

Spin-polarized transport through two quantum dots Interference and Coulomb correlation effects^{*}

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Electronic transport through two single-level quantum dots attached in parallel to ferromagnetic leads has been analyzed theoretically. The intra-dot Coulomb correlation was taken into account, while the inter-dot hopping and Coulomb repulsion have been neglected. The dots, however, may interact *via* the external leads when the off-diagonal elements of the coupling matrix do not vanish. Conductance and tunnel magnetoresistance associated with the magnetization rotation from antiparallel to parallel configurations are calculated by the non-equilibrium Green function technique. The relevant Green functions are derived from the appropriate equation of motion in the Hartree–Fock approximation. We focus on the interference effects due to nonzero off-diagonal elements of the coupling matrix.

Key words: *quantum dot; tunnel magnetoresistance; quantum interference*

1. Introduction

Owing to a recent progress in nanotechnology, it is now possible to attach quantum dots (QDs) to magnetic/nonmagnetic electrodes (leads) and investigate spin and charge transport through the dots. This, in turn, leads to a significant theoretical activity aimed at understanding details of electronic transport through single QDs as well as through the arrays of dots [1–8]. In this paper, we consider electronic transport through two QDs which are coupled in parallel to two external ferromagnetic leads. The inter-dot hopping and inter-dot Coulomb interaction are neglected, while the intra-dot electron correlations are taken into account. The two quantum dots interact with the ferromagnetic leads, and the corresponding interaction matrix includes both diagonal and off-diagonal elements. The latter are of particular interest here as they give rise to indirect interaction of the dots and lead to some interference effects.

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Transport characteristics of the system in the linear response regime are calculated using the Green function formalism [9–14]. Since the systems with Coulomb interaction cannot be treated exactly, we applied the Hartree–Fock decoupling scheme to calculate the higher order Green functions from the corresponding equations of motion. The average values of the occupation numbers (which enter the expressions for the Green functions) and the Green functions have been calculated self-consistently. In section 2, we briefly describe the model as well as the theoretical method. Numerical results and their discussion are presented in section 3, whereas summary and final conclusions – in section 4.

2. Model and method

We consider two single-level quantum dots attached to ferromagnetic leads with collinear (parallel or antiparallel) magnetic moments. The system is described by the Hamiltonian of the general form:

$$H = H_{\text{leads}} + H_{DQD} + H_{\text{tunnel}}$$

The first term, H_{leads} , describes the left (L) and right (R) electrodes in the non-interacting quasi-particle approximation:

$$H_{\text{leads}} = H_L + H_R \quad \text{with} \quad H_\alpha = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\alpha\sigma} \quad \text{for } \alpha = L, R \quad (\text{for } \alpha = L, R)$$

The second term describes the two quantum dots

$$H_{DQD} = \sum_{i\sigma} \varepsilon_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \sum_i U_i n_{i\sigma} n_{i\bar{\sigma}}$$

where $\varepsilon_{i\sigma}$ is the energy of the i th dot bare level, $n_{i\sigma} \equiv d_{i\sigma}^\dagger d_{i\sigma}$ is the particle number operator, and U_i denotes the corresponding Coulomb integral. The last term of the Hamiltonian, H_{tunnel} , describes electron tunneling from the leads to dots (and *vice versa*)

$$H_{\text{tunnel}} = \sum_{\mathbf{k}\alpha} \sum_{i\sigma} V_{i\mathbf{k}\sigma}^\alpha c_{\mathbf{k}\alpha\sigma}^\dagger d_{i\sigma} + \text{h.c.}$$

where $V_{i\mathbf{k}\sigma}^\alpha$ are the relevant matrix elements. Coupling of the dots to external leads can be parameterized in terms of

$$\Gamma_{ij\sigma}^\alpha(\varepsilon) = 2\pi \sum_{\mathbf{k}} V_{i\mathbf{k}\sigma}^\alpha V_{j\mathbf{k}\sigma}^{\alpha*} \delta(\varepsilon - \varepsilon_{\mathbf{k}\alpha\sigma})$$

We assume that the matrix elements $\Gamma_{ij\sigma}^\alpha(\varepsilon)$ are constant within the energy band, $\Gamma_{ij\sigma}^\alpha(\varepsilon) = \Gamma_{ij\sigma}^\alpha = \text{const}$ for $\varepsilon \in \langle -D, D \rangle$, and $\Gamma_{ij\sigma}^\alpha(\varepsilon) = 0$ otherwise (here $2D$ is the electron bandwidth).

