Eur. Phys. J. B (2015) 88: 110
DOI: 10.1140/epjb/e2015-50821-3

THE EUROPEAN PHYSICAL JOURNAL B

Regular Article

Ferromagnets-induced splitting of molecular states of T-shaped double quantum dots

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Received 27 November 2014 / Received in final form 11 February 2015
Published online 4 May 2015
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Abstract. The exchange field for molecular states of double quantum dot, induced by two ferromagnets coupled to the device in T-shaped configuration, is defined and calculated. It is found, that in the regime of strong coupling between quantum dots, the dependence of the exchange field on this coupling becomes nontrivial. In particular, it changes the sign a few times to eventually vanish in the limit of infinite inter-dot coupling. The excitation energies of double quantum dot are calculated and the results used to predict the conditions for suppression of the two-stage Kondo effect in the considered nanostructure.

1 Introduction

When a discrete level is coupled to a large system of continuous energy spectrum, it is not only broadened, but also shifted [1]. This applies, in particular, to a quantum dot (QD) coupled to a metallic lead: the charge fluctuations give rise to the renormalization of the dot level [2]. If the coupling to the lead is spin dependent, this renormalization also depends on spin, leading to the splitting of the dot's level, often called *the exchange field*. It can be estimated through the Anderson's scaling approach [3,4] or numerical renormalization group calculations [5,6], as well as within the perturbation theory, second order in the interaction with the lead, where usual logarithmic divergences cancel out when one takes the difference of the shifts for levels of opposite spins [7]. The exchange field was also observed experimentally [8,9]. Its values are of the order of fraction of meV; the magnetic field corresponding to such a splitting for an electron with spin $s = 1/2$ and gyromagnetic ratio $g = 2$ is a few Tesla [9]. The estimations of the exchange field based on numerical renormalization group calculations were found to be in good agreement with experiment [9]. Moreover, as dependent significantly on the dot's energy level, the exchange field is very important for spintronic applications, as a tool enabling manipulation of the single electron's spin (localized on the quantum dot) by only electrical means [10].

In the past few years, transport properties of double quantum dots (DQDs), from which only one is coupled directly to the leads, and the second is side-coupled to the first one, were addressed in a number of papers [11–14][1]. This configuration is often referred to as T-shaped DQD. In such systems, the two-stage Kondo effect occurs: the usual Kondo effect is suppressed at sufficiently low temperatures, due to singlet formation in DQD subsystem [12,15,16]. This singlet, however, can be broken by the magnetic field, which restores the Kondo effect [17]. In the present paper a similar system with ferromagnetic electrodes (Fs) is considered (see Fig. 1). It is shown, by means of perturbative calculation, that the exchange field can be considered as an alternative mechanism of breaking the singlet and restoring the Kondo effect. This is confirmed by numerical renormalization group calculations [18].

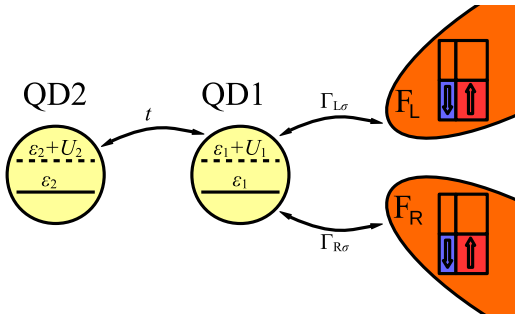

Fig. 1. Scheme of the considered system.

It is worth stressing, that all the correlations in DQD subsystem are treated analytically. The exchange field is properly defined for all the eigenstates, whose energies are obtained exactly for a rather general case[2]. In particular, adjusting of Coulomb energies and energy levels of both dots independently is allowed. The latter is especially important for applications, where one should be able to tune the exchange field by changing the energy levels of QDs.

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[1] See also references cited in references [11–14].

[2] Less general case was studied in reference [19].

The article is organized as follows. In Section 2 the Hamiltonian of DQD is presented and its eigenvalues and eigenstates are calculated. Then, in Section 3 the exchange field for eigenstates of DQD is defined and the formula for it is derived. Finally, the results are presented in Section 4.

2 The double-dot system

The Anderson model is used to describe quantum dots. It is also assumed, that their mutual interaction is reduced to the hopping between the dots. Thus, the Hamiltonian of DQD subsystem has the form

$$H_{\mathrm{DQD}} = \sum_{\alpha\sigma} \varepsilon_\alpha d^\dagger_{\alpha\sigma} d_{\alpha\sigma} + \sum_\sigma t \left(d^\dagger_{1\sigma} d_{2\sigma} + h.c. \right) + \sum_\alpha \frac{U_\alpha}{2} \left(\sum_\sigma d^\dagger_{\alpha\sigma} d_{\alpha\sigma} - 1 \right)^2 - \frac{U_1 + U_2}{2}. \quad (1)$$

The constant term is set such that unoccupied DQD has energy equal to 0. The index $\alpha \in \{1, 2\}$ corresponds to number of QD (see Fig. 1), while $\sigma = \pm 1$ denotes direction of the spin. t denotes the hopping between the dots. $d^{(\dagger)}_{\alpha\sigma}$ annihilates (creates) an electron of spin σ in dot α. The Coulomb energy of dot α is U_α, while the energy level for an electron of spin σ in the dot α is ε_α. The mean detuning of dot's level from particle-hole symmetric point is $\varepsilon = (\varepsilon_2 + \varepsilon_1)/2 + U$, where $U = (U_2 + U_1)/4$. For convenience the following notation is used: $\Delta = (U_2 - U_1)/4$, $\delta = (\varepsilon_2 - \varepsilon_1)/2 + \Delta$.

In addition, q denotes the normal-ordered charge of DQD. Similarly, S denotes the total spin of DQD, and S_z is used for its z component. Eigenstates are denoted $|e_i\rangle$, with $i \in \{1, \ldots, 16\}$, while states from the basis of definite occupation numbers have form $|\chi_1\chi_2\rangle$, where $\chi_\alpha \in \{0, \uparrow, \downarrow, 2\}$ is the state of QDα.

