

# Interference and Coulomb correlation effects in spin-polarized transport through coupled quantum dots

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Spin-dependent transport through two coupled single-level quantum dots attached to ferromagnetic leads with collinear (parallel and antiparallel) magnetizations is analyzed theoretically. The intra-dot Coulomb correlation is taken into account, whereas the inter-dot Coulomb repulsion is neglected. Transport characteristics, including conductance and tunnel magnetoresistance associated with the magnetization rotation from parallel to antiparallel configurations, are calculated by the nonequilibrium Green function technique. The relevant Green functions are derived by the equation of motion method in the Hartree-Fock approximation. We have found a splitting of the Fano peak, induced by the intra-dot Coulomb interaction. Apart from this, the intra-dot electron correlations are shown to lead to an enhancement of the tunnel magnetoresistance effect.

Key words: *quantum dot; tunnel magnetoresistance; Fano effect*

## 1. Introduction

The Fano effect originates from quantum interference between resonant and non-resonant transmission processes [1]. The effect appears in experiments as an asymmetric line shape of the transmission spectra. Owing to a tunability of the parameters describing quantum dots (QDs), experimental investigation of the Fano effect in systems including QDs offers new possibilities, not accessible in traditional situations.

The Fano effect in electrical conductance occurs when the phase of electron wave in the non-resonant channel changes insignificantly within the energy  $\Gamma$  centred at the resonance level, where  $\Gamma$  stands for the discrete level width. The Fano line shape in various QD systems has been recently observed experimentally, and the experiments initiated extensive theoretical works on the coherent transport through coupled QDs

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[2–4]. However, in most theoretical works, the electron–electron interaction was neglected. Moreover, the considered situations were limited to transport through two quantum dots coupled either in series or in parallel to nonmagnetic electron reservoirs. The electron correlations in two QDs coupled in series to nonmagnetic leads have been taken into account in a recent paper [5]. As concerns transport through double quantum dots (DQDs) attached to magnetic leads, only a few papers have addressed this issue up to now [6–8].

In this paper we consider electronic transport through two QDs which are coupled to two ferromagnetic leads. The tunnel barrier between the dots is assumed to be magnetic, hence the inter-dot hopping parameter is spin dependent. The considerations are limited to QDs with vanishing inter-dot Coulomb interaction, while the intra-dot electron correlation is taken into account. Transport characteristics in the linear response regime are calculated using the Green function formalism [9–13]. Since the systems with Coulomb interaction usually cannot be treated exactly, we applied the Hartree–Fock approximation scheme to calculate the Green functions from the relevant equations of motion. The average values of the occupation numbers (which enter the expressions for the Green functions) have been calculated self-consistently.

## 2. Model and analytical solution

We consider two single-level quantum dots attached to ferromagnetic leads, and for simplicity we restrict our considerations to the case where magnetic moments of the leads are either parallel or antiparallel. The system is then described by Hamiltonian of the general form  $H = H_{\text{leads}} + H_{\text{DQD}} + H_{\text{tunnel}}$ . The term  $H_{\text{leads}}$  describes the left ( $L$ ) and right ( $R$ ) electrodes in the non-interacting quasi-particle approximation,  $H_{\text{leads}} = H_L + H_R$ , with  $H_\alpha = \sum_{k\sigma} \varepsilon_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma}$  (for  $\alpha = L, R$ ). Here,  $c_{k\alpha\sigma}^\dagger$  ( $c_{k\alpha\sigma}$ ) is the creation (annihilation) operator of an electron with the wave number  $k$  and spin  $\sigma$  in the lead  $\alpha$ , whereas  $\varepsilon_{k\alpha\sigma}$  denotes the corresponding single-particle energy.

