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Influence of external magnetic field on transport properties of a quantum dot attached to non-collinearly polarized magnetic electrodes

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Transport properties of a single level quantum dot attached to non-collinearly polarized magnetic leads and under the influence of external magnetic field have been analyzed theoretically. Description of the considered system has been modelled by the Anderson Hamiltonian with the finite Coulomb repulsion parameter. The analysis has been performed using the equation of motion method for the non-equilibrium Green function within the Hartree–Fock approximation. Numerical illustration of the transport properties such as differential conductance, tunnelling magnetoresistance and spin accumulation on the dot under influence of external magnetic field has been presented.

Key words: *quantum dot; Hartree–Fock approximation; spin accumulation; tunnelling magnetoresistance*

I. Introduction

Spin polarized transport through quantum dots attached to ferromagnetic leads has recently raised a great interest. It is not only because of possible area of studying new physical phenomena but also due to promising applications in spinelectronics or microelectronic devices as well as for storage and processing information.

In this paper, an interacting single level quantum dot has been studied. The dot is coupled symmetrically to external ferromagnetic electrodes whose magnetic moments are, in general, non-collinear and may be rotated independently [1–4], the dot being under the influence of an external magnetic field. The orientation of the magnetic moments of the electrodes and direction of the external magnetic field is such that they all are in a common plane.

Further considerations are focused on the bias dependence of the differential conductance, tunnel magnetoresistance effect (TMR) and spin accumulation under the

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influence of external magnetic field on the dot. Moreover, the dependences of TMR and spin accumulation on the angles between the spin moments of the leads is shown for a few values of the external magnetic field.

2. Model

The system under consideration is an interacting single-level quantum dot attached to ferromagnetic leads with non-collinear magnetizations. Degeneration of the discrete level of the dot is removed by an external magnetic field which is, in general, non-collinear with the magnetizations of the electrodes. The field and magnetizations, however, are in a common plane. The axis z of the reference frame is assumed to be along the field, whereas the net spin moments of the leads are in the xz plane and form the angles ϕ_R (right lead) and ϕ_L (left lead) with the z axis [1, 3].

The whole system is described by the Anderson-like Hamiltonian of a general form

$$H = \sum_{\alpha} H_{\alpha} + H_D + H_T \tag{1}$$

where H_α describes the electrodes

$$H_{\alpha} = \sum_{\mathbf{k}} \sum_{\beta=\pm} \varepsilon_{\alpha\mathbf{k}\beta}\, a^{+}_{\alpha\mathbf{k}\beta} a_{\alpha\mathbf{k}\beta}, \tag{2}$$

for $\alpha = L, R$ (left and right electrodes, respectively). Here, $\varepsilon_{\alpha\mathbf{k}\beta}$ is the energy of an electron with the wave vector $\mathbf{k}$ and spin $\beta = +$ (–) that refers to majority (minority) spins in the electrode α, whereas $a^{+}_{\alpha\mathbf{k}\beta}$ ($a_{\alpha\mathbf{k}\beta}$) stands for the creation (annihilation) operators. The single-particle energy $\varepsilon_{\alpha\mathbf{k}\beta}$ includes the electrostatic energy, $\varepsilon_{\alpha\mathbf{k}\beta} = \varepsilon^{0}{}_{\alpha\mathbf{k}\beta} + eU_e^{\alpha}$, where e ($e < 0$) stands for the electron charge, $\varepsilon^{0}_{\alpha\mathbf{k}\beta}$ is the single-particle energy for the unbiased system, whereas U_e^{α} is the electrostatic potential of the αth electrode. Electrostatic potentials $U_e^L = V_t/2$ and $U_e^R = -V_t/2$ are applied to the left and right electrodes, respectively with V_t as the transport voltage.

The dot is described by the Hamiltonian including the Coulomb interaction term

$$H_D = \sum_{\sigma} \varepsilon_d^{\sigma} c^{+}_{\sigma} c_{\sigma} + U n_{\uparrow} n_{\downarrow}, \tag{3}$$

where c^{+}_{σ}, c_{σ} are the creation and annihilation operators for spins $\sigma = \uparrow, \downarrow$, the arrows denote projection of the dot spin on the global quantization z axis, and ε_d^{σ} is the energy level of the dot for spin σ. The Coulomb repulsion parameter is denoted by U, whereas $n_{\sigma} = c^{+}_{\sigma} c_{\sigma}$ denotes the particle number operator. The Zeeman splitting of the dot level due to external magnetic field is $\Delta_Z = \varepsilon_d^{\uparrow} - \varepsilon_d^{\downarrow}$, where $\varepsilon_d^{\sigma} = \varepsilon_d \pm \Delta_Z/2$ is the energy level of the dot for spin σ.

