A study of inelastic electron–phonon interactions on tunneling magnetoresistance of a nano-scale device

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ABSTRACT

In this research, we have studied the effect of inelastic electron–phonon interactions on current–voltage characteristic and tunneling magnetoresistance of a polythiophene molecule that is sandwiched between two cobalt electrodes using modified Green's function method as proposed by Walczak. The molecule is described with a modified Su–Schrieffer–Heeger Hamiltonian. The ground state of the molecule is obtained by Hellman–Feynman theorem. Electrodes are described in the wide-band approximation and spin-flip is neglected during conduction. Our calculation results show that with increase in voltage the currents increase and tunneling magnetoresistance decreases. Change in tunneling magnetoresistance due to inelastic interactions is limited in a small bias voltage interval and can be neglected in the other bias voltages.

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1. Introduction

Due to its application in electronic devices, spin transport through molecules has been the focus of many researchers’ attention in the recent years. Several theoretical and experimental works confirm that conducting polymers can also act as spin-polarized materials [1–4]. Many studies have been done on transport properties of organic semiconductors that are sandwiched between two electrodes using the Su–Schrieffer–Heeger (SSH) Hamiltonian [1,4,5]. In these studies inelastic electron–phonon interactions have been neglected. In the presence of magnetic field, magnetic moments in the electrodes are oriented in the same direction, and as a result conduction of system changes. In this paper, we study spin-dependent transport and tunneling magnetoresistance (TMR) in a polythiophene (PTh) molecule in the presence of inelastic electron–phonon interactions. We consider an organic spin-valve consisting of a PTh molecule sandwiched between two cobalt electrodes as schematically shown in Fig. 1.

Because of the weakness in spin–orbit coupling and hyperfine interactions in the organic materials, spin relaxation length is long and spin-flip process during conduction can be neglected [2,6]. In addition, we do not consider the presence of phonon in electrodes in the present work. Walczak [7,8] developed a Green’s function approach to study the electron transport through DNA molecule in the presence of electron–phonon interactions. We exploited the same approach for investigating transport problem in organic semiconductors. This paper is organized as follows: details of the selected model that has been used are presented in Section 2. In Section 3 we discuss the results of calculations and our conclusion is given in Section 4.

2. Model and method

The electronic part of the Hamiltonian can be written as

\[ H = H_1 + H_{dl} + H_0 + H_T \]

where \( H_{dl} \) denotes the Hamiltonian of left/right electrode and \( H_0 \) represents molecular Hamiltonian. Both the electrodes are described in the wide-band approximation [7,8]. The PTh molecule is considered as a quasi-one-dimensional chain with N rings, which can be described by means of modified SSH Hamiltonian as follows [1,9]:

\[ H_{PTh} = \sum_{i=1}^{4N} \sum_{\sigma} \left( t_{i\sigma} C_{i\sigma} C_{i\sigma} + t_{i+1\sigma} (C_{i+1\sigma} C_{i\sigma} + C_{i\sigma}^+ C_{i+1\sigma}^+) \right) + \sum_{n=1}^{N} \sum_{\sigma} \left( \epsilon^{(t)} (C_{4n\sigma}^+ C_{4n-3\sigma} + C_{4n-3\sigma}^+ C_{4n-3\sigma}) + \epsilon^{(c)} (C_{4n\sigma} C_{4n-3\sigma} + C_{4n-3\sigma}^+ C_{4n-3\sigma}) \right) \]

where

\[ t_{i,i+1} = t_0 - t_f \cos \left( \frac{i\pi}{N} \right) - \alpha (u_{i+1} - u_i) \]

The index \( i \) runs over the orbitals of carbon chain of the molecule. The operator \( C_{i\sigma} (C_{i\sigma}^+) \) creates/annihilates a \( \sigma \) electron with

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Fig. 1. Schematic representation of polythiophene molecule sandwiched between two ferromagnetic electrodes in the presence of magnetic field.

