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SPIN-POLARIZED CURRENT IN A MAGNETIC TUNNEL JUNCTION: MESOSCOPIC DIODE BASED ON A QUANTUM DOT

W. Rudziński

Department of Physics, Adam Mickiewicz University, Ul. Umultowska 85, 61-614 Poznan, Poland

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Abstract. Theoretical analysis of electronic transport through a two-barrier magnetic tunnel junction based on a single-level interacting quantum dot (QD) is carried out. The key point of our considerations is diode-like behavior of transport characteristics of an asymmetric tunnel junction with one electrode being half-metallic. A number of mechanisms leading to modifications of the diode-like behavior have been discussed by means of the nonequilibrium Green-function technique. It is found that the diode effect is reduced for a nonmagnetic QD coupled to external ferromagnetic electrodes with noncollinear magnetic moments, whereas it is significantly enhanced for a magnetic QD in the antiparallel configuration. By taking into account spin-flip processes in the barriers, some suppression of the diode effect is found for a wide range of transport voltages. Finally, interaction of the quantum dot with a phonon field has been included in the theoretical description. It is shown that the electron-phonon interaction gives rise to oscillations of the tunnel magnetoresistance. In asymmetrical junctions, the electron-phonon coupling may lead to a significant suppression or enhancement of the tunneling current, depending on the bias polarization.

1. INTRODUCTION

Transport properties of structures based on quantum dots (QDs) have been extensively studied both experimentally [1-5] and theoretically [6-10]. It has been shown that electron-electron interactions in single electron transistors including quantum dots may lead to such effects as the Coulomb blockade, Kondo resonance, or diode-like behaviour. In this paper, we analyze electron tunneling through an interacting quantum dot with a single discrete level, which is coupled via tunneling barriers to two ferromagnetic leads. In contrast to theoretical models investigated so far, we consider a more realistic model of a mesoscopic diode by including spin-flip processes, spin-splitting of the discrete level, as well as effects due to electron-phonon interactions on the dot. The latter effects, as reported in recent experiments [4,5], are especially important in systems based on molecular quantum dots. Our considerations apply to arbitrary configuration of the magnetic moments of the external source and drain ferromagnetic electrodes. Thus, the previous analysis [9] of the diode effect found 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 state.

Corresponding author: W. Rudziński, e-mail: wojrudz@amu.edu.pl

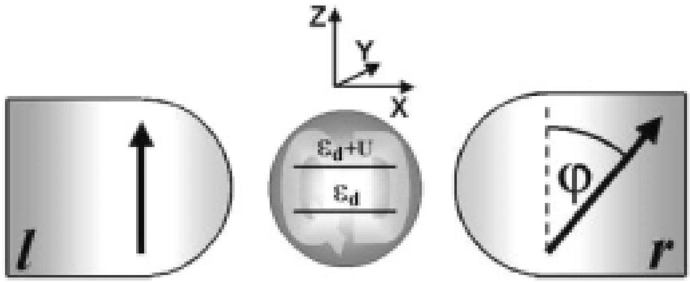

Fig. 1. Schematics of the system considered in this paper. The coordinate system used to describe states of the dot is also shown.

2. MODEL

Consider a single-level QD coupled to two ferromagnetic leads by tunneling barriers. Magnetic moments of the external leads lie in the common plane and form an arbitrary angle φ. Geometry of the device and the orientation of the coordinate system are shown schematically in Fig. 1. The whole system can be described by the model Hamiltonian of the form:

$$H = H_\nu + H_d + H_{ph} + H_{el-ph} + H_t\,. \qquad (1)$$

The left (ν=*l*) and right (ν=*r*) ferromagnetic electrodes in Eq. (1) are taken in the noninteracting quasiparticle limit,

$$H_\nu = \sum_{\beta k \nu} \varepsilon_{\beta k \nu} a^+_{\beta k \nu} a_{\beta k \nu}\,, \qquad (2)$$