The second term of the Hamiltonian describes the two coupled quantum dots:

$$H_{\text{DQD}} = \sum_{i\sigma} \varepsilon_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \sum_{\sigma} (t_\sigma d_{1\sigma}^\dagger d_{2\sigma} + h.c.) + \sum_i U_i n_{i\sigma} n_{i\bar{\sigma}} \quad (1)$$

where  $\varepsilon_{i\sigma}$  is the energy of an  $i$ th dot level,  $t_\sigma$  is the inter-dot hopping parameter, and  $n_{i\sigma} \equiv d_{i\sigma}^\dagger d_{i\sigma}$  is the particle number operator. Both  $t_\sigma$  and  $\varepsilon_{i\sigma}$  are assumed to be spin-dependent in a general case. The last term in Eq. (1) describes the intra-dot Coulomb interactions, with  $U_i$  ( $i = 1, 2$ ) denoting the corresponding Coulomb integrals.

The last term of the Hamiltonian,  $H_{\text{tunnel}}$ , describes electron tunneling from the leads to dots (and *vice versa*), and takes the form:

$$H_{\text{tunnel}} = \sum_{k\alpha} \sum_{i\sigma} (V_{ik\sigma}^\alpha c_{k\alpha\sigma}^\dagger d_{i\sigma} + h.c.) \quad (2)$$

where  $V_{ik\sigma}^\alpha$  is the relevant matrix element. Coupling of the dots to external leads can be parameterized in terms of  $\Gamma_{ij\sigma}^\alpha(\varepsilon) = 2\pi \sum_k V_{ik\sigma}^\alpha V_{jk\sigma}^{\alpha*} \delta(\varepsilon - \varepsilon_{k\alpha\sigma})$ . We assume that  $\Gamma_{ij\sigma}^\alpha(\varepsilon)$  is 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,  $2D$  denotes the electron band width in the electrodes.

Electric current  $J$  flowing through the system can be determined from the following standard formula [12, 13]:

$$J = \sum_\sigma J_\sigma = \frac{ie}{2\hbar} \sum_\sigma \int \frac{d\varepsilon}{2\pi} \text{Tr} \left\{ \left[ \Gamma_\sigma^L - \Gamma_\sigma^R \right] \mathbf{G}_\sigma^<(\varepsilon) + \left[ f_L(\varepsilon) \Gamma_\sigma^L - f_R(\varepsilon) \Gamma_\sigma^R \right] \left[ \mathbf{G}_\sigma^r(\varepsilon) - \mathbf{G}_\sigma^a(\varepsilon) \right] \right\} \quad (3)$$

where  $f_\alpha(\varepsilon) = [\exp\{(\varepsilon - \mu_\alpha)/k_B T\} + 1]^{-1}$  is the Fermi–Dirac distribution function in the lead  $\alpha$ ,  $\mathbf{G}_\sigma^<(\varepsilon)$  and  $\mathbf{G}_\sigma^{r(a)}(\varepsilon)$  are the Fourier transforms of the lesser and retarded (advanced) Green functions of the dots, and  $\Gamma_\sigma^\alpha$  describes coupling of the dots to the lead  $\alpha$  ( $\alpha = L, R$ ),

$$\Gamma_\sigma^\alpha = \begin{pmatrix} \Gamma_{11\sigma}^\alpha & \sqrt{\Gamma_{11\sigma}^\alpha \Gamma_{22\sigma}^\alpha} \\ \sqrt{\Gamma_{11\sigma}^\alpha \Gamma_{22\sigma}^\alpha} & \Gamma_{22\sigma}^\alpha \end{pmatrix} \quad (4)$$

In the parallel magnetic configuration one can write:

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

for  $\sigma = \uparrow$  (upper sign) and  $\sigma = \downarrow$  (lower sign). Here,  $p_\alpha$  is the polarization strength of the  $\alpha$ th lead,  $\Gamma_0$  is a constant, the parameter  $\beta$  takes into account the difference in the coupling strengths of a given electrode to the two dots, whereas  $\gamma$  describes asymmetry in the coupling of the dots to the left and right leads. For  $\beta = 0$  one finds DQDs connected in series.

