}=\nu_i\\
&Y_{ji}^{\sigma-\sigma1}=\alpha_j\mu_i+\beta_j\nu_i\\
&Y_{ji}^{\sigma-\sigma2}=\delta_j\nu_i+\gamma_j\mu_i\\
&Y_{ji}^{\sigma\sigma1}=\nu_i;\quad Y_{ji}^{\sigma\sigma2}=\mu_i\\
&Z_{mj}^{\sigma\sigma-\sigma1}=p_m\gamma_j+q_m\delta_j\\
&Z_{mj}^{\sigma\sigma-\sigma2}=p_m\alpha_j+q_m\beta_j\\
&Z_{mj}^{\sigma-\sigma-\sigma1}=p_m;\quad Z_{mj}^{\sigma-\sigma-\sigma1}=q_m\\
&W_m^{\sigma-\sigma-\sigma1}=q_m;\quad W_m^{\sigma-\sigma-\sigma2}=p_m
\end{aligned} \tag{11}$$

The constraint on the space of the possible system states has to be taken into account:

$$\hat{n}_b+\sum_{i\sigma}\hat{n}_{fi\sigma}+\sum_{j\sigma\sigma'}\hat{n}_{dj}^{\sigma\sigma'}+\sum_{m\sigma}\hat{n}_{\psi m\sigma}+\hat{n}_{\varphi}=1 \tag{12}$$

Condition (12) means that states with only one pseudo-particle are allowed.

Electron filling numbers in the coupled QDs can be expressed in terms of the pseudo-particles filling numbers:

$$\hat{n}_{\sigma}^{el}=\sum_l c_{\sigma l}^{+}c_{\sigma l}=\sum_{i,l}|X_i^{\sigma l}|^2\hat{n}_{fi\sigma}+\sum_{i,j,l}|Y_{ji}^{\sigma-\sigma l}|^2\hat{n}_{dj}^{\sigma-\sigma}+\sum_{i,l}|Y_{ji}^{\sigma\sigma l}|^2\hat{n}_{dj}^{\sigma\sigma}+\sum_{m,j,l}|Z_{mj}^{\sigma\sigma-\sigma l}|^2\hat{n}_{\psi m-\sigma}+\sum_{m,l}|Z_{mj}^{-\sigma-\sigma\sigma l}|^2\hat{n}_{\psi m\sigma}+\sum_{m,l}|W_m^{\sigma-\sigma-\sigma l}|^2\hat{n}_{\varphi} \tag{13}$$