with β=+(-) denoting spin projection on the local quantization axis for majority (minority) electrons. The term corresponding to the dot, H_d,

$$H_d = \sum_\sigma \varepsilon_{d\sigma} c^+_\sigma c_\sigma + U c^+_\uparrow c_\uparrow c^+_\downarrow c_\downarrow\,, \qquad (3)$$

includes the spin-dependent single particle energy level $\varepsilon_{d\sigma}$, with σ = ↑, ↓ denoting spin projection on the global quantization axis aligned parallel to the *z*-axis (Fig.1), and Coulomb correlations described by the Hubbard parameter *U*. In order to include the effect of a phonon field on transport properties, the model has been extended by adding the phonon Hamiltonian H_{ph},

$$H_{ph} = \hbar\omega b^+ b\,, \qquad (4)$$

where ω is a vibrational frequency of the phonon mode, whereas b^+ and *b* are the corresponding phonon creation and anihilation operators. In turn, the electron-phonon interaction term $H_{el\text{-}ph}$ reads

$$H_{el\text{-}ph} = \lambda(b + b^+) c^+_\sigma c_\sigma\,, \qquad (5)$$

with the parameter λ denoting the strength of the electron-phonon coupling. Finally, the tunneling part H_t includes spin-dependent tunneling processes which conserve electron spin, as well as tunneling processes with spin reversal,

$$H_t = \sum_{\beta\sigma k} \{T^l_{k\mp\beta} a^+_{lk\mp\beta} c_\sigma + [T^r_{k\mp\beta} a^+_{lk\mp\beta} \cos\frac{\varphi}{2} \mp\beta T^r_{k\pm\beta} a^+_{lk\pm\beta} \sin\frac{\varphi}{2}] c_\sigma + hc.\}. \qquad (6)$$

Spin asymmetry of the tunneling rates, $\Gamma^\nu_\beta \sim |T^\nu_{k\beta}|^2$,

$$\Gamma^l_\pm = \Gamma_0(1 \pm p_l)\,, \qquad (7)$$

$$\Gamma^r_\pm = \alpha\Gamma_0(1 \pm p_r)\,, \qquad (8)$$

is described by the parameters p_l and p_r. The parameter α in Eq. (8) describes the ratio of tunneling matrix elements through the right and left barriers, whereas Γ_0 in Eqs. (7) and (8) determines tunneling rates for the case of $p_l = p_r = 0$. We also introduce the factor Λ which describes the ratio of the average tunneling matrix elements for tunneling with and without spin reversal. Finally the electrostatic potential of the dot is assumed to be the average value of the electrostatic potentials of the electrodes.

To calculate the density matrix for the system we used nonequilibrium Green-function technique based on equation of motion in the Hartree-Fock approximation. Thus, having found occupations numbers for the dot, we have calculated the tunneling current from the Meir-Wingreen formula [11]. The corresponding tunnel magnetoresistance (TMR) was defined quantitatively as TMR=[I_P- $I(\varphi)$]/$I(\varphi)$, with I_P denoting electric current in the parallel configuration, and $I(\varphi)$ being the current when magnetic moments of the leads form an angle φ.

