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Phonon-assisted tunnelling through a quantum dot coupled to magnetic leads

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Spin-polarized transport has been theoretically studied in double barrier tunnelling junctions based on a single level quantum dot interacting with a local phonon mode. It was shown that the electron –phonon interaction gives rise to oscillations of the tunnel magnetoresistance (TMR). In asymmetrical junctions, the polaronic transport through the junction may lead to a significant suppression of the diode-like behaviour. The case of negative effective charging energy has also been analyzed numerically. It was shown in particular that for a mesoscopic diode an interplay between the single-electron cotunnelling and the pair tunnelling processes leads to inversion of TMR.

Key words: *quantum dot; spin-polarized tunnelling; phonons*

1. Introduction

Electronic transport through discrete levels of single molecules, carbon nanotubes or quantum dots (QDs) coupled to vibrational degrees of freedom has been investigated recently in a number of experimental as well as theoretical works (see, e.g., [1–3]). The present paper extends studies on phonon-assisted electronic transport in mesoscopic systems to the case of tunnelling through a single-level quantum dot coupled to ferromagnetic electrodes. One of the most widely studied spin-dependent effects in such magnetic tunnel junctions is the tunnel magnetoresistance (TMR) [4]. Here, TMR is analyzed numerically in the context of polaronic transport through an interacting quantum dot and the both induced by the polaron shift cases of positive and negative effective charging energy are taken into account.

2. Model and method

Consider a single-level QD coupled to two ferromagnetic leads by tunnelling barriers, with the magnetic moments of the leads assumed to be aligned parallel (P) or

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antiparallel (AP). The whole system can be described by the model Hamiltonian of the form:

$$H = H_v + H_d + H_{ph} + H_{el-ph} + H_t \tag{1}$$

The term H_v describes the left ($v = l$) and right ($v = r$) electrodes taken in the non-interacting quasiparticle limit

$$H_v = \sum_{\sigma k v} \varepsilon_{\sigma k v} a^+_{\sigma k v} a_{\sigma k v} \tag{2}$$

where $\varepsilon_{\sigma k v}$ is the single electron energy in the ν-th electrode for the wave vector **k** and spin $\sigma(\sigma = \uparrow, \downarrow)$. The term corresponding to the dot, H_d

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

includes the spin-dependent single particle energy level ε_d, and Coulomb correlations described by the Hubbard parameter U. In order to include the effect of a phonon field, the model has been extended by

$$H_{ph} = \hbar\omega_0 \, b^+ b \tag{4}$$

where ω_0 is a vibrational frequency of the phonon mode, whereas b^+ and b are the corresponding phonon creation and anihilation operators. Moreover, the electron-phonon interaction part of the Hamiltonian (1) reads

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

with the parameter λ denoting the strength of the electron-phonon coupling. Finally, the tunnelling part H_t includes spin-dependent tunnelling processes

$$H_t = \sum_{\sigma k v} T^v_{k\sigma} a^+_{\sigma k v} c_\sigma + \text{h.c.} \tag{6}$$

Spin asymmetry of the tunnelling rates, $\Gamma^v_\sigma \sim \left| T^v_{k\sigma} \right|^2$, is described by the parameters p_l and p_r

$$\Gamma^l_{\uparrow(\downarrow)} = \Gamma_0 \left(1 \pm p_l\right) \tag{7}$$

$$\Gamma^r_{\uparrow(\downarrow)} = \alpha \Gamma_0 \left(1 \pm p_r\right) \tag{8}$$

where α denotes the ratio of tunnelling matrix elements through the right and left barriers, and where Γ_0 is a parameter.

To calculate the density matrix for the system we used non-equilibrium Green function technique based on the equation of motion in the Hartree–Fock approximation. The assumption of strong electron-phonon interactions on the dot allowed us to combine the non-equilibrium Green function method with a canonical Lang–Firsov transformation [5]. Consequently, the electron part of the model (1) is reshaped to the standard form of the Anderson Hamiltonian with renormalized energy of the dot discrete level, $\varepsilon_d' = \varepsilon_d - \lambda^2$, and with renormalized Coulomb charging energy, $U' = U - 2\lambda^2$. Thus, having found the occupation numbers of the dot, we have finally calculated the tunnelling current from the Meir–Wingreen formula [6] as well as the corresponding TMR defined quantitatively as TMR = $(I_P - I_{AP})/I_{AP}$, with I_P and I_{AP} denoting electric current in the P and AP configurations, respectively.

3. Numerical results

Let a QD be separated by non-equivalent barriers from both electrodes assuming that the right electrode is half-metallic (fully spin-polarized in one direction) whereas the left one is ferromagnetic. Assume further that the discrete level ε_d' is empty in equilibrium, $\varepsilon_d' > 0$.

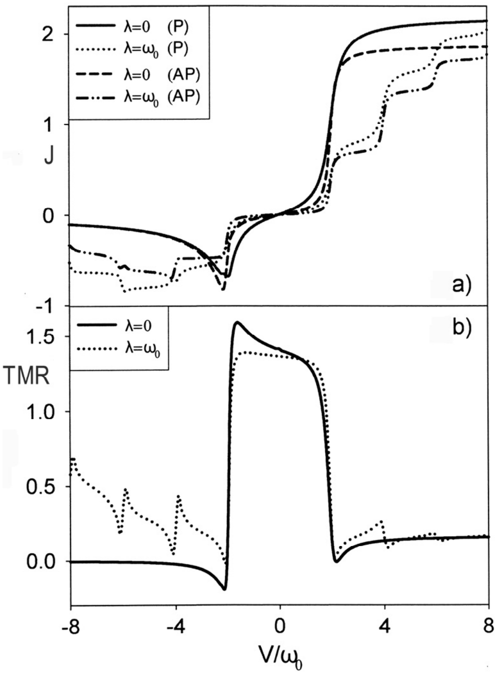

Fig. 1. Bias dependence of the electric current (a) and of TMR (b) for the asymmetrical junction with $U >> 0$. The current–voltage characteristics for $\lambda = 0$ are compared to the case of strong electron–phonon coupling, $\lambda = \omega_0$. The energy is measured in units of the frequency of the phonon mode ω_0, and the parameters are: $p_l = 0.4$, $p_r = 1$, $\alpha = 0.1$, $\varepsilon' = \lambda$, $\Gamma_0 = 0.2\omega_0$ and $T = 0$