The eigenvalues of H_{DQD} are listed in Table 1. One can clearly see charge U(1) and spin SU(2) symmetries. The energies of the states in the $q = 0$, $S = 0$ subspace are the roots of the following cubic polynomial,

$$\omega^3 + (2U - 6\varepsilon)\omega^2 - 4\left(t^2 + 2U\varepsilon + \delta^2 - 3\varepsilon^2\right)\omega + 8\left[t^2\varepsilon + U\left(\varepsilon^2 - \delta^2\right) + \delta^2\varepsilon - \varepsilon^3\right] = 0. \quad (2)$$

They can be expressed through radicals, but the resulting expressions are somewhat cumbersome and for this reason were not explicitly listed in Table 1. However, for special cases they significantly simplify. Eigenvalues for some of these cases are presented in Table 2. For $\varepsilon = \delta = 0$ ($\varepsilon_1 = -U_1/2$, $\varepsilon_2 = -U_2/2$) the charge symmetry also becomes SU(2). Then, states: $|e_1\rangle$, $|e_{11}\rangle$, and $|e_{16}\rangle$, form the triplet of $E = 0$ (see column $\delta = 0$ in Tab. 2 for E_{11}). Simultaneously, $S = 1/2$ doublets with $q = \pm 1$ become degenerated.

In turn, the eigenstates are listed in Table 3. These corresponding to highest quantum numbers ($q = \pm 2$, $S = 1$) are trivial. Expressions for states forming doublets are only a bit more complicated. They all can be written using coefficients

$$\nu_\pm = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\delta - \Delta}{\sqrt{t^2 + (\delta - \Delta)^2}}}, \quad (3)$$

$$\tilde{\nu}_\pm = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\delta + \Delta}{\sqrt{t^2 + (\delta + \Delta)^2}}}. \quad (4)$$

Note, that for $t = 0$, $\nu_\pm$ ($\tilde{\nu}_\pm$) are either 0 or 1, depending on the sign of $\delta - \Delta$ ($\delta + \Delta$), correspondingly. The three remaining states, $|e_9\rangle$, $|e_{10}\rangle$, $|e_{11}\rangle$, can be reasonably simply expressed through the coefficients dependent on the respective eigenvalues,

$$\xi^1_i = \frac{P_i Q_i/t - 2t}{\sqrt{8t^2 + 2P_i^2 - 4P_iQ_i + P_i^2Q_i^2/t^2}}, \quad (5)$$

$$\xi^2_i = -\frac{\sqrt{2}P_i}{\sqrt{8t^2 + 2P_i^2 - 4P_iQ_i + P_i^2Q_i^2/t^2}}, \quad (6)$$

$$\xi^3_i = \frac{2t}{\sqrt{8t^2 + 2P_i^2 - 4P_iQ_i + P_i^2Q_i^2/t^2}}, \quad (7)$$

where $P_i = 2(\varepsilon + \delta) - E_i$ and $Q_i = 2(\varepsilon - U) - E_i$. Note, that dependence of ξ^a_i on E_i (through P_i and Q_i), means in fact a complicated dependence on all the parameters of the model. Moreover, if two of the energies E_9, E_{10}, E_{11}

Table 1. Exact eigenvalues of H_{DQD}. Solutions of cubic secular equation in $q = 0, S = 0$ subspace were not written explicitly.

State	q	S_z	E_i
$\|e_1\rangle$	-2	0	0
$\|e_2\rangle$, $\|e_3\rangle$	-1	$-\frac{1}{2}, \frac{1}{2}$	$\varepsilon - U - \sqrt{(\Delta - \delta)^2 + t^2}$
$\|e_4\rangle$, $\|e_5\rangle$	-1	$-\frac{1}{2}, \frac{1}{2}$	$\varepsilon - U + \sqrt{(\Delta - \delta)^2 + t^2}$
$\|e_6\rangle$, $\|e_7\rangle$, $\|e_8\rangle$	0	$-1, 0, 1$	$2(\varepsilon - U)$
$\|e_9\rangle$	0	0	E_9
$\|e_{10}\rangle$	0	0	E_{10}
$\|e_{11}\rangle$	0	0	E_{11}
$\|e_{12}\rangle$, $\|e_{13}\rangle$	$+1$	$-\frac{1}{2}, \frac{1}{2}$	$3\varepsilon - U - \sqrt{(\Delta + \delta)^2 + t^2}$
$\|e_{14}\rangle$, $\|e_{15}\rangle$	$+1$	$-\frac{1}{2}, \frac{1}{2}$	$3\varepsilon - U + \sqrt{(\Delta + \delta)^2 + t^2}$
$\|e_{16}\rangle$	$+2$	0	4ε

Table 2. Values of eigenenergies E_9, E_{10} and E_{11} for different limiting cases [19]. Each row corresponds to one of the three solutions of equation (2) expressed through radicals.

State	$t = 0$	$\delta = 0$	$U = 0$
$\|e_9\rangle$	$2(\varepsilon + \delta)$	$2\varepsilon - U + \sqrt{U^2 + 4t^2}$	$2\left(\varepsilon + \sqrt{t^2 + \delta^2}\right)$
$\|e_{10}\rangle$	$2(\varepsilon - U)$	$2\varepsilon - U - \sqrt{U^2 + 4t^2}$	$2\left(\varepsilon - \sqrt{t^2 + \delta^2}\right)$
$\|e_{11}\rangle$	$2(\varepsilon - \delta)$	2ε	2ε

Table 3. Eigenvectors of H_{DQD}.