When the matrix elements $V_{ik\sigma}^\alpha$ can be assumed real and constant, the coupling matrix Γ_σ^α can be written in the form,

$$\Gamma_\sigma^\alpha = \begin{pmatrix} \Gamma_{11\sigma}^\alpha & \sqrt{\Gamma_{11\sigma}^\alpha \Gamma_{22\sigma}^\alpha} \\ \sqrt{\Gamma_{11\sigma}^\alpha \Gamma_{22\sigma}^\alpha} & \Gamma_{22\sigma}^\alpha \end{pmatrix}$$

The above form of Γ_σ^α corresponds to the case of maximum off-diagonal elements. In a general case, however, the off-diagonal matrix elements can be significantly reduced in comparison to those given in the equation, or even can be totally suppressed due to complete destructive interference. To include these effects, we introduce a prefactor $q \in \langle 0, 1 \rangle$ in the off-diagonal matrix elements. Moreover, the off-diagonal elements can be complex in a general case. Here, however, we assume them real. Thus, in the parallel magnetic configuration one can write:

$$\begin{aligned} \Gamma_{11\sigma}^L &= \Gamma_0(1 \pm p_L), & \Gamma_{22\sigma}^L &= \alpha \Gamma_0(1 \pm p_L), & \Gamma_{12\sigma}^L &= \Gamma_{21\sigma}^L = q \Gamma_0 \sqrt{\alpha}(1 \pm p_L) \\ \Gamma_{11\sigma}^R &= \gamma \alpha \Gamma_0(1 \pm p_R), & \Gamma_{12\sigma}^R &= \Gamma_{21\sigma}^R = q \gamma \Gamma_0 \sqrt{\alpha}(1 \pm p_R), & \Gamma_{22\sigma}^R &= \gamma \Gamma_0(1 \pm p_R) \end{aligned}$$

for $\sigma = \uparrow$ (upper sign) and $\sigma = \downarrow$ (lower sign). Here, p_α is the polarization strength of the α -th lead, γ_0 is a constant, the factor α takes into account a difference in the coupling strengths of a given electrode to the two dots, whereas γ describes asymmetry in the coupling of the dots to the left and right leads. Similar formula can be written for antiparallel configuration.

Electric current J flowing through the system can be determined from the following formula [13, 14]:

$$\begin{aligned} J &= \sum_\sigma J_\sigma \\ &= \frac{ie}{2\hbar} \sum_\sigma \int \frac{d\varepsilon}{2\pi} \text{Tr} \left\{ [\Gamma_\sigma^L - \Gamma_\sigma^R] \mathbf{G}_\sigma^<(\varepsilon) + [f_L(\varepsilon) \Gamma_\sigma^L - f_R(\varepsilon) \Gamma_\sigma^R] [\mathbf{G}_\sigma^r(\varepsilon) - \mathbf{G}_\sigma^a(\varepsilon)] \right\}, \end{aligned}$$

where

$$f_\alpha(\varepsilon) = \left[\exp\left(\frac{\varepsilon - \mu_\alpha}{k_B T}\right) + 1 \right]^{-1}$$

is the Fermi–Dirac distribution function for the α -th lead, whereas $\mathbf{G}_\sigma^<(\varepsilon)$ and $\mathbf{G}_\sigma^{r(a)}(\varepsilon)$ are the Fourier transforms of the lesser and retarded (advanced) Green functions of the dots. To calculate the Green functions $\mathbf{G}_\sigma^{r(a)}(\varepsilon)$, we write the corresponding equation of motion and apply the Hartree–Fock decoupling scheme for higher order Green functions. In turn, the lesser Green function $G_{ij\sigma}^<(\varepsilon)$ has been calculated

from the corresponding equation of motion, with the higher order Green functions calculated on taking into account the Langreth theorem [14] and the Hartree–Fock decoupling scheme assumed when calculating $\mathbf{G}_\sigma^{r(a)}(\varepsilon)$. Details of the calculations will be presented elsewhere. We only note that these formulas include the expectation values $\langle n_{i\sigma} \rangle$, $\langle d_{i\bar{\sigma}}^\dagger c_{k\alpha\bar{\sigma}} \rangle$ and $\langle c_{k\alpha\sigma}^\dagger d_{i\bar{\sigma}} \rangle$, which can be determined taking into account the identities:

$$\langle n_{i\sigma} \rangle = -i \int \frac{d\varepsilon}{2\pi} G_{ii\sigma}^<(\varepsilon)$$

$$\langle d_{i\bar{\sigma}}^\dagger c_{k\alpha\bar{\sigma}} \rangle = -i \int \frac{d\varepsilon}{2\pi} \langle \langle c_{k\alpha\sigma} | d_{j\sigma}^\dagger \rangle \rangle^<$$

and a similar one for $\langle c_{k\alpha\sigma}^\dagger d_{i\bar{\sigma}} \rangle$. The averages $\langle n_{i\sigma} \rangle$, $\langle d_{i\bar{\sigma}}^\dagger c_{k\alpha\bar{\sigma}} \rangle$, $\langle c_{k\alpha\sigma}^\dagger d_{i\bar{\sigma}} \rangle$ and the Green functions have been determined self-consistently.