Consider first the large U limit, which implies that the dot may be either empty or singly occupied. The basic transport property of the asymmetrical tunnelling junction is the asymmetry of its current–voltage characteristics with respect to the bias reversal. As shown in Fig. 1a, for $\lambda = 0$ such a system can work as a mesoscopic diode [4]. At positive bias, the current flows for both P and AP configurations and thus TMR is significantly suppressed. By contrast, when electrons tunnel through the dot from the left electrode to the half-metallic one, then the sequential tunnelling is exponentially suppressed below the threshold voltage and only the higher-order tunnelling processes may occur. The latter property results in a significant TMR maximum for bias voltages at which sequential tunnelling is exponentially suppressed. At a sufficiently large bias voltage, the dot energy level ε_d ($\varepsilon'_d = \varepsilon_d$ at $\lambda = 0$) enters the tunnelling window, and electric current starts to flow through the junction. This takes place only in a small voltage range in the vicinity of the first threshold voltage, where the resonant bump is observed. Above the bump, the current is suppressed by an electron which has tunnelled to the discrete level from the left electrode, and which cannot tunnel further because there are no states available for it in the half-metallic drain electrode.

When the electron-phonon interactions are switched on, then at positive bias the exponential suppression of the tunnelling rates gives rise to a suppression of the electric current (Fig. 1a). Also, additional Franck–Condon steps appear in the current and the corresponding TMR exhibits oscillations beyond the Coulomb blockade regime (Fig. 1b). By contrast, at negative bias voltages, the current suppression is lifted above the elastic resonance threshold. This reduction of the diode-like behaviour becomes possible when at a sufficiently large bias voltage a phonon energy level enters the tunnelling window. Phonon emission induced at $T = 0$ may then increase the probability of the following two-electron processes: one electron with spin antiparallel to the magnetization of the half-metallic lead is tunnelling back to the source ferromagnetic electrode, while the second electron with the opposite spin is tunnelling to the drain electrode thus lifting the current suppression. Consequently, an enhancement of the oscillating TMR occurs.

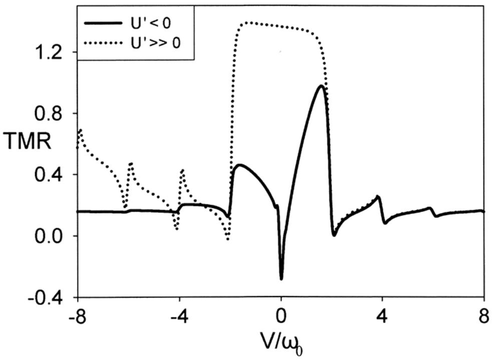

Fig. 2. Bias dependence of TMR for a large positive charging energy $U' >> 0$ and $\lambda = \omega_0$ compared to TMR for a negative effective charging energy, $U' = -2\ \omega_0$. The other parameters are as in Fig. 1

Let us now discuss the current voltage characteristics for our mesoscopic diode assuming that the polaron shift gives rise to a negative *effective* charging energy, $U' < 0$. It is known [2] that at a finite effective $U' < 0$ two electrons can hop onto the dot simultaneously from (or out to) opposite leads and charge transport may be dominated by tunnelling of electron pairs. As shown in Fig. 2, such a pair tunnelling leads to a remarkable modification of the TMR characteristics for the asymmetrical system considered here. The central maximum of TMR (dotted curve in Fig. 2) originating from the single-electron higher-order tunnelling processes is now split due to pair-tunnelling into the two TMR maxima (solid curve in Fig. 2). In case of the asymmetrical magnetic junctions discussed here, pair-tunnelling processes are blocked at negative bias voltages since there are no states available for electrons with spins opposite to the magnetization of the half-metallic drain lead. Then, only single-electron cotunnelling is possible around $V = 0$. On the other hand, at small positive bias voltages, besides single-electron cotunnelling also pair-tunnelling is allowed contributing to a larger TMR ratio. Thus, an interplay between the single-electron cotunnelling and pair-tunnelling processes leads to inversion and asymmetry of TMR in the vicinity of $V = 0$, the visible in Fig. 2.

4. Conclusions

The polaronic transport through a tunnelling device based on an interacting single-level QD coupled to ferromagnetic electrodes results in a typical step-like electric current behaviour with additional Franck–Condon steps appearing at threshold bias voltages at which phonon-assisted electron transmission takes place. Consequently, oscillations of the corresponding tunnel magnetoresistance have been observed. It has also been found that the electron–phonon interactions in asymmetrical junctions may lift the current suppression above the threshold voltages at which the elastic resonance occurs, thus giving rise to a reduction of the diode-like behaviour.

When the polaron shift induces a negative effective charging energy, then a competition between the single-electron cotunnelling and pair-tunnelling processes leads to a splitting of the TMR maximum in the Coulomb blockade regime. The latter feature may be accompanied by an inversion of the TMR ratio in the vicinity of zero bias voltage.

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