spin \( \sigma \) at the \( i \)th site of the PTh molecule. \( e_{0} \) is the onsite energy of carbon atoms and \( t_{L}+1 \) denotes the hopping integral between two neighboring sites. \( t_{0} \) is the transfer integral in an undimerized molecule and \( t_{i} \) is the confinement constant, which guarantees the nondegenerate characteristics of the ground state [10]. The electron–phonon coupling constant denoted by \( z \), \( We \) and \( r \) shows the effect of sulfur atom on the Hamiltonian of molecule and \( u_{i} \) is the displacement of the \( i \)th carbon atom. Finally in Eq. (1) \( H_{r} \) denotes coupling between molecule and electrodes. Electron states in the chain accompanied with \( m \) phonons can be written as [7,8]:

\[
|n\sigma,m\rangle = d_{n}^{m}(a_{\sigma}^{\dagger})^{m}\sqrt{m!}|0\rangle
\]

where \( a_{\sigma} \) and \( a_{\sigma}^{\dagger} \) are phonon creation and annihilation operators, respectively, and \( |0\rangle \) shows the vacuum state. For the sake of simplicity, we consider only one phonon mode with energy \( \omega \). In this new formalism Hamiltonian of the scattering region can be written as:

\[
H_{M} = \sum_{i} \sum_{\sigma,\pi} (\varepsilon_{0} + m\omega)|i,\sigma,m\rangle \langle i,\sigma,m| - \sum_{i=1,\sigma,m}^{N} t_{i,i+1}(|i,\sigma,m\rangle \langle i+1,\sigma,m| + |i+1,\sigma,m\rangle \langle i,\sigma,m|) - \sum_{\sigma,\pi}^{N}(\varepsilon_{4n+3,\sigma,m}\langle 4n+3,\sigma,m| + |4n,\sigma,m\rangle \langle 4n,\sigma,m|) + \Gamma_{4}(\langle 4n,\sigma,m| + |4n+3,\sigma,m\rangle \langle 4n+3,\sigma,m|) - \sum_{i=1,\sigma,m}^{N} \lambda_{i}i\sigma,m + 1(i,\sigma,m + 1) \langle i,\sigma,m| + |i,\sigma,m\rangle \langle i,\sigma,m + 1|)
\]

where \( \lambda \) is the energy of electron–phonon interaction; in this work we assume that \( |\lambda| = |\varepsilon_{4}|. If we neglect inelastic electron–phonon interactions during conduction process, electron states will be changed from \( |1,\sigma,m\rangle \rightarrow |4N+1,\sigma,m\rangle. But if we consider inelastic interactions, electrons can absorb/emits phonons and enter from \( |1,\sigma,m\rangle \rightarrow |4N,\sigma,m\rangle \); for such a process we can write the transmission coefficient as follows [7]:

\[
T_{m,m}^{\sigma,\sigma}(\epsilon) = \Gamma_{\sigma}^{R} \Gamma_{\sigma}^{L} \left| G_{m+1,m+1,\sigma}^{\sigma}\right|^{2}
\]

where \( \Gamma_{\sigma}^{R} = 2\pi|\gamma_{\sigma}^{R}|^{2} \rho_{\sigma}^{R} \gamma_{\sigma}^{R} \) is the coupling strength between molecule and electrodes, \( \rho_{\sigma}^{R} \) is the density of state in the electrodes for spin \( \sigma \) and Green's function is defined as follows [1,7,8]:

\[
G_{m+1,m+1,\sigma}^{\sigma}(\epsilon) = \left[ E - H_{M} - \sum_{\sigma'}^{\sigma} - \sum_{\sigma}^{\sigma'} \right]^{-1}
\]

The interaction between molecule and leads is described through self-energy terms. In the wide-band approximation, \( \Gamma_{\sigma}^{R} \) is independent of energy and \( \Sigma_{\sigma}^{R} = \varepsilon_{L}^{R} \).

On calculating the transmission coefficients for all the possible transmission mechanisms we can define the total transmission function as a sum of all the incoming channels \( m \) and all the outgoing channels \( m' \), weighted by the appropriate factor \( P_{nn} \), which is the Boltzmann distribution function [7,8]:

\[
T_{m,n}^{\sigma,\sigma}(\epsilon) = \sum_{m'\sigma'} P_{m,m'} T_{m,m'}^{\sigma,\sigma}(\epsilon)
\]

Elastic part of transmission occurs when \( m \) and \( m' \) are equal and can be written as [7,8]:

\[
T_{el}(\epsilon) = \sum_{m,\sigma} P_{m,m} T_{m,m}^{\sigma,\sigma}(\epsilon)
\]

The current total through junction is derived as follows:

\[
I_{tot} = \frac{2e}{h} \int_{-\infty}^{\infty} d\epsilon \sum_{m,\sigma} T_{m,m}^{\sigma,\sigma}(\epsilon) [P_{m}f_{L}^{m}(1-f_{R}^{m}) - P_{m}f_{R}^{m}(1-f_{L}^{m})]
\]