3. Numerical results

Using the formulas derived above, one can calculate numerically the current, conductance, and tunnel magnetoresistance. The latter quantity describes the change in the system resistance when magnetic configuration of the system varies from antiparallel to parallel, and is described quantitatively by the ratio $(R_{AP} - R_P)/R_P$, where R_{AP} and R_P are the resistances in the antiparallel and parallel magnetic configurations, respectively. In the following discussion, we assume spin degenerate and equal bare dot levels, $\varepsilon_i\sigma = \varepsilon_0$ (for $i = 1, 2$ and $\sigma = \uparrow, \downarrow$). We also assume the same spin polarization of both leads ($p_L = p_R = p = 0.4$), the same intra-dot Coulomb parameters for both dots ($U_1 = U_2 = U$), and left-right symmetry of the coupling ($\gamma = 1$). We also note that energy in this paper is measured in the units of γ_0 , and that the numerical results are valid for temperatures above the corresponding Kondo temperature.

Let us consider first the case of nonmagnetic electrodes and $U = 0$. Figure 1 shows the linear conductance (per spin) in function of the dots' level position, calculated for two different values of the parameter α and two limiting values of the parameter q . For $q = 1$ (maximum off-diagonal elements of $\mathbf{\Gamma}_\sigma^\alpha$) and $\alpha \neq 1$ (in our case $\alpha = 0.15$), the conductance has a dip when the bare dot levels cross the Fermi level of the leads. The dip is a consequence of destructive quantum interference of electron waves transmitted through the two effective levels of the DQD system, i.e. through the dot levels renormalized due to their interaction *via* the electrodes (owing to non-zero off-diagonal elements of the matrix $\mathbf{\Gamma}_\sigma^\alpha$). The dip, however, disappears when $\alpha = 1$, but the conductance maximum does not reach $2e^2/h$ as it does for the totally decoupled dots ($q = 0$ and $\alpha = 1$). It is also worth noting that the width of the peak for $q = 1$ and $\alpha = 1$ is

two times higher than that for totally decoupled dots, and is of the order of $4\gamma_0$. The dip also disappears when $q = 0$, independently of the value of the parameter α .

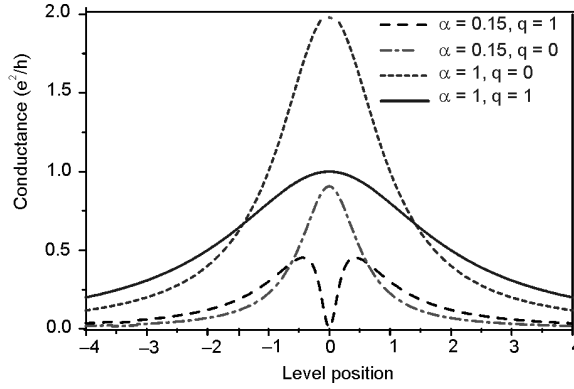


Fig. 1. Linear conductance per spin in function of the position of bare dot levels (ε_0), calculated for indicated values of the parameters α and q and for $p = 0$, $U = 0$ and $k_B T = 0.01$. The energy is measured in the units of Γ_0