To calculate the Green functions  $\mathbf{G}_\sigma^{r(a)}(\varepsilon)$ , we apply the method of equation of motion. First we write the equation of motion for the casual Green function

$$\begin{aligned} G_{ij\sigma}(\varepsilon) &\equiv \langle \langle d_{i\sigma} | d_{j\sigma}^+ \rangle \rangle \\ \varepsilon \langle \langle d_{i\sigma} | d_{j\sigma}^+ \rangle \rangle &= \langle \{ d_{i\sigma}, d_{j\sigma}^+ \} \rangle + \langle \langle [d_{i\sigma}, H] | d_{j\sigma}^+ \rangle \rangle \end{aligned} \quad (5)$$

where  $H$  denotes the full Hamiltonian of the system. Taking into account the explicit form of  $H$ , one arrives at the equation

$$(\varepsilon - \varepsilon_{i\sigma})\langle\langle d_{i\sigma} | d_{j\sigma}^+ \rangle\rangle = \delta_{ij} + \delta_{i1}t_\sigma\langle\langle d_{2\sigma} | d_{j\sigma}^+ \rangle\rangle + \delta_{i2}t_\sigma^*\langle\langle d_{1\sigma} | d_{j\sigma}^+ \rangle\rangle + \sum_{k\alpha} V_{ik\sigma}^{\alpha*}\langle\langle c_{k\alpha\sigma} | d_{j\sigma}^+ \rangle\rangle + U_i\langle\langle n_{i\bar{\sigma}}d_{i\sigma} | d_{j\sigma}^+ \rangle\rangle. \quad (6)$$

Applying equation of motion to the Green function  $\langle\langle c_{k\alpha\sigma} | d_{j\sigma}^+ \rangle\rangle$  one finds

$$\langle\langle c_{k\alpha\sigma} | d_{j\sigma}^+ \rangle\rangle = \frac{1}{\varepsilon - \varepsilon_{k\alpha\sigma}} \sum_{i'} V_{i'k\sigma}^\alpha \langle\langle d_{i'\sigma} | d_{j\sigma}^+ \rangle\rangle \quad (7)$$

Now, the Hartree–Fock approximation is applied to the higher-order Green function generated on the right hand side of Eq. (6):

$$\langle\langle n_{i\bar{\sigma}}d_{i\sigma} | d_{j\sigma}^+ \rangle\rangle \approx \langle n_{i\bar{\sigma}} \rangle \langle\langle d_{i\sigma} | d_{j\sigma}^+ \rangle\rangle \quad (8)$$

Applying the above decoupling procedure and introducing:

$$\Sigma_{ij\sigma} = \Sigma_{ij\sigma}^L + \Sigma_{ij\sigma}^R \quad (9)$$

where

$$\Sigma_{ij\sigma}^\alpha = \sum_k \frac{V_{ik\sigma}^\alpha V_{jk\sigma}^{\alpha*}}{\varepsilon - \varepsilon_{k\alpha\sigma}} \quad (10)$$

one can rewrite Eq.(6) in the form,

$$(\varepsilon - \varepsilon_{i\sigma} - U_i \langle n_{i\bar{\sigma}} \rangle) \langle\langle d_{i\sigma} | d_{j\sigma}^+ \rangle\rangle = \delta_{ij} + \delta_{i1}t_\sigma\langle\langle d_{2\sigma} | d_{j\sigma}^+ \rangle\rangle + \delta_{i2}t_\sigma^*\langle\langle d_{1\sigma} | d_{j\sigma}^+ \rangle\rangle + \sum_{i'} \Sigma_{i'i\sigma} \langle\langle d_{i'\sigma} | d_{j\sigma}^+ \rangle\rangle \quad (11)$$

Now, the set of equations is closed and the casual Green function can be calculated. Having found the casual Green function, one can calculate the retarded and advanced Green functions  $G_{ij\sigma}^{r(a)}(\varepsilon)$  as  $G_{ij\sigma}^{r(a)}(\varepsilon) = G_{ij\sigma}(\varepsilon \pm i0^+)$ . Writing the Green functions in the matrix form one arrives at the following formula:

$$\mathbf{G}_\sigma^{r(a)}(\varepsilon) = \frac{1}{\Omega_{r(a)\sigma}^2(\varepsilon)} \begin{pmatrix} \varepsilon - \varepsilon_{2\sigma} - \Sigma_{22\sigma}^{r(a)}(\varepsilon) - U_2 \langle n_{2\bar{\sigma}} \rangle & t_\sigma + \Sigma_{21\sigma}^{r(a)}(\varepsilon) \\ t_\sigma^* + \Sigma_{12\sigma}^{r(a)}(\varepsilon) & \varepsilon - \varepsilon_{1\sigma} - \Sigma_{11\sigma}^{r(a)}(\varepsilon) - U_1 \langle n_{1\bar{\sigma}} \rangle \end{pmatrix} \quad (12)$$

where  $\Omega_{r(a)\sigma}$  is defined as

$$\begin{aligned} \mathcal{Q}_{r(a)\sigma}^2(\varepsilon) = & (\varepsilon - \varepsilon_{1\sigma} - \Sigma_{11\sigma}^{r(a)} - U_1 \langle n_{1\bar{\sigma}} \rangle)(\varepsilon - \varepsilon_{2\sigma} - \Sigma_{22\sigma}^{r(a)} - U_2 \langle n_{2\bar{\sigma}} \rangle) \\ & - (t_\sigma + \Sigma_{21\sigma}^{r(a)})(t_\sigma^* + \Sigma_{12\sigma}^{r(a)}) \end{aligned} \quad (13)$$

In Equation (13), the energy dependence of the self energies  $\Sigma_{ij\sigma}^{r(a)}$  is not indicated explicitly for clarity reasons. The self-energies have the form:

$$\Sigma_{ij\sigma}^{r(a)}(\varepsilon) = A_{ij\sigma}(\varepsilon) \mp \frac{i}{2} \Gamma_{ij\sigma} \quad (14)$$

with

$$\Gamma_{ij\sigma} = \Gamma_{ij\sigma}^L + \Gamma_{ij\sigma}^R \quad (15)$$

and

$$A_{ij\sigma}(\varepsilon) = \frac{1}{2\pi} \Gamma_{ij\sigma} \ln \left( \frac{D - \varepsilon}{D + \varepsilon} \right) \quad (16)$$

The lesser Green function  $\mathbf{G}_\sigma^<(\varepsilon)$  can be derived from the Keldysh equation:

$$\mathbf{G}_\sigma^<(\varepsilon) = \mathbf{G}_\sigma^r(\varepsilon) \Sigma_\sigma^<(\varepsilon) \mathbf{G}_\sigma^a(\varepsilon) \quad (17)$$

In the zero bias (equilibrium) limit, the lesser self-energy  $\Sigma_\sigma^<(\varepsilon)$  is given by the expression:

$$\Sigma_\sigma^<(\varepsilon) = i[f_L(\varepsilon)\Gamma_\sigma^L + f_R(\varepsilon)\Gamma_\sigma^R]$$

Finally, the average values of the occupation numbers,  $\langle n_{i\sigma} \rangle$ , have to be calculated self-consistently using the formula

$$\langle n_{i\sigma} \rangle = -i \int \frac{d\varepsilon}{2\pi} G_{ii\sigma}^<(\varepsilon) \quad (18)$$

### 3. Numerical results

Using the formulas derived above, one can calculate numerically basic transport characteristics, like conductance and tunnel magnetoresistance. The latter quantity describes the change in the system resistance when magnetic configuration of the system varies from parallel to antiparallel, 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. For the following discussion, we assume that the dot levels are spin-degenerate and equal,  $\varepsilon_{i\sigma} = \varepsilon_0$  (for  $i = 1, 2$  and  $\sigma = \uparrow, \downarrow$ ). The inter-

dot hopping parameter is assumed to be real and independent of the spin orientation,  $t_\sigma = t = t^*$  (for  $\sigma = \uparrow, \downarrow$ ), and for numerical calculations we take  $t = 0.6$  (the energy in this paper is measured in the units of  $\Gamma_0$ ). We note that for positive  $t$ , the symmetric (anti-symmetric) state becomes anti-bonding (bonding) – the situation is reversed for negative  $t$ . Apart of this, we assume the same spin polarizations of the leads ( $p_L = p_R = p = 0.4$ ), different coupling of a given electrode to the two dots (described by the parameter  $\beta = 1/3$ ), and left-right symmetry of the coupling ( $\gamma = 1$ ). Finally, we assume the same intra-dot Coulomb parameters for both dots:  $U_1 = U_2 = U$ . We point that the numerical results shown in this paper are valid for temperatures above the corresponding Kondo temperature  $T_K$ .