The elastic part of the current can be obtained from the above equation by the assumption of \( m = m' \) [7,8]:

\[
I_{el} = \frac{2e}{h} \int_{-\infty}^{\infty} d\epsilon \sum_{m,\sigma} T_{m,m}^{\sigma,\sigma}(\epsilon) f_{R}^{m}(1-f_{L}^{m})
\]

where \( f_{L}^{m} \) and \( f_{R}^{m} \) is the Fermi function of the left/right electrode with chemical potential \( \mu_{L/R} = \mu_{L/R}^{m} = (eV/2) \) and Fermi energy \( e_{L/R} \)

\[
I_{el}(\epsilon) = \text{[exp}(\beta(e-\mu_{L/R})(1+1)]^{-1}
\]

The displacement of the \( i \)th carbon atom is evaluated with the help of the Hellmann–Feynman theorem as follows [10,11,12]:

\[
u_{i} = \sum_{\sigma} \left[ \nu_{i1} + \nu_{i2} + 2(2\pi)^{-1} \sum_{k,\sigma} \sum_{\mu} \langle \Psi_{i1,\mu,\sigma}^{+} \Psi_{i1,\mu,\sigma} - \Psi_{i1,\mu,\sigma}^{+} \Psi_{i1,\mu,\sigma} \rangle \text{J}_{i}(x,\text{int}) \right]
\]

where \( \lambda(x,\text{int}) = \begin{cases} 1 & x \text{ is integer} \\ 0 & \text{otherwise} \end{cases} \)

We assume that the system is in the ground state and only the lowest levels are occupied. The calculations are performed as follows.

Eqs. (13) and (14) are solved self-consistently and the ground state of the isolated molecule is obtained. Then we calculate the transmission coefficient in the presence \( T_{\sigma}^{\sigma} \) and absence \( T_{\sigma}^{\sigma} \) of magnetic field. Total current and elastic part of the current can be calculated from Eqs. (10) and (11). Finally, tunneling magnetoresistance can be defined using the following equation [12]:

\[
TMR(V) = \frac{I_{b}^{p}(V)}{I_{b}^{p}(0)}
\]

where \( I_{b}^{p} \) is the current in the presence/absence of magnetic field. Calculations are performed for the total current and the elastic part of the current and the TMR is compared in these two situations.

3. Numerical result and discussion

Numerical calculations are carried out for a molecule with 8 rings (8 sites) and the parameters for a PTh chain are chosen as
These parameters can significantly reproduce the experimental band gap [1]. We have used the following set of parameters for describing cobalt electrodes (given in 1/eV), \( \rho^I = 0.1367 \), \( \rho^J = 0.5772 \), and we set \( \gamma_L = \gamma_R = 0.2 \) eV, \( \epsilon_f = -1 \) eV and \( \omega = 0.1 \) eV. Maximum number of allowed phonon quanta is chosen to be five and all of the calculations are done at room temperature. In the presence of magnetic field, magnetic moments of electrodes point to the field direction. As a result density of states and transmission coefficient are different for spin up and down. Fig. 2 shows the total and elastic part of transmission spectrum as a function of incident electron energy for spin up and down. Fig. 3 shows the current–voltage characteristic of PTh molecule in the presence of magnetic field. The magnitude of the current flowing through the PTh molecule is in the order of micro-Ampere, which is comparable to the experimental result with gold leads [13]. As can be seen, the non-Ohmic behavior of the...
molecule is evident. Regarding the current–voltage characteristic of PTh it can be suggested as a switch in the electronic circuit. Fig. 4(a) presents TMR versus bias voltage in the presence and absence of inelastic electron–phonon interactions. The difference between these two situations is plotted in Fig. 4(b). As expected, in the presence of electron–phonon interaction, due to spin-independent nature of interaction, TMR decreases. In the low-voltage regime the current is small and TMR is constant. With increasing voltage energy-window opens and resonant tunneling occurs, and as a result, current increases while TMR decreases. In the presence of inelastic electron–phonon interaction polaron formation shifts the current peak and reduces the conductance gap [14]. As a result rapid decreasing of TMR starts at a lower voltage. At higher voltages, TMR does not change with the increase in voltage and the changes made by inelastic interactions disappear.

4. Conclusion

In summary, based on Walczak formulation we have investigated the effect of inelastic electron–phonon interactions on TMR in a polyiopiphene molecule. Our calculations indicate that the change in TMR due to inelastic interaction is limited in a small bias voltage interval and can be neglected in other bias voltages.

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