Finally, the tunnelling term H_T in the Hamiltonian (1) has the form

$$H_T = \sum_{\alpha}\sum_{k}\left(\left(T_{\alpha k+}a^{+}_{\alpha k+}\cos\frac{\phi_\alpha}{2} - T_{\alpha k-}a^{+}_{\alpha k-}\sin\frac{\phi_\alpha}{2}\right)c_{\uparrow} + \left(T_{\alpha k+}a^{+}_{\alpha k+}\sin\frac{\phi_\alpha}{2} + T_{\alpha k-}a^{+}_{\alpha k-}\cos\frac{\phi_\alpha}{2}\}c_{\downarrow}\right)\right) + \text{h.c.} \tag{4}$$

where $T_{\alpha k\beta}$ stands for the appropriate tunneling matrix element.

3. Method

In order to calculate the quantities of interest, we have applied the equation of motion technique for the Green function of the dot $G_{\sigma\sigma'} = \ll c_\sigma \mid c^{+}_{\sigma'} \gg$. In the Hartree –Fock approximation [4, 5], the current flowing from the αth electrode to the dot is given by the formula

$$J_\alpha = \frac{ie}{\hbar}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{2\pi}\mathrm{Tr}\left(\mathbf{\Gamma}_\alpha\left(G^{<}(\varepsilon) + f_\alpha(\varepsilon)\left(G^{r}(\varepsilon) - G^{a}(\varepsilon)\right)\right)\right) \tag{5}$$

where

$$f_\alpha(\varepsilon) = \frac{1}{1 + \exp\dfrac{\varepsilon - e\mu_\alpha}{k_B T}}$$

is the Fermi–Dirac distribution function with potentials $\mu_L = eU_e^L = eV_t/2$ and $\mu_R = eU_e^R = -eV_t/2$, $G^{r(a)} = G(\varepsilon \pm i\eta)$ stands for the retarded (advanced) Green function, and $G^{<}(\varepsilon)$ is the lesser Green function. The matrix $\mathbf{\Gamma}_\alpha$ is of the form

$$\mathbf{\Gamma}_\alpha = \Gamma_0\begin{pmatrix} 1 + p_\alpha\cos\phi_\alpha & p_\alpha\sin\phi_\alpha \\ p_\alpha\sin\phi_\alpha & 1 - p_\alpha\cos_\alpha \end{pmatrix}, \tag{6}$$

where p_α denotes polarization of the αth electrode. The coupling between the dot and the leads is given by the formula

$$\Gamma^{\alpha}_{\beta}(\varepsilon) = 2\pi\sum_k |T_{\alpha k\beta}|^2\,\delta(\varepsilon - \varepsilon_{\alpha k\beta})$$

and $\Gamma^{\alpha}_{\beta}(\varepsilon)$ is assumed to be energy independent within the electron bandwidth and zero otherwise.

Hence, one may write

$$\Gamma_{\pm}^{\alpha}(\varepsilon) = \Gamma_{\pm}^{\alpha} = \Gamma_{0}^{\alpha}(1 \pm p_{\alpha}) \qquad \text{with} \qquad \Gamma_{0}^{L} = \Gamma_{0}^{R} = \Gamma_{0}$$

In order to perform numerical calculations on the considered Green functions, one needs to find self-consistently the average values of the occupation numbers,

$$< n_{\sigma} >=< c_{\sigma}^{+}c_{\sigma} >= \mathrm{Im}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{2\pi}G_{\sigma\sigma}^{<}, \tag{7}$$

and

$$< n_{-\sigma\sigma} >=< c_{\sigma}^{+}c_{-\sigma} >= -i\int_{-\infty}^{+\infty}\frac{d\varepsilon}{2\pi}G_{-\sigma\sigma}^{<}. \tag{8}$$

The differential conductance is defined as $G_{\mathrm{diff}} = dJ/dV$ where the total current flowing through the system is $J = (1/2)(J_L - J_R)$, whereas

$$\mathrm{TMR} = \frac{G_{\mathrm{diff}}(\phi_L = 0, \phi_R = 0) - G_{\mathrm{diff}}(\phi_L, \phi_R)}{G_{\mathrm{diff}}(\phi_L = 0, \phi_R = 0)}$$

and the spin accumulation on the dot is $< S_z >= (n_{\uparrow} - n_{\downarrow})/2$.