$\lvert e_1\rangle = \lvert 00\rangle,$
$\lvert e_2\rangle = \nu_+\lvert\downarrow 0\rangle - \nu_-\lvert 0\downarrow\rangle,$
$\lvert e_3\rangle = \nu_+\lvert\uparrow 0\rangle - \nu_-\lvert 0\uparrow\rangle,$
$\lvert e_4\rangle = \nu_-\lvert\downarrow 0\rangle + \nu_+\lvert 0\downarrow\rangle,$
$\lvert e_5\rangle = \nu_-\lvert\uparrow 0\rangle + \nu_+\lvert 0\uparrow\rangle,$
$\lvert e_6\rangle = \lvert\downarrow\downarrow\rangle,$
$\lvert e_7\rangle = (\lvert\downarrow\uparrow\rangle + \lvert\uparrow\downarrow\rangle)/\sqrt{2},$
$\lvert e_8\rangle = \lvert\uparrow\uparrow\rangle,$
$\lvert e_9\rangle = \xi_9^1\lvert 20\rangle + \xi_9^2\frac{\lvert\downarrow\uparrow\rangle - \lvert\uparrow\downarrow\rangle}{\sqrt{2}} + \xi_9^3\lvert 02\rangle,$
$\lvert e_{10}\rangle = \xi_{10}^1\lvert 20\rangle + \xi_{10}^2\frac{\lvert\downarrow\uparrow\rangle - \lvert\uparrow\downarrow\rangle}{\sqrt{2}} + \xi_{10}^3\lvert 02\rangle,$
$\lvert e_{11}\rangle = \xi_{11}^1\lvert 20\rangle + \xi_{11}^2\frac{\lvert\downarrow\uparrow\rangle - \lvert\uparrow\downarrow\rangle}{\sqrt{2}} + \xi_{11}^3\lvert 02\rangle,$
$\lvert e_{12}\rangle = \tilde{\nu}_-\lvert\downarrow 2\rangle - \tilde{\nu}_+\lvert 2\downarrow\rangle,$
$\lvert e_{13}\rangle = \tilde{\nu}_-\lvert\uparrow 2\rangle - \tilde{\nu}_+\lvert 2\uparrow\rangle,$
$\lvert e_{14}\rangle = \tilde{\nu}_+\lvert\downarrow 2\rangle - \tilde{\nu}_-\lvert 2\downarrow\rangle,$
$\lvert e_{15}\rangle = \tilde{\nu}_+\lvert\uparrow 2\rangle - \tilde{\nu}_-\lvert 2\uparrow\rangle,$
$\lvert e_{16}\rangle = \lvert 22\rangle.$

should happen to coincide, these expressions must become ill-defined, because they constitute the components of the eigenvectors, which must be different even if the eigenvalues are the same. Thus, one must be careful when analyzing cases possessing special symmetries, where such degeneracy may occur.

Similarly to the eigenvalues E_i, the coefficients ξ_i^a simplify tremendously in some special cases, in particular

$$\begin{aligned}
\lim_{t\to 0}\left(\xi_9^1,\xi_9^2,\xi_9^3\right) &= (0,0,\pm 1),\\
\lim_{t\to 0}\left(\xi_{10}^1,\xi_{10}^2,\xi_{10}^3\right) &= (0,\pm 1,0),\\
\lim_{t\to 0}\left(\xi_{11}^1,\xi_{11}^2,\xi_{11}^3\right) &= (\pm 1,0,0),\\
\lim_{\delta\to 0}\left(\xi_9^1,\xi_9^2,\xi_9^3\right) &= (-1,0,1)/\sqrt{2},\\
\lim_{\delta\to 0}\left(\xi_{10}^1,\xi_{10}^2,\xi_{10}^3\right) &= \left(1,-\sqrt{2},1\right)/2,\\
\lim_{\delta\to 0}\left(\xi_{11}^1,\xi_{11}^2,\xi_{11}^3\right) &= \left(1,+\sqrt{2},1\right)/2.
\end{aligned}$$

Note, that for $t = 0$ the eigenstates correspond to states of definite occupation. The signs may vary depending on model parameters.

3 The exchange field

Ferromagnets (Fs) are modeled very simply, neglecting the Stoner splitting and the dependence of density of states and hoppings on energy (for energies smaller than the cutoff $\pm W$, with 0 at the Fermi energy). The ferromagnetism is then taken into account via spin-dependent coupling between Fs and DQD. In the linear response regime, these assumptions allow for showing that two parallely magnetized leads are equivalent by the unitary transformation [20] to the one effective lead F. Denoting by $a_{r\omega\sigma}$ annihilation operator of an electron of energy ω and spin σ in left ($r = L$) or right ($r = R$) ferromagnet, normalized such that the anti-commutator $\{a_{r\omega\sigma}, a^\dagger_{r'\omega'\sigma'}\} = \delta_{rr'}\delta_{\sigma\sigma'}\delta(\omega-\omega')$, the transformation reads the introduction of new operators,

$$c_{\omega\sigma} = u_\sigma a_{L\omega\sigma} + v_\sigma a_{R\omega\sigma}, \tag{8}$$
$$f_{\omega\sigma} = -v_\sigma a_{L\omega\sigma} + u_\sigma a_{R\omega\sigma}, \tag{9}$$

where $u_\sigma = \sqrt{\Gamma_{L\sigma}/(\Gamma_{L\sigma}+\Gamma_{R\sigma})}$ and $v_\sigma = \sqrt{1-u_\sigma^2}$. Then, both new operators fulfill the fermionic anticommutation relations. Moreover, f-operators do not appear in the tunnelling term of the Hamiltonian and can be omitted. On the other hand, c-operators' coupling is $\Gamma_\sigma = \Gamma_{L\sigma} + \Gamma_{R\sigma}$.

In order to treat the coupling between DQD and F with a perturbation theory, we write the Hamiltonian as $H = H_0 + H_I$, with

$$H_0 = H_{\mathrm{DQD}} + \sum_\sigma \int_{-W}^{W} \omega c^\dagger_{\omega\sigma} c_{\omega\sigma} d\omega\,, \tag{10}$$

$$H_I = \sum_\sigma \int_{-W}^{W} \sqrt{\frac{\Gamma_\sigma}{\pi}}\left(d^\dagger_{1\sigma} c_{\omega\sigma} + h.c.\right) d\omega. \tag{11}$$

The coupling can be expressed as $\Gamma_\sigma = (1+p\sigma)\Gamma$, where p denotes the spin polarization of F. Denoting by $\lvert e_i^*\rangle$ the state of the system, in which DQD is in the state $\lvert e_i\rangle$ and the effective F is in its ground state (all single-electron levels below the Fermi surface are occupied, all above are empty), one can write the zero-temperature expression for the shift of the energy level E_i in the second order in H_I,

$$\delta E_i = \sum_{\psi\neq e_i^*} \langle e_i^*|H_I|\psi\rangle \frac{1}{E_i - E_\psi}\langle\psi|H_I|e_i^*\rangle, \tag{12}$$

where $\lvert\psi\rangle$ runs through all of the intermediate states in the basis $\lvert e_i^*\rangle$. Note that if the intermediate states had been taken from the basis $\lvert\chi_1\chi_2\rangle$, their unperturbed energy E_ψ would not have been defined and the operator $(E_i - H_0)^{-1}(1 - \lvert e_i^*\rangle\langle e_i^*\rvert)$ would have to be considered instead of the sum over intermediate states in equation (12).