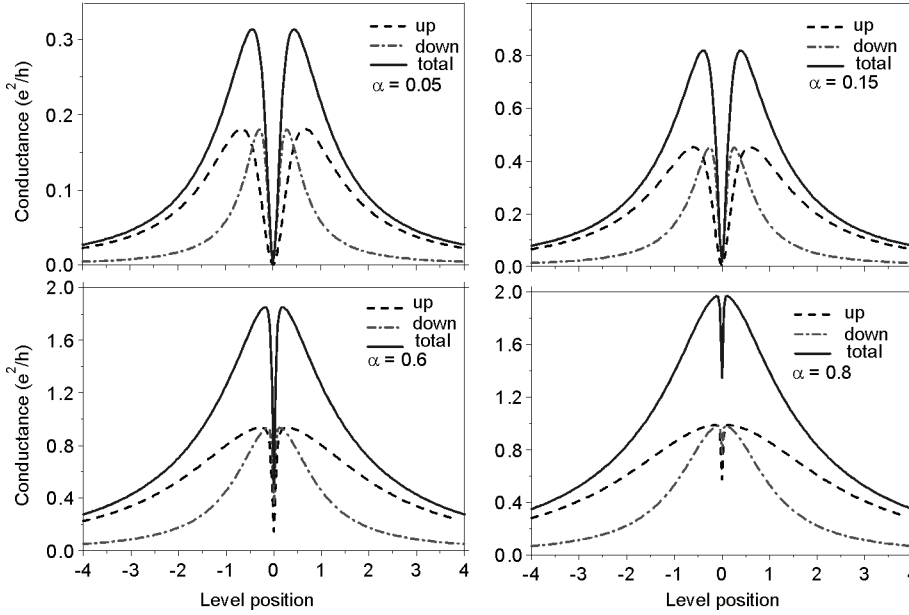


Fig. 2. Linear conductance for parallel magnetic configuration (total and for both spin channels) in function of the position of the dot levels (ε_0), calculated for indicated values of the parameter α and for $q = 1$, $p = 0.4$, $U = 0$, and $k_B T = 0.01$. The energy is measured in the units of Γ_0

In Figure 2, we show the linear conductance (total and for both spin channels) in the situation when the QDs are coupled to ferromagnetic leads, calculated for indicated values of the parameter α and for $q = 1$. The dip in the conductance emerges

when α departs from 1 ($\alpha < 1$), and increases with decreasing α . However, the conductance also decreases with decreasing α and disappears for $\alpha = 0$ (the dots are then coupled to one lead only and transport is suppressed). Thus, the conductance dip appears when there is an asymmetry in the coupling of a given electrode to the two dots, but only if the off-diagonal coupling elements are non-zero ($q > 0$).

Consider now the influence of the Coulomb interaction on the interference effects described above. First, the Coulomb interaction leads to splitting of the structure from Fig. 2. As a result, Coulomb counterparts of the spectra from Fig. 2 appear on their negative energy side, with characteristic gaps between the two parts of the spectra, as shown in Fig. 3. It is also worth to note that the Coulomb interaction generally breaks the symmetry of the spectra. Such symmetry is clearly seen in Fig. 2, but is absent in Fig. 3, particularly for α close to 1.

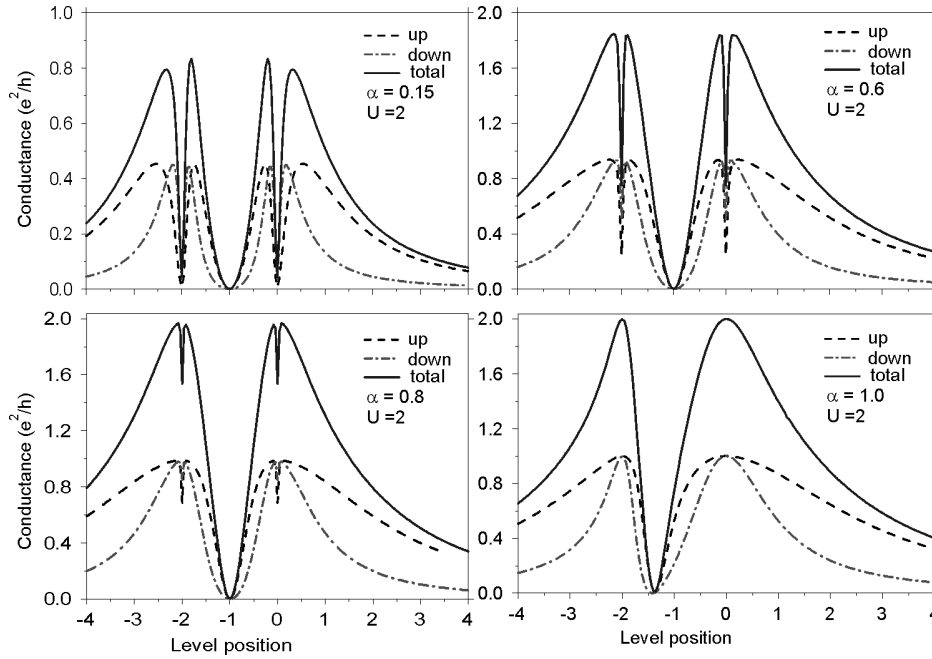


Fig. 3. Linear conductance for parallel magnetic configuration (total and for both spin channels) in function of the position of the dot levels (ε_0), calculated for indicated values of the parameters α and U , and for $q = 1$, $p = 0.4$, and $k_B T = 0.01$. The energy is measured in the units of Γ_0

The spectra shown in Fig. 3 are for a relatively large value of U ($U = 2$). The Coulomb counterparts are then well separated from the main spectra and the gap between them is well defined. The situation is more complex when the parameter U is smaller, as shown in Fig. 4. The four-peak structure is still present for $U = 0.6$, but only three peaks survive for $U = 0.2$ (see Fig. 4a).

