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A solvable model for spin-dependent electronic transmission of ferromagnetic nanowires

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ABSTRACT

We present an exact analytical method to calculate the electronic transmission coefficient of ferromagnetic nanowires based on Green's function theory and tight-binding approach. To this end, we obtain the spin-dependent self-energies of the nanowire due to the existence of ferromagnetic leads and derive the elements of system Green's function matrix. Spin-dependent electron transport via some configurations of a ferromagnetic nanowire including magnetic defects is investigated in detail. Further, we analyze the electron reflection from an ideal semi-infinite magnetic chain with different moments at the edge. The results can be useful to simulate and develop magnetic and spintronic nano-devices.

1. Introduction

To combine the miniaturization of nanoelectronics and spin phenomena, the role of low dimensionality in the magnetic and transport properties of materials becomes important [1,2]. Thanks to the modern nanotechnology, it is possible today to build low dimensional magnetic devices and to examine the interesting results predicted by theoreticians. The Rashba [1,3], Aharonov–Bohm [4–6], spin–orbit coupling [7] and Zeeman [1,8] effects are usually studied in the mesoscopic systems under a magnetic field. The last one deals with interaction of electron spin by internal or external magnetic field and leads us to spintronics. Spintronics, a branch of electronics that employs the spin of electron, becomes a fast growing research field over the past decades [2,8,9]. The giant magnetoresistance [10–12], spin valve behavior [8,13], magnetic storage [14], spin filter [15] and injection of spin polarized currents from ferromagnetic materials to paramagnetic materials [16,4] are some important spintronic phenomena. Further, to investigate the electrical spin injection such as spin transport, spin detection and spin accumulation in magnetic and nonmagnetic nanowires usually the electrodes are chosen to be ferromagnetic materials [2,17–19]. Accordingly, the theoretical and experimental studies of spintronic including ferromagnetic leads have been attracted a great deal of interests in recent years.

The aim of this paper is to formulate the spin-dependent electron transport through the nanostructures sandwiched between two ferromagnetic leads at the tight-binding approach. Two most important techniques which have been developed to solve the transport problem of quasi-one-dimensional systems are Green's function and transfer matrix methods. We employ the transfer matrix method to obtain Green's function matrix elements analytically. We focus on spin-dependent transmission coefficient of ferromagnetic nanowires and derive an analytical formalism for the self-energies and transmission coefficients of up and down spins. Moreover, we use the model to study the effect of the magnetic defects on the electronic transport of an ideal ferromagnetic chain.

The paper is organized as follows. In Section 2, we present an analytical formalism to consider spin-dependent electronic transmission of magnetic chain including three different parts. Further, we apply this analytic formalism to some interesting configurations of magnetic chains. In Section 3, we give some conclusions and remarks. In Appendix A, we derive the