Since H_I allows only single hops, all the possible intermediate states are of the form $c^{(\dagger)}_{\omega\sigma}\lvert e_j^*\rangle$, with the energy $E_\psi = E_i + [\pm\omega + (E_j - E_i)]$. This results in the shift,

$$\delta E_i = \sum_{j\sigma}\frac{\Gamma_\sigma}{\pi}\left\{|\langle e_j|d^\dagger_{1\sigma}|e_i\rangle|^2\int_{-W}^{W}\frac{1-\theta(\omega)}{\omega-(E_j-E_i)}d\omega - |\langle e_j|d_{1\sigma}|e_i\rangle|^2\int_{-W}^{W}\frac{\theta(\omega)}{\omega+(E_j-E_i)}d\omega\right\}. \tag{13}$$

Notice that δE_i is linear in Γ and contains two parts: one independent of p, and one linear in p. Let the exchange field in the state $\lvert e_i\rangle$ be denoted $\Delta\varepsilon_i^{\mathrm{ex}}$ and defined as the

latter of those, normalized by the z-component of the spin of $|e_i\rangle$, i.e. $\delta E_i = \delta E_i|_{p=0} + S_z \Delta\varepsilon_i^{\mathrm{ex}}$, if only $S_z \neq 0$. For $S_z = 0$, the modules of respective matrix elements of $d_{1\sigma}^{(\dagger)}$ do not depend on spin direction, nor do the energies of all states, thus, the terms corresponding to different σ cancel out and the exchange field is 0. Extracting the part proportional to p and performing elementary integrals, one obtains the general, exact expression for the exchange field,

$$\Delta\varepsilon_i^{\mathrm{ex}} = \sum_{j\sigma} \frac{\sigma p \Gamma}{\pi S_z} \log\left|\frac{E_j - E_i}{W + (E_j - E_i)}\right| \times \left(|\langle e_j|d_{1\sigma}^{\dagger}|e_i\rangle|^2 + |\langle e_j|d_{1\sigma}|e_i\rangle|^2\right). \quad (14)$$

S_Z was introduced to the definition of the exchange field to make the clear correspondence between $\Delta\varepsilon^{\mathrm{ex}}$ and the effective magnetic field $B = \Delta\varepsilon^{\mathrm{ex}}/(g\mu_B)$, which would cause the same splitting of the multiplets.

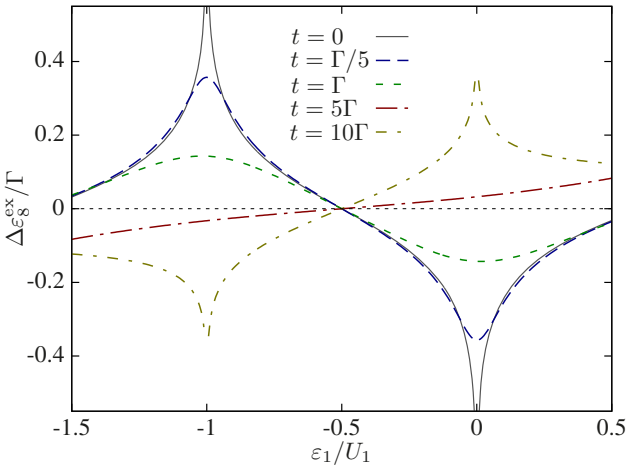

Fig. 2. The dependence of the exchange field in the spin-up triplet component $|e_8\rangle$ on QD1 level position, for finite $U_1 = W/2 = 5\Gamma$, $p = 0.4$, $U_2 = \varepsilon_2 = 0$ and different t.

4 Results

In Section 4.1 it is shown, how the exchange field obtained for a single QD is affected by the presence of QD2. Then, in Section 4.2 the exchange fields in different states are compared and their influence on the ground state of the DQD subsystem is analyzed. The signature of the exchange field in the conductance of the system is discussed in Section 4.3. Finally, in Section 4.4, the limitations of the considered method are examined.

4.1 The role of inter-dot interaction

Setting $t = 0$ and $U_2 = \varepsilon_2 = 0$, one practically obtains a single QD coupled to the ferromagnet, plus a free orbital of zero energy. For $t = 0$ the basis states $|e_i\rangle$ coincide with states $|\chi_1\chi_2\rangle$, except for $|e_7\rangle$ and $|e_8\rangle$, where, respectively, the sum and the difference of two such states occurs. For any of basis state $|e_i\rangle$ having the form $|\sigma\chi_2\rangle$, the result (14) simplifies to

$$S_z \Delta\varepsilon_{|\sigma\chi_2\rangle}^{\mathrm{ex}} = \frac{\sigma p \Gamma}{\pi} \log\left|\frac{\varepsilon_1}{\varepsilon_1 + U_1} \cdot \frac{W + (\varepsilon_1 + U_1)}{W - \varepsilon_1}\right|, \quad (15)$$

which has a nice limit for $W \to \infty$, namely

$$S_z \Delta\varepsilon_{|\sigma\chi_2\rangle}^{\mathrm{ex}} \underset{W\to\infty}{\longrightarrow} \frac{\sigma p \Gamma}{\pi} \log\left|\frac{\varepsilon_1}{\varepsilon_1 + U_1}\right|. \quad (16)$$

This is the result obtained by Martinek et al. in reference [4] for a single quantum dot coupled to a ferromagnetic lead.

Note, that $U_1 = 0$ implies $\Delta\varepsilon^{\mathrm{ex}} = 0$, also for finite W. This is caused by the fact, that particle-like and hole-like processes cancel each other. The exchange field diverges for resonant positions of the dot's level and vanishes in the particle-hole symmetric point (cf. Fig. 2), solid line. Notice, that in general also $\Delta\varepsilon^{\mathrm{ex}}$ may become divergent in the limit $W \to \infty$. For this reason that limit was avoided and W of the order of the highest relevant energy scale was used, as suggested by the scaling theory [2].