3. NUMERICAL RESULTS

Consider a QD separated by non-equivalent barriers from both electrodes and assume that the right electrode is half-metallic whereas the left one is a normal ferromagnetic metal like Co or Fe. Assume further, that the discrete level $\varepsilon_{d\sigma}$ is empty in equilibrium, $\varepsilon_{d\sigma} > 0$. It is known that in collinear configurations such a system can work as a mesoscopic diode, i.e. electric current can flow for one bias polarization, whereas it is suppressed or even totally blocked for the opposite bias polarization [9]. This is the case of current-voltage characteristics in Fig 1a. For positive bias, the current flows above the threshold voltage for arbitrary value of the angle φ. On the other hand, the current suppression, clearly visible in Fig. 2a above the resonant bump for negative bias in the collinear configurations, is due to the fact that the electron which has tunneled to the discrete level from the left electrode cannot tunnel further because there are no states available for it in the half-metallic drain electrode. When the energy level $\varepsilon_{d\sigma}+U$ crosses the Fermi energy of the source (left) lead, the current increases and finally saturates at a certain level. When the angle φ is different from $\varphi = 0$ or $\varphi = \pi$, the electron tunneling from the source lead has both spinor components that allow it to tunnel further. Thus, for a non-collinear situation the probability of tunneling to the drain lead does not vanish and consequently a reduction of the diode effect is observed. A significant modifications of the latter property due to the applied external magnetic field applied, as well as due to spin-flip processes in the tunneling barriers are presented in Figs. 2b and 2c, respectively.

When the discrete level of the dot is spin-split due to the applied external magnetic field, a significant enhancement of the diode-like behaviour occurs. It is clearly shown in Fig. 2b, where the resonant bump at the threshold voltage almost disappears in the AP configuration. The physical mechanism responsible for this behavior follows from the spin splitting of the QD level due to magnetic field. The tunneling current is suppressed in the vicinity of the first threshold voltage by an elec-

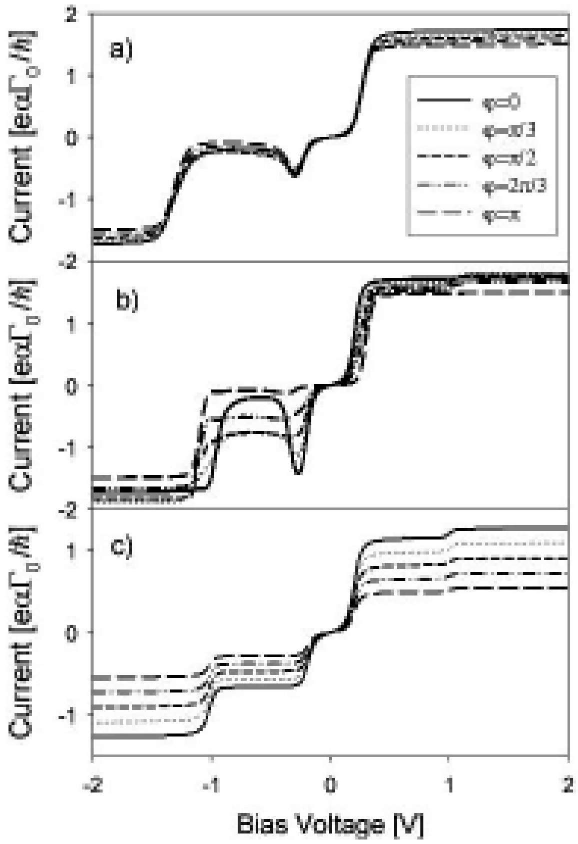

Fig. 2. Bias dependence of electric current for indicated values of the angle j and for the parameter Λ=0 (a,b) and Λ=1 (c). The dot energy levels are: $\varepsilon_{d\uparrow} = \varepsilon_{d\downarrow} = 0.1$ eV (a,c) and $\varepsilon_{d\uparrow} = 0.1$ eV, $\varepsilon_{d\downarrow} = 0.15$ eV (b). The other parameters are: U=0.4 eV, $p_l = 0.4$, $p_r = 1$, Γ_0=0.01 eV, $\alpha = 0.1$, T=100K.

tron residing on the dot in the spin-up tunneling channel. In turn, spin-flip processes in the tunneling barriers diminish the asymmetry in the current-voltage characteristics. Such tunneling events accompanied by spin reversal enhance electric current between the two threshold bias voltages and consequently lead to suppression of the diode effect (Fig. 2c).