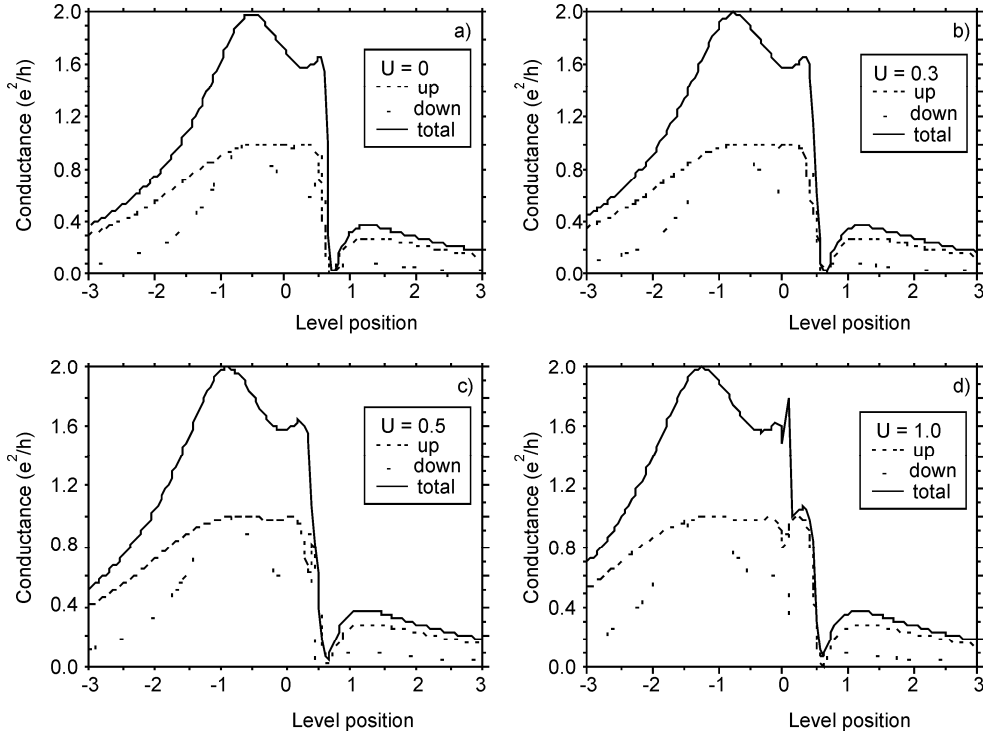


Fig. 1. Linear conductance in the parallel configuration as a function of the position of the dot levels ( $\varepsilon_0$ ), calculated for indicated values of the intra-dot Coulomb repulsion parameter  $U$  and for  $p = 0.4$ ,  $t = 0.6$ , and  $k_B T = 0.01161$ . The energy is measured in the units of  $\Gamma$

Let us consider first a noninteracting ( $U = 0$ ) case (see Fig. 1a). The inter-dot coupling lifts the level degeneracy. Consequently, the peak in the density of states becomes split into two components: a broad peak centred at the anti-bonding state and a narrow one corresponding to the bonding state [2, 8]. The conductance associated with the bonding state reveals the antiresonance behaviour with the characteristic Fano line shape clearly seen in Fig. 1a. In turn, the peak associated with the anti-

bonding state is relatively broad. As the asymmetry of the dot coupling to a given electrode is reduced, the width of the anti-bonding (bonding) resonance increases (decreases). Numerical results for  $\beta = 1$  (not presented in this paper) show that the resonance corresponding to the bonding state becomes  $\delta$ -like, while the resonance due to the anti-bonding state acquires the width  $\sim 4\Gamma_0$ . Since coupling of the dots to external leads is spin-dependent, the corresponding level widths depend on the spin orientation, too. This is the reason why the splitting for the down spin orientation is clearly seen, whereas the one for the spin-up orientation is not well resolved (there is rather an abrupt drop in the conductance for  $\varepsilon_0 \sim t$ ).