In Figure 2, it is shown how the result from equation (16) changes, when t becomes nonzero (for both dots occupied with a single spin-up electron each). It is clearly seen, that the divergences at the resonances are then removed and the peaks diminish, eventually the exchange field changes sign for really strong t. In the particle-hole symmetric point, $\varepsilon_1 = -U_1/2$, $\Delta\varepsilon_8^{\mathrm{ex}} = 0$ for all t.

Finally, in Figure 3, the density plots of a dependence of the exchange field in the triplet state on both dots' energy levels are presented, for different values of t, in the case of equal Coulomb interactions on both dots. In Figure 3a, one can clearly see, that for $t = 0$ the results are qualitatively equivalent to those obtained in Figure 2, where only QD1 was interacting. In agreement with intuition, ε_2 plays no role in such a situation. However, with increasing t, the importance of the QD2 level position becomes clear (cf. Fig. 3b). Further increase of t causes the peaks of $\Delta\varepsilon^{\mathrm{ex}}$ to change their positions (see Figs. 3c–3e), such that for $t = 10\Gamma$ the sign of the exchange field is at most of the dots' level positions opposite to the one for $t = 0$ (see Fig. 3f). After another significant changes of peaks positions while increasing t even further (cf. Figs. 3g and 3h), the exchange field starts to diminish for $t = 20\Gamma$ (see Fig. 3i), to vanish completely in the limit $t \to \infty$. Actually, the fact that $\Delta\varepsilon_i^{\mathrm{ex}} \to 0$ for $t \to \infty$ is rigorously true for all the molecular states and can be proven as follows.

At first, note, that all the matrix elements of $d_{\alpha\sigma}^{(\dagger)}$ in the eigenbasis have finite limits. On the contrary, all the energies of states with $S = 1/2$ asymptotically equal $\pm t$. E_8 and E_9 asymptotically equal $\pm 2t$, the other energies have finite, nonzero limits for $t \to \infty$. In equation (14) energies are present under the logarithm, always as differences. The logarithm containing energy difference $(E_j - E_i)$ has nonzero coefficient only for such pairs (i, j), that some of

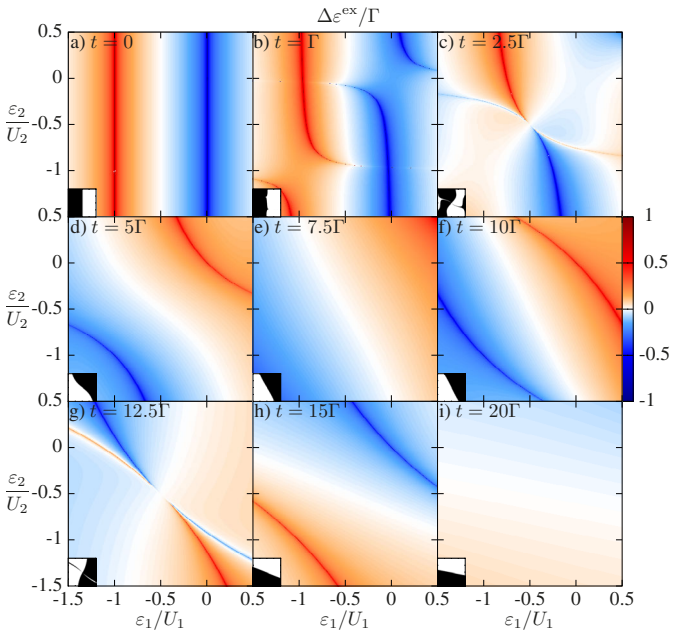

Fig. 3. The dependence of the exchange field in the spin-up triplet component $\Delta\varepsilon_8^{\rm ex}$ on the level positions of both dots for $U_1 = U_2 = W/2 = 5\Gamma$, $p = 0.4$ and different t, as indicated in the figure. Insets in the bottom left corners indicate the range of positive (negative) data in black (white), for readability of the plots in the gray-scale.

$\langle e_i|d^{(\dagger)}_{\alpha\sigma}|e_j\rangle$ is nonzero. As can be easily checked case by case, all the important energy differences diverge in the limit $t \to \infty$, so the corresponding logarithms vanish (cf., Eq. (14)). This means, that for very large t, the eigenstates of DQD are too far from each other (in the sense of energy difference) to allow significant charge fluctuations.

4.2 The exchange field for different states

In the case of a single quantum dot coupled to F, the exchange field is either zero (for states of $S_z = 0$), or given by equation (16). This means that it influences the energy spectrum of the dot identically to the magnetic field $B = \Delta\varepsilon^{\rm ex}/(g\mu_B)$. It is not exactly the case for DQD. Here, the corresponding magnetic field must be different for different states. However, the multiplet structure of the eigenbasis is preserved. This is illustrated in Figure 4. If the corresponding magnetic field were the same in all the states, all the curves in Figure 4 would coincide. Instead, the peaks appear at different positions for different curves. In the range of small negative values of ε_1, $\Delta\varepsilon_i^{\rm ex}$ even changes the sign, depending on i.

Even more interesting result is obtained, when one analyzes the ground state of the DQD subsystem with correction coming form the exchange field. Having defined the ground state energy as $E_{\rm GS} \equiv \min_i E_i$ (for a fixed set of model parameters), the unperturbed excitation energies $E_i - E_{\rm GS}$ are plotted as functions of QD1 level position in Figure 5a, and the excitation energies corrected by the exchange field, $E_i + S_z\Delta\varepsilon_i^{\rm ex} - E_{\rm GS}$, are shown in

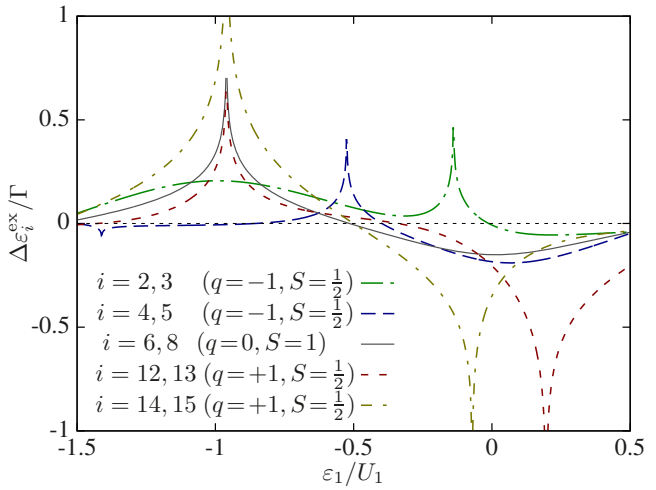

Fig. 4. The dependence of the exchange field on the QD1 level position, for $U_1 = U_2 = W/2 = 5\Gamma$, $p = 0.4$, $\varepsilon_2 = 0$ and $t = \Gamma$. In the states not listed in the legend, $\Delta\varepsilon_i^{\rm ex} = 0$.