2. Numerical results and discussion

In this section, we discuss some numerical results for nonlinear transport, assuming empty dot level at equilibrium, $\varepsilon_d = 0.1$ eV, the Coulomb parameter $U = 0.4$ eV, temperature $T = 100$ K, polarization $p_L = p_R = 0.5$, $\Gamma_0 = 0.01$ eV, and the electron bandwidth extending from –3.3 eV to 3.3 eV.

The differential conductance is shown in Figs. 1a and 2a for the parallel configuration, $\phi_L = \phi_R = 0$ (solid line), perpendicular configuration, $\phi_L = 0$, $\phi_R = \pi/2$ (dashed line), and the anti-parallel configuration, $\phi_L = 0$, $\phi_R = \pi$ (dotted line). The TMR is presented in Figs. 1b and 2b, whereas the spin accumulation $<S_z>$ in Figs. 1c and 2c. Figure 1 represents the case in the absence of external magnetic field, $\Delta_Z = 0$. Figure 2, in turn, corresponds to the case with magnetic field applied to the dot, leading to the Zeeman splitting of $\Delta_Z = 0.2$ eV. The differential conductance in the absence of external magnetic field reveals two peaks, appearing symmetrically for positive as well as negative bias resulting from symmetrical coupling to left and right electrodes. The central peaks correspond to the situation when the Fermi level of the source electrode crosses the dot level ε_d (first transport window, the dot becomes singly occupied). This enables the current flow through the system and appears as a peak in the differential conductance. The outermost peaks correspond to the situation when the electrochemical potential of the source electrode crosses the level $\varepsilon_d + U$, also enabling the current flow through the system; the dot may be doubly occupied.

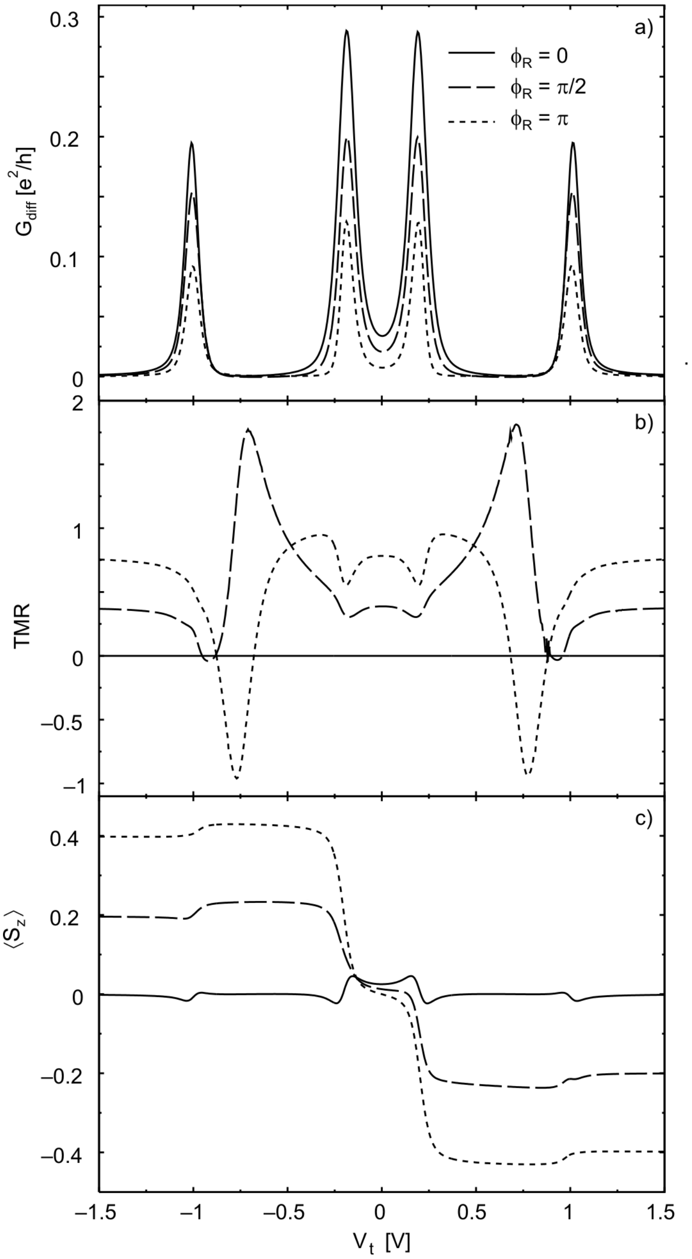

Fig. 1. Transport characteristics in function of bias voltage V_t for $\phi_L = 0$ in the absence of the external magnetic field, $\Delta_Z = 0$: a) bias dependence of the differential conductance in the configuration $\phi_R = 0$ (solid line), $\phi_R = \pi/2$ (dashed line), $\phi_R = \pi$ (dotted line), b) the magnitude of the TMR effect corresponding to the differential conductance shown in (a), c) the bias dependence of the $<S_z>$ component on the dot

