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Effective exchange interaction in tunnelling junctions based on a quantum dot with non-collinear magnetic moments of the leads

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Electron tunnelling through a spin-split discrete level of an interacting quantum dot coupled to two ferromagnetic electrodes (leads) is investigated theoretically in the sequential-tunnelling regime. Spin-splitting of the dot level is induced by an effective exchange interaction between the spin on the dot and spins in the leads. The calculations apply to arbitrary angles enclosed between the magnetizations of the external electrodes. It is shown that the interplay between effective exchange field and Coulomb correlations on the dot may enhance the tunnel magnetoresistance at certain bias voltages. It is also found that a large spin splitting appearing for strong Coulomb correlations gives rise to an enhanced diode-like effect. Finally, it is shown that by rotating the magnetization of one of the electrodes, one can modulate the amplitude of the spin-polarized current, from a blockade in the parallel or antiparallel configuration to its maximum value in the non-collinear case.

Key words: *quantum dot; tunnelling; spin-valve effect; spin-polarized transport*

1. Introduction

Extensive studies on spin-polarized transport phenomena in microelectronic devices have contributed recently to progress in fabricating extremely small transistors, consisting of metallic grains or semiconductor quantum dots (QD) coupled through tunnel barriers to external electrodes [1, 2]. In this paper, we consider sequential electron tunnelling through an atomic spacer coupled to two ferromagnetic leads with magnetic moments polarized at an arbitrary angle Θ with respect to each other. The atomic spacer is assumed to be an interacting QD with a single discrete level, which is spin-split due to effective exchange interaction between the spin on the dot and spins

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in the electrodes. It is shown that the interplay of Coulomb correlations on the dot and the effective molecular field can significantly enhance tunnel magnetoresistance (TMR) in systems with non-collinearly polarized external source and drain ferromagnetic electrodes. Moreover, a previous analysis [3, 4] of the diode effect, predicted for collinear magnetic configurations in a device with one electrode being half metallic, is extended by taking into account modifications due to non-collinear magnetic states as well as due to the effective field. Therefore, an enhancement of the diode-like behaviour in a junction with collinearly aligned lead magnetizations is found. In turn, by presenting the angular dependencies of the transport characteristics, we show that a suppression of the diode effect occurs in non-collinear configurations.

2. Model

In the model Hamiltonian of the system, the left and right ferromagnetic electrodes are taken in the non-interacting quasi-particle limit. The term corresponding to the dot includes a single-particle energy level ε_d and the Coulomb correlation described by the parameter U. The spin eigenstates of the dot are denoted by $\sigma = \uparrow$ for spin-up electrons and $\sigma = \downarrow$ for spin-down electrons. In turn, the tunnelling part describes spin-dependent tunnelling processes through the left and right barrier. Since the magnetic moments of the external electrodes form an arbitrary angle Θ, the tunnelling terms of the model Hamiltonian are written in the corresponding local reference frames, where the tunnelling matrices are diagonal in the spin space. The spin asymmetry of the tunnelling rates across the left (l) and right (r) barriers, $\Gamma_l^{\pm} = \Gamma_0(1 \pm p_l)$ and $\Gamma_r^{\pm} = \alpha\Gamma_0(1 \pm p_r)$ (+ and – denote majority and minority electrons, respectively), is described by the parameters p_l and p_r. We also introduce a parameter Γ_0, which is the value of the tunnelling rate $\Gamma_{l,r}^{\pm}$ at $p_{l,r} = 0$, and α, which determines the ratio of the tunnelling matrix elements through the right and left barriers. Finally, the electrostatic potential of the dot is assumed to be an average value of the electrostatic potentials of the electrodes.

The transport properties of the system will be described in the sequential tunnelling regime. In order to calculate the current–voltage characteristics in a stationary state, we have generalized the master equation method [5]. The master equation allows the occupation numbers for the dot to be obtained, which in turn can be used to calculate the tunnelling current $J(\Theta)$ for arbitrary magnetic configurations Θ. The corresponding TMR has been defined qualitatively as TMR = $[J_P - J(\Theta)]/J(\Theta)$, with J_P denoting the electric current for the parallel ($\Theta = 0$) configuration. The bias variations of transport characteristics in the non-equilibrium situation are governed by the bias voltage (V_t) dependencies of the effective exchange interaction between the dot spin and spin of electrons in the external magnetic leads. To determine the exchange interaction energy, E_{eff}, we adopted the second-order perturbation theory, developed for the Anderson Hamiltonian [6]. The explicit formula for E_{eff} is given by