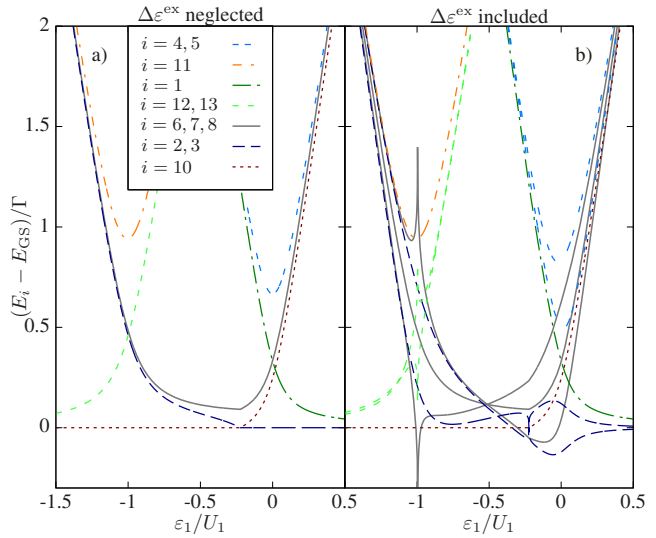

Fig. 5. (a) The difference between E_i and the ground state energy $E_{\rm GS}$ vs. ε_1, for $U_1 = U_2 = W/2 = 5\Gamma$, $p = 0.4$, $\varepsilon_2 = 0$ and $t = \Gamma/3$. (b) The same for $E_i + S_z\Delta\varepsilon_i^{\rm ex}$ instead of E_i, with $E_{\rm GS}$ still obtained without $\Delta\varepsilon_i^{\rm ex}$.

Figure 5b. It is visible, that in the Coulomb blockade regime, the ground state of isolated DQD is either the singlet state $|e_{10}\rangle$, or degenerate doublet, $|e_2\rangle, |e_3\rangle$. The triplet $|e_6\rangle, |e_7\rangle, |e_8\rangle$ is a low-lying excited state. However, when DQD is coupled to F, due to strong renormalization by the exchange field, the state $|e_6\rangle$ becomes the ground state for $\varepsilon_1 \approx -U_1$, while in very narrow region around $\varepsilon_1 \approx -0.25U_1$, $|e_8\rangle$ is the ground state. Moreover, $|e_6\rangle$ becomes degenerate with a singlet state $|e_{10}\rangle$ in the vicinity of $\varepsilon_1 = -U_1$. Because these two states differ in S_z by unity and have the same charge, they are degenerate states connected by a single spin-flip process, and as so, they can contribute to the formation of the single-stage Kondo effect. The second stage, when the singlet is non-degenerate ground state of DQD, is suppressed. Thus, the

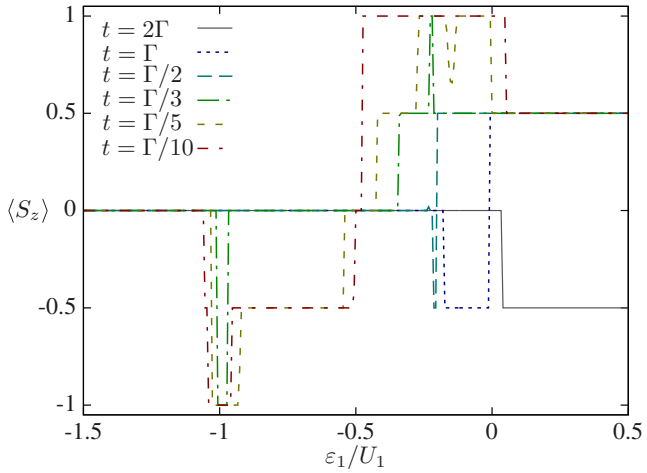

Fig. 6. The average value of z-component of DQD spin for $T = 10^{-4}\Gamma$, different t and other parameters the same as in Figure 5.

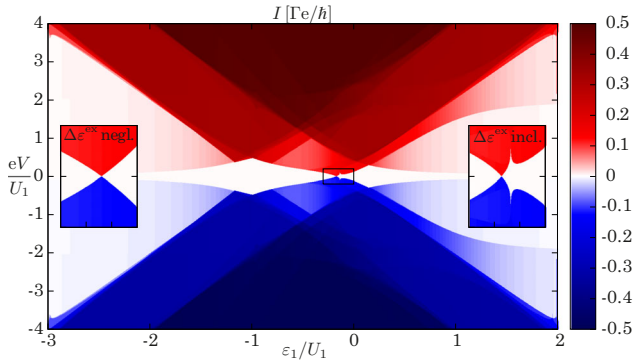

Fig. 7. The current through DQD for $T = 10^{-4}\Gamma$, $t = \Gamma$ and other parameters the same as in Figure 5, obtained with DQD eigenstates energies corrected by the exchange field. Right inset shows enlarged region $\varepsilon_1 \in [-0.3, 0]U_1$, $eV \in [-0.2, 0.2]U_1$, marked also with a rectangle in the main plot. The left inset shows the same region as the right one, but with the exchange field neglected.

large exchange field in triplet state is the condition for the two-stage Kondo effect to be suppressed. This is indeed confirmed by the numerical renormalization group calculations [18].