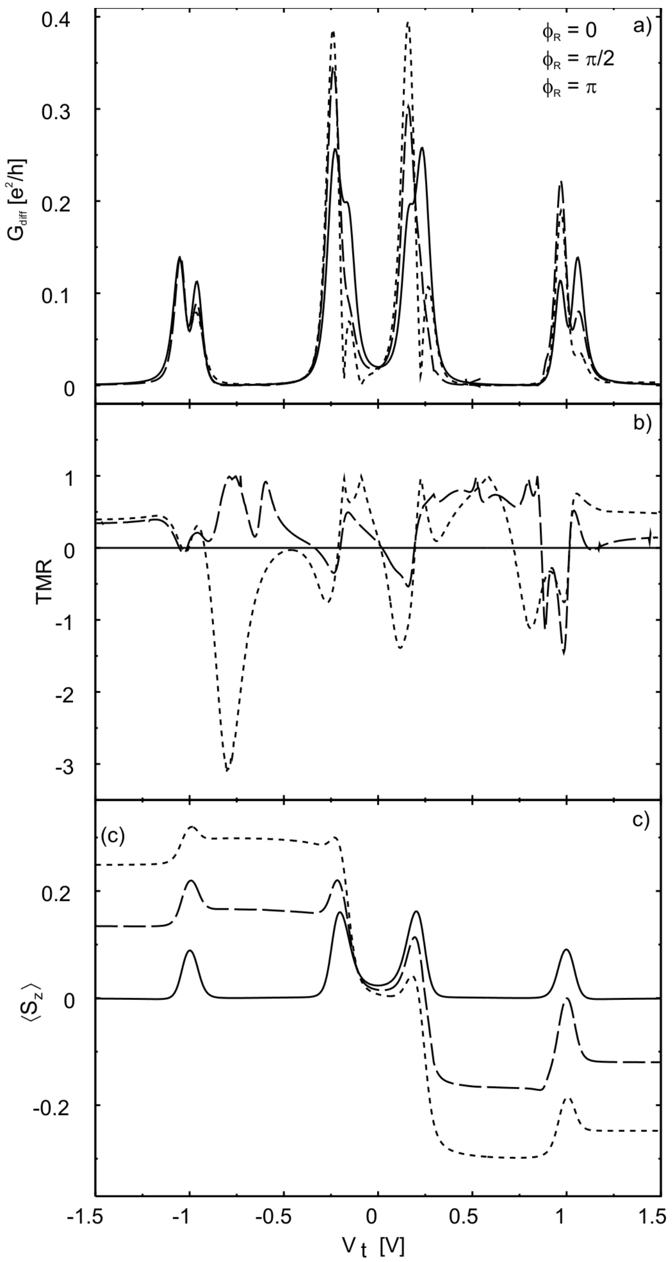

Fig. 2. The transport characteristics in function of bias voltage V_t for $\phi_L = 0$ in the presence of the external magnetic field $\Delta_Z = 0.2$ eV: a) bias dependence of the differential conductance in the configuration $\phi_R = 0$ (solid line), $\phi_R = \pi/2$ (dashed line), $\phi_R = \pi$ (dotted line), b) the magnitude of the TMR effect corresponding to the differential conductance shown in (a), c) the bias dependence of the $\langle S_z \rangle$ component on the dot

Intuitively, the larger conductance is observed for the parallel configuration, when homogeneously polarized spins can freely tunnel through the system, whereas the lower conductance is observed for the anti-parallel configuration. If the electrodes were semimetallic, the transport through the dot would be blocked in the antiparallel configuration [4]. The configuration ϕ_L =0, ϕ_R = π/2 corresponds to an intermediate situation. In the presence of external magnetic field, the dot level degeneracy is removed and the transport through the system goes via "spin-up" and "spin-down" Zeeman levels. Thus one observes splitting of the conductance peaks. This is more