$$E_{\text{eff}} = \sqrt{\Delta E_l^2 + \Delta E_r^2 + 2\Delta E_l \, \Delta E_r \cos\Theta} \tag{1}$$

$$\Delta E_{l,r} = (\Gamma_{l,r}^{-} - \Gamma_{l,r}^{+})\left[\operatorname{Re}\Psi\left(\frac{1}{2} + \frac{\varepsilon_d + U - \mu_{l,r}}{2\pi\, K_B T} i\right) - \operatorname{Re}\Psi\left(\frac{1}{2} + \frac{\varepsilon_d - \mu_{l,r}}{2\pi\, K_B T} i\right)\right] \tag{2}$$

where the symbol $\Psi(z)$ is the digamma function, and $\mu_{l,r}$ denotes the chemical potential of the left or right electrode. Using Eqs. (1) and (2), one finally obtains the energies of the spin-split discrete level, $\varepsilon_{d\downarrow(\uparrow)} = \varepsilon_d \pm E_{\text{eff}}/2$. The external magnetic leads are thus considered as the source of mean fields which influence the tunnelling processes through the QD spin channels $\varepsilon_{d\sigma}$ and $\varepsilon_{d\sigma} + U$.

3. Numerical results

Consider first non-linear transport through a symmetrical junction, assuming an empty level at equilibrium, $\varepsilon_d > 0$. In Figure 1a we show the bias dependence of the difference between the energies of the dot spin channels $\varepsilon_{d\downarrow}$ and $\varepsilon_{d\uparrow}$, plotted for selected Θ angles. A maximum of spin-splitting appears at a threshold voltage, for which either the level ε_d or $\varepsilon_d + U$ crosses the Fermi level of the source electrode. For voltages below the first peak in Fig. 1a, the discrete level of the dot lies above the Fermi level of the source electrode and the sequential tunnelling processes are exponentially suppressed. For voltages between the maxima, QD may be singly occupied. Finally, above the second threshold voltage two electrons may reside on the dot. A minimum in Fig. 1a is observed at the bias voltage for which a reorientation of the effective field occurs, relative to the spin quantization axes of the magnetic electrodes. The latter feature originates from bias-dependent dot–lead exchange interactions. In non-collinear cases, the interplay between these interactions and Coulomb correlations on the dot may lead to a negative differential conductance in the bias range between the threshold voltages, as is clearly seen in Fig. 1b (the curve for $\Theta = \pi/2$).

Since in this voltage range the dot is singly occupied, then in a non-collinear configuration one may observe an increased accumulation of the average spin component $\langle S_z \rangle$ on the dot. This is due to the fact that the mean field tends to align parallel relative to the magnetization of the source lead with increasing bias, and thus the number of spin states available for an electron residing on the dot in the local reference system of the drain electrode effectively diminishes. Consequently, as displayed in Fig. 1c, a significant enhancement of the corresponding TMR may be observed between the two threshold voltages. This is the case until the probability of occupying the level $\varepsilon_d + U$ starts to increase at a certain bias voltage. When $\varepsilon_d + U$ crosses the Fermi level of the source lead, both tunnelling channels become active, the spin-polarized current increases relatively quickly and finally saturates at a certain level.

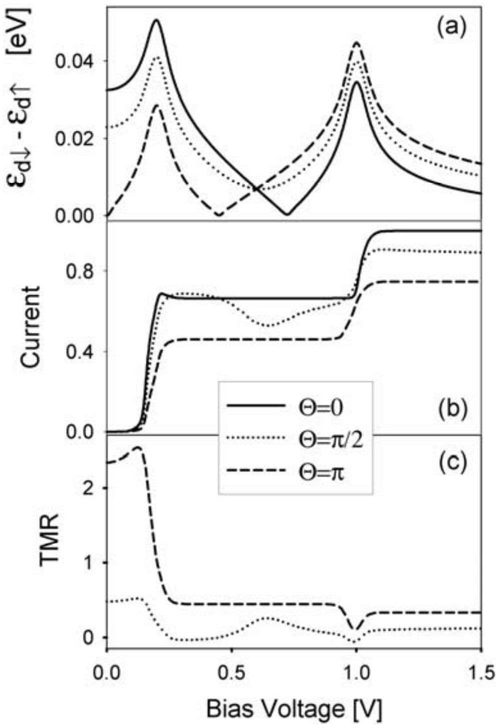

Fig. 1. Bias dependence of the difference between the energies $\varepsilon_{d\downarrow}$ and $\varepsilon_{d\uparrow}$ (a), tunnelling current (b), and the corresponding TMR (c) for the indicated angles Θ. The parameters are: $\varepsilon_d = 0.1$ eV, $p_l = p_r = 0.5$, $U = 0.4$ eV, $\alpha = 1$, and $T = 100$ K