In any real material an electron tunneling through a double-barrier structure will interact with phonons and the resulting changes in the transmission will be manifested in the current [4]. In the strong electron-phonon interaction regime it is appropriate to eliminate the electron-phonon coupling terms in the Hamiltonian by using the Lang-Kirsov

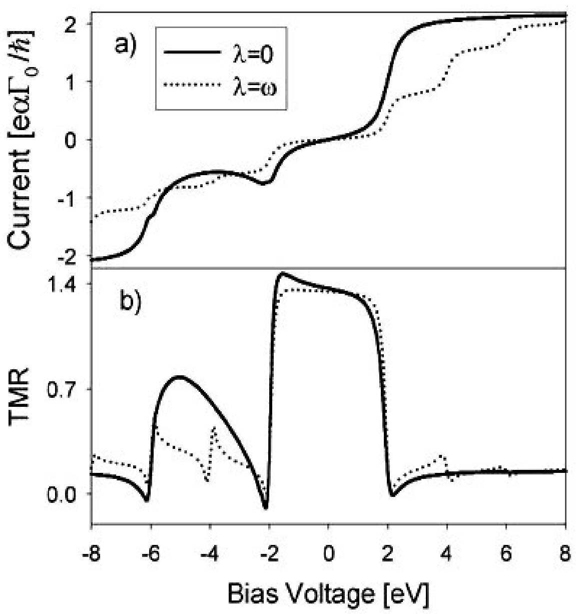

Fig. 3. Bias dependence of electric current (a) in the parallel (φ=0) configuration and TMR (b) for the system with (λ=ω eV, dashed curves) and without (λ=0, solid curves) electron-phonon interactions on the dot. The other parameters are $\varepsilon_{d\uparrow} = \varepsilon_{d\downarrow} = 2\omega$ eV, $U = 4\omega$ eV, $p_l = 0.4$, $p_r = 1$, $\Gamma_0 = 0.2\omega$ eV, $\alpha = 0.1$, $\Lambda = 0$, $T = 0$K.

canonical transformation [12]. Consequently, the phonon part, H_{ph}, of the Hamiltonian remains unchanged, whereas the electron part is reshaped to the standard form of the Anderson Hamiltonian with renormalized energy of the dot discrete level, $\varepsilon_{d\sigma} - \lambda^2$, and renormalized Coulomb charging energy, $U - 2\lambda^2$. The tunneling amplitudes are also renormalized, which describes the fact that the electron hopping will be accompanied by a phonon cloud.

In the nonequilibrium situation, when the bias voltage is applied to the external electrodes, electric current and TMR exhibit new features. First, as seen in Fig. 3a, besides the two steps in the current corresponding to the two threshold bias voltages at which the dot level crosses the Fermi level of the source electrode, also the Franck-Condon steps spaced at the phonon energy appear. Second, when the electron-phonon interactions are switched on, a significant suppression of the current flowing from the right half-metallic electrode to the left ferromagnetic one is observed. For the opposite bias polarization the current suppression occurring between the two threshold bias voltages is now lifted due to tunneling processes mediated by the phonon energy levels. Third, the discussed here electric current modifications are accompanied by strong oscillations in TMR (Fig. 3b) above the threshold voltage, at which the dot energy level $\varepsilon_d\sigma$ enters the tunneling window. A specific profile of these oscillations is due to the fact that between the Franck-Condon steps spin accumulation slowly increases and then at phonon resonances it is abruptly diminished due to an increased electron transmission through the phonon energy levels.

4. CONCLUSIONS

Concluding, the present work reveals that enhancement of the diode-like behaviour is possible in single-electron systems based on a magnetic quantum dot separated by nonequivalent barriers from ferromagnetic leads (one being half-metallic). If the ferrromagnetic electrodes are non-collinearly magnetized then the diode like behaviour is always reduced. Similarly, other mechanisms considered here, namely spin-flip processes in the tunneling barriers as well as electron-phonon interactions on the dot lead to suppression of the diode effect.

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