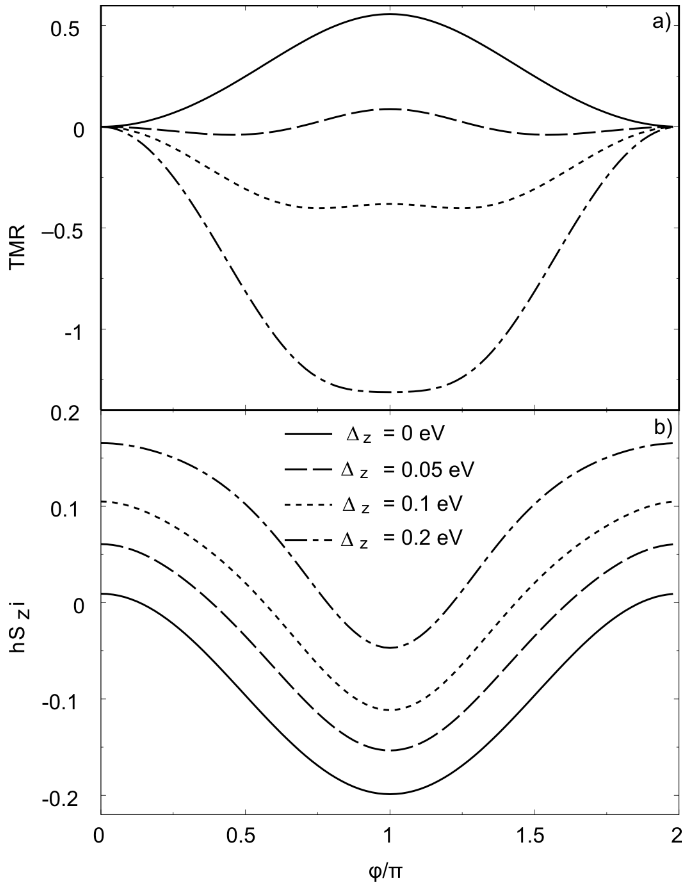

Fig. 3. Transport characteristics for $\phi_L = 0$ in function of $\phi_L = \phi$ for the transport window at $V_t = 0.5$ V. The magnitude of the TMR effect (a), and the $<S_z>$ component (b) for various values of Δ_Z. Polarization $p_L = p_R = 0.8$, the other parameters are as in Fig. 1

visible for peaks corresponding to electronic transport *via* the $\varepsilon_d + U$ level (outermost peaks). The amplitude of the outermost peaks for the parallel configuration in external magnetic field becomes suppressed compared to that for $\Delta_Z = 0$, whereas for the other presented configurations such a tendency is not visible and additionally an asymmetry for the negative and positive bias appears. We propose that the asymmetry is the result of the difference in spin σ = ↑ and spin σ = ↓ populations for the right and the left electrodes when changing the electrode configuration from the parallel to the antiparallel one. Such a behaviour is visible for the $\varepsilon_d^{\uparrow} + U$ and $\varepsilon_d^{\downarrow} + U$, as well as $\varepsilon_d^{\uparrow}$ and $\varepsilon_d^{\downarrow}$ spin levels. Moreover, the amplitude of the central peaks in the conductance tends to increase with increasing $\phi_R = \phi$, that is an inverse effect compared to the situation in the absence of external magnetic field.

The plot of TMR effect in function of the bias voltage shows a complex behaviour that is, in general, the result of spin accumulation on the dot, see Figs. 1b, c, 2b, c. In Figure 3a, the angular dependence of the TMR effect is shown for a few values of the external magnetic field and for $V_t = 0.5$ V. Namely, the magnetization angle of the left electrode is fixed, $\phi_L = 0$, while the right angle is rotated from $\phi_R = 0$ to $\phi_R = 2\pi$. As one may see, the TMR vanishes for $\phi = 0$ and $\phi = 2\pi$, for all indicated values of the Zeeman splitting. In the absence of external magnetic field, the TMR is positive at $V_t = 0.5$ V. One also observes that increasing the external magnetic field leads to negative values of the TMR.

The average $< S_z > = < (n_{\uparrow} - n_{\downarrow})/2 >$ component is given in $\hbar$ units. As shown in Figs. 1c, 2c and 3b, the absolute value of the average $<S_z>$ increases with increasing the angle ϕ_R in the absence as well as in the presence of external magnetic field. Moreover, the $<S_z>$ component is symmetrical with respect to the bias only in a parallel configuration, also for the dot under the influence of external magnetic field.

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