Now consider the situation when the drain electrode (the right one) is half metallic, whereas the source electrode is an ordinary 3D ferromagnet, like Co or Fe. Moreover, assume again that at $V_t = 0$ one has $\varepsilon_d > 0$, whereas $\varepsilon_d + U >> 0$, which implies that the dot may only be empty or singly occupied. From [3, 4] it is known that in collinear configurations such a junction can work as a mesoscopic diode, i.e. the electric current can flow for one bias polarization, whereas it is suppressed or even blocked for the opposite bias polarization. The results for the electric current in the considered device with the mean field switched on, and for different angles Θ, are shown in Fig. 2. As discussed above, the effective field yields a maximum of discrete level spin-splitting at the threshold voltage. The spin-up electrons of energy $\varepsilon_{d\uparrow}$, which enter the electron window first, may hence tunnel through the QD, giving rise to a significant enhancement of the resonant bump that occurs at a positive bias ($V_t > 0$) in the parallel configuration ($\Theta = 0$). This is true until the spin channel $\varepsilon_{d\downarrow}$ crosses the Fermi level of the source electrode. After that, at voltages above the bump, a blockade of the electric current appears, due to the spin-down electron that tunnelled to the dot from the source (left) lead. When the magnetic configuration of the junction becomes non-collinear, then in general an electron that has tunnelled to the QD has spin with both spinor components in the local reference. If only the spin channel $\varepsilon_{d\uparrow}$ is active in tunnelling, then effectively both leads contain less available spin states for these electrons, and a suppression of the resonant bump occurs.

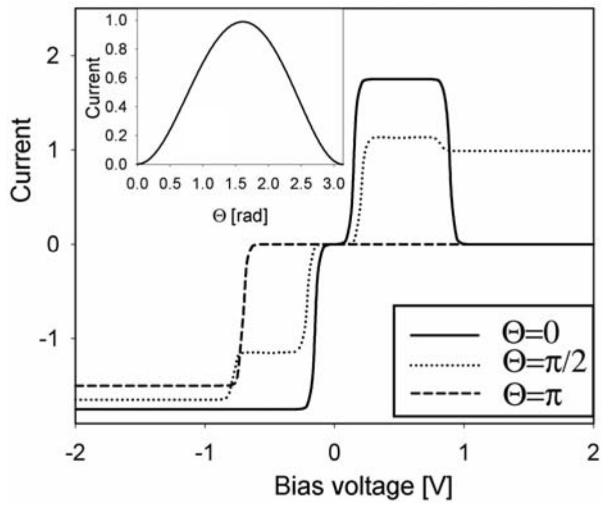

Fig. 2. Bias dependence of the electric current, calculated for the large U limit, with the empty state in equilibrium and for the indicated angles Θ. The inset shows the angular dependence of the electric current, calculated for a bias voltage of $V_t = 1$ V. The other parameters are: $\varepsilon_d = 0.25$ eV, $p_l = 0.4$, $p_r = 1$, $\alpha = 0.1$, and T = 100 K

The same mechanism is also responsible for current suppression in the vicinity of the threshold voltage at negative bias ($V_t < 0$). On the other hand, when both spin channels are in the tunnelling window, then for positive voltages above the bump the current blockade is lifted. Finally, in the antiparallel case the current is blocked in the entire range of positive bias voltages and also in a certain range of negative bias. The diode effect presented here for $\Theta = \pi$ is thus more pronounced as compared to the previous predictions, evaluated for a system with spin-degenerate discrete levels [3, 4]. The inset in Fig. 2 shows in detail how the current varies with the angle Θ at selected bias voltages above the resonant bump. From this it evidently follows that collinear configurations are important for diode behaviour. Furthermore, the amplitude of the current can be modulated with Θ, from a blockade in collinear configurations to a maximum intensity in the non-collinear case.

To summarize, we have investigated sequential tunnelling through a spin-split discrete level of an interacting quantum dot coupled to non-collinearly polarized external ferromagnetic electrodes. In particular, we have shown that in non-collinear configurations the interplay of the effective exchange field, originating from the external electrodes, and Coulomb correlations on the dot may lead to a negative differential conductance between the threshold voltages, at which a new transport channel becomes open for tunnelling. Moreover, we have found that in systems with a half-metallic electrode the diode effect is suppressed when the magnetic moments of the leads are non-collinear. On the other hand, an interesting enhancement of diode-like behaviour is found in the antiparallel configuration. We predict that the latter feature is most significant in junctions with strong Coulomb repulsion between electrons on the dot.

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