Let us discuss now the influence of intra-dot Coulomb repulsion on the picture described above (Fig. 1) for  $U > 0$ . One can note a splitting of the Fano resonance in the total conductance, which occurs for a sufficiently large Coulomb integral  $U$  (of the order or larger than the Fano-line width) and increases with increasing  $U$ . On the other hand, no such splitting can be seen for the anti-bonding peak. This is because the line width of the anti-bonding level (strongly coupled to the leads) is much larger than  $U$  assumed in Fig. 1. It is also worth noting that no splitting of the Fano peak occurs for a sufficiently small value of  $U$  (smaller than the Fano-line width).

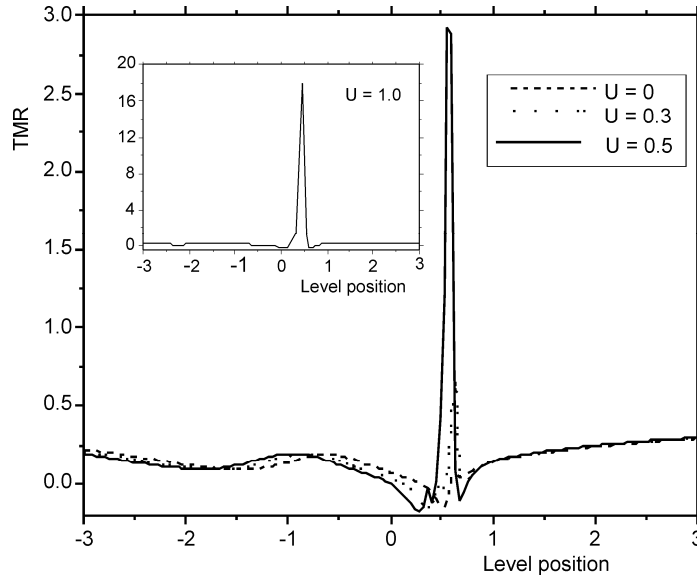


Fig. 2. TMR in the linear response regime as a function of the level position ( $\varepsilon_0$ ) calculated for indicated values of the intra-dot Coulomb parameter  $U$ , leads polarization  $p = 0.4$ , inter-dot coupling  $t = 0.6$ , and  $k_B T = 0.01161$

The splitting of the Fano antiresonance line, induced by the Coulomb correlation in the dots, is also visible in each spin contribution of the conductance, as clearly visible in Fig. 1 for  $U = 1$ . However, the conductance vanishes only for one component of the split Fano line, while the second component corresponds to a finite and

positive conductance. This behaviour gives rise to the splitting of the Fano line in the total conductance, observed in Fig. 1. The two components of the Fano resonance are well separated, and the separation is of the order of  $U$ . Positions of the two Fano resonances are approximately at  $\varepsilon_0 \sim t$  and  $\varepsilon_0 \sim (t-U)$ , as one could expect.

In Figure 2, we show TMR for indicated values of the Coulomb repulsion  $U$ . When the dot levels are well above or well below the Fermi level of the leads, TMR tends to the Julliere value,  $2p^2/(1-p^2)$ , 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 for  $\varepsilon_0 \sim t$ .

#### 4. Summary and conclusions

In this paper, we considered transport through two coupled quantum dots attached to ferromagnetic leads. We have found the Lorentzian line shape resonance associated with the anti-bonding state, and the Fano line shape resonance associated with the bonding state. The influence of the resonances on the tunnel magnetoresistance was also analyzed and we found some enhancement of the magnetoresistance due to the intra-dot Coulomb correlations. These results have been obtained in the Hartree-Fock approximation. However, we have also performed calculations using higher order decoupling schemes, in particular we have analyzed transport in the Kondo regime. The details will be presented elsewhere.

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