Knowing energies of DQD states, corrected by $\Delta\varepsilon^{ex}$, one can calculate expectation values of different operators, assuming equilibrium probabilities for eigenstates. Here, the z component of DQD spin is considered (see Fig. 6). Small finite temperature, $T = 10^{-4}\Gamma$, was used to make the curves smoother in the regions of degenerated ground state. For weak t, see curve for $t = \Gamma/10$, $\langle S_z \rangle \neq 0$ in the region of Coulomb blockade. It is negative $(-1/2)$ for negative detuning, and reaches $+1$ for positive detuning. However, it vanishes in the small region around particle-hole symmetric point. For $\varepsilon_1 \approx -U_1$ the triplet component becomes the ground state, resulting in $\langle S_z \rangle = -1$. For large, positive detunings, $\langle S_z \rangle = +1/2$. On the contrary to the case of small t, for $t = 2\Gamma$, $\langle S_z \rangle = 0$ for most of QD1 level positions. Only when $\varepsilon_1 > 0$, the average spin becomes $-1/2$, which is opposite to what happens for $t = \Gamma/10$. This is caused by the fact, that $\Delta\varepsilon^{ex}$ can change the sign with increasing t; compare Figure 2. For intermediate values of the inter-dot coupling, $\Gamma/5 < t < \Gamma$, the region of $\langle S_z \rangle = 0$ in the center of Coulomb valley becomes larger upon increasing t, and the region of $\langle S_z \rangle = +1/2$ appears for ε_1 slightly larger than $-U_1/2$. Moreover, for $\varepsilon_1 \approx -0.25U_1$ the t-dependence of $\langle S_z \rangle$ becomes highly nontrivial. For $t = \Gamma/5$, there occurs a dip, suggesting degeneracy between states of $S_z = 1$ and $S_z = 1/2$. For $t = \Gamma/3$, the $S_z = 1$ state is the ground state only in very narrow region of ε_1 (see also Fig. 5). For $t = \Gamma/2$, one sees a sharp dip, reaching $\langle S_z \rangle = -1/2$, instead of peak reaching $\langle S_z \rangle = 1$, present for $t = \Gamma/3$. This dip is significantly wider for $t = \Gamma$. Nevertheless, even in this case, for $\varepsilon_1 > 0$, $\langle S_z \rangle = +1/2$, contrary to the case of $t = 2\Gamma$. The fact that large range of $\langle S_z \rangle$ values is possible in the region $-0.25U_1 < \varepsilon_1 < 0$ corresponds to large variety of values of $\Delta\varepsilon^{ex}$ for different states, visible in Figure 4 for the case of $t = \Gamma$. In particular, note that $\Delta\varepsilon^{ex}$ can have different sign for different multiplets, thus, states possessing different sign of $\langle S_z \rangle$ may become the ground state.

4.3 The I-V characteristics

The exchange field influences not only the static properties, such as the magnetization of DQD presented in Figure 6. As claimed earlier, also the conductance exhibits its signatures. To present this, the current through the system was calculated using master equation method [21,22], with tunneling rates given by the Fermi golden rule. Moreover, in this subsection we use two leads, with $\Gamma_{r\sigma} = (1 + \sigma p)\Gamma/2$, because the transformation given by equations (8) and (9) does not decouple f operators outside the equilibrium. The results, presented in Figure 7, are valid only in the sequential tunneling regime, since any higher terms are neglected. However, the influence of the exchange field on the I-V characteristics near the resonance is clearly visible.

In general, one can see large regions of approximately constant current. Each such region corresponds to a fixed set of many-body DQD states, whose energy differences fit in the energy window of a voltage bias. The whole plot resembles a bit a structure characteristic of single interacting QD. However, the inter-dot interaction t causes the edges of fixed-current regions to band, and the increased number of states reflects itself in the splitting of just a few regions present in the single-QD case. The fact that the plot is not symmetric with respect to $\varepsilon_1 = -U_1/2$ comes from the lack of particle-hole symmetry in QD2, since $\varepsilon_2 = 0 \neq -U_2/2$ was assumed. All these features, visible in Figure 7, are valid also when one neglects the existence of $\Delta\varepsilon^{ex}$.

The effects of $\Delta\varepsilon^{ex} \neq 0$ are explicitly shown in the insets. The right one shows the enlargement of the region $-0.3U_1 < \varepsilon_1 < 0$, $|V| < 0.2U_1/e$. The left one – the results obtained in the same region by neglecting $\Delta\varepsilon^{ex}$.

Note, that according to Figure 5, in this region the ground state becomes magnetic due to the exchange field. The result is clearly visible: the lack of degeneracy leads to the splitting of the X-like structure, which resembles the effect of external magnetic field (here magnetic field is absent).

4.4 Limitations of the method

The considerations in this paper rely on the perturbative expansion in Γ. For transport properties, this is very strong assumption, which limits the range of validity of the results obtained in Section 4.3. One can expect the best accuracy in the sequential tunneling regime, worse in the co-tunneling regime, and completely false in the Kondo regime. However, the inter-dot interaction t was treated exactly, so the interference effects between different conduction paths, containing arbitrary number of hops of an electron between the dots are properly taken into account.

On the other hand, the renormalization of levels caused by the interaction with magnetically polarized bath obtained with second order perturbation theory proved to be in a good agreement with more sophisticated methods, in particular with numerical renormalization group calculations, for different systems and also in the strong coupling regime [7,14]. For this reason, one can hope that they can be quite generally valid in the linear response regime. Nevertheless, higher order terms may play an important role for particle-hole symmetric point, where $\Delta\varepsilon^{\mathrm{ex}} = 0$. For QDs possessing large-spin ground state, they give rise to formation of the effective magnetic quadrupolar field, not vanishing at the symmetric point [23].