Linear conductance in the parallel configuration is different from that in the anti-parallel one. This leads to a nonzero tunnel magnetoresistance (TMR), shown in Fig. 5

for indicated values of the Coulomb parameter U . When the dots' levels are well above or well below the Fermi level of the leads, TMR tends to the Julliere value,

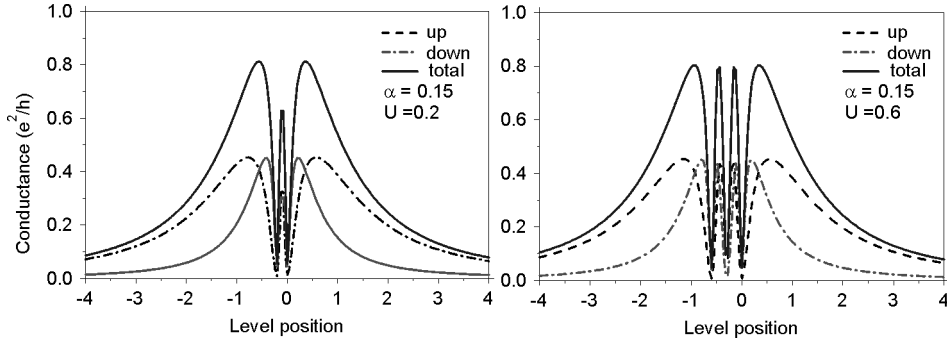


Fig. 4. Linear conductance for parallel magnetic configuration (total and for both spin channels) in function of the position of the dot levels (ε_0), calculated for indicated values of the parameters α and U , and for $q = 1$, $p = 0.4$, and $k_B T = 0.01$. The energy is measured in the units of Γ_0 .

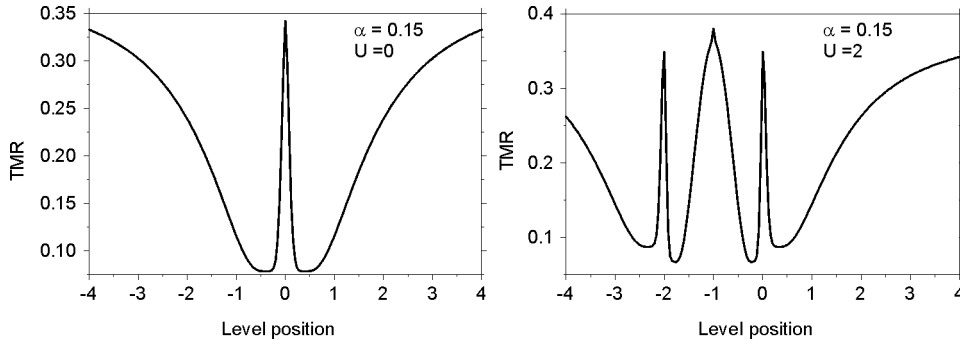


Fig. 5. TMR in the linear response regime in function of the level position (ε_0) calculated for indicated values of the parameter U , $p = 0.4$, $k_B T = 0.01$

$2p^2/(1-p)^2$, observed in planar magnetic junctions with the same ferromagnetic electrodes. When the dot levels approach the Fermi energy, the situation becomes more complex and TMR displays new features, as for instance some enhancement (peaks) and/or suppression (dips) seen in Fig.5. This is particularly seen for $U > 0$, where the number of peaks and dips in TMR is larger than for $U = 0$.

4. Summary and conclusions

We considered transport through two quantum dots attached in parallel to two ferromagnetic leads. The dots do not interact directly, however, they can interact indirectly *via* the leads provided the off-diagonal elements of the coupling matrix are nonzero. We have found a splitting in the conductance peak for $U = 0$, which is a result of

quantum interference. Apart from this, we have shown that including Coulomb correlations leads to splitting of the spectra and additional Coulomb counterparts to the main spectra appear, with characteristic Coulomb gaps between.

The influence of quantum interference and Coulomb correlation on TMR was also analyzed and we found some additional features of the magnetoresistance. These new features follow from the interplay of Coulomb interaction and quantum interference.

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