Moreover, an important note can be done, if one considers the case $U_2 = 0$. Then, one can propose a definition of the exchange field induced on QD2 by both F and QD1 (as opposed to the exchange field for molecular states defined earlier). This is done as follows. Since the only nonquadratic terms in the Hamiltonian are related to the Coulomb interactions, the subsystem containing F and QD1 can now be diagonalized exactly. The whole model is then equivalent to the Anderson impurity (corresponding to QD2) coupled to the lead possessing Lorentzian density of states (corresponding to the diagonalized subsystem containing F and QD1) [24]. Then, treating t perturbatively to the second order and defining $\Delta\varepsilon^{\mathrm{ex}}_{\mathrm{QD2}}$ to be the difference between the shifts of different spins for the singly occupied QD2, we obtain [14]

$$\begin{aligned}\Delta\varepsilon^{\mathrm{ex}}_{\mathrm{QD2}} = &\sum_{\sigma}\sigma\frac{t^2}{2}\left[L_{U_2+\tilde{\delta}}(\Gamma_\sigma) - L_{-\tilde{\delta}}(\Gamma_\sigma)\right]\\ &-\sum_{\sigma}\sigma\frac{t^2}{\pi}\arctan\left(\frac{\varepsilon_{-1}}{\Gamma_\sigma}\right)\\ &\times\left[L_{U_2+\tilde{\delta}}(\Gamma_\sigma) + L_{-\tilde{\delta}}(\Gamma_\sigma)\right]\\ &-\sum_{\sigma}\sigma\frac{t^2}{2\pi}L_{\Gamma_\sigma}\left(U_2+\tilde{\delta}\right)\log\frac{(\varepsilon_2+U_2)^2}{\varepsilon_1^2+\Gamma_\sigma^2}\\ &+\sum_{\sigma}\sigma\frac{t^2}{2\pi}L_{\Gamma_\sigma}\left(-\tilde{\delta}\right)\log\frac{\varepsilon_2^2}{\varepsilon_1^2+\Gamma_\sigma^2},\end{aligned}\tag{17}$$

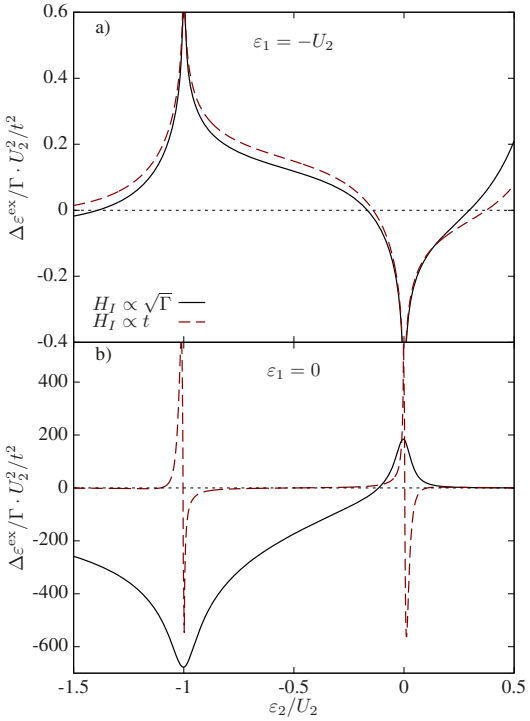

Fig. 8. The dependence of the exchange field on QD2 level position calculated from equation (14) for the state $|e_{13}\rangle$ ($q = +1$, $S_z = +1/2$, solid line), and from equation (17) (dashed line), for $U_1 = 0$, $U_2 = W/2$, $t = \Gamma = W/100$, $p = 0.4$, and (a) $\varepsilon_1 = -U_2$, (b) $\varepsilon_1 = 0$.

where $L_y(x) = y/(x^2+y^2)$ and $\tilde{\delta} \equiv \varepsilon_2 - \varepsilon_1 = 2\delta - U_2/2$. Interestingly, $\Delta\varepsilon^{\mathrm{ex}}_{\mathrm{QD2}}$ does not vanish for $U_2 = 0$. This peculiarity changes if equation (17) is expanded in the power series in Γ. Then, zeroth order vanishes, and in the first order one obtains the result, in which $U_2 = 0$ implies $\Delta\varepsilon^{\mathrm{ex}}_{\mathrm{QD2}} = 0$.

The question if the result (17) can be reasonably compared with equation (14) is not trivial. First of all, while in equation (14) we treated t exactly and Γ perturbatively, it was the other way around in equation (17). Thus, if these two are to be correct simultaneously, both t and Γ must be small, when compared to U_2. This is, however, not the whole story yet. The even bigger problem is that equation (17) corresponds to the situation, in which QD2 is singly occupied, while the subsystem containing F and QD1 is in its ground state. The occupancy of QD1 in this ground state is not well defined for the general case. Thus, the reasonable comparison can be made only in the special cases. One of them is the case of large $|\varepsilon_1|$. Indeed, QD1 is practically doubly occupied for $\varepsilon_1 \ll -\Gamma$ and practically unoccupied for $\varepsilon_1 \gg \Gamma$. The comparison of $\Delta\varepsilon^{\mathrm{ex}}$ obtained in this case from equations (14) and (17) is presented in Figure 8a. The same comparison for $\varepsilon_1 = 0$ does not make sense, which is illustrated in Figure 8b. This demonstrates, that the validity of the results obtained in this paper is limited to the case of Γ weak enough for DQD occupation to be determined from H_{DQD} eigenenergies only. In particular, the spin-dependent Fano-like interference occurring

at extremely low temperatures is better described with the aid of formula (17) then by equation (14) [14].

5 Conclusions

In the present article we have defined and calculated the exchange field induced in the molecular states of a double quantum dot by the coupling to the ferromagnetic leads in the T-shaped configuration. It was shown that the exchange field is different in different molecular states, so it is not acting exactly like a real magnetic field. However, it acts very similarly, reversing the sign of the shift upon spin-reversal in the considered state.

The results for small t agree with well-known formula (16). However, the dependence on t for stronger inter-dot hopping is complex, and perturbative treatment of t would have to be performed to very high order to give results consistent with equation (14), in particular for the parameters used in Figure 3. Because changing t can change sign and magnitude of $\Delta\varepsilon^{\mathrm{ex}}$, it can be used to tune the exchange field as well as ε_1 or ε_2.

The validity of equation (14) is limited by the validity of perturbative treatment of Γ and by the assumption, that the molecular states are relevant for the physical situation of the interest. For the case of strong Γ and weak t, this is not the case.

The author thanks I. Weymann for fruitful discussions and P. Baláž for critical reading of the manuscript. Research was supported by the National Science Center in Poland through Project No. DEC-2013/10/E/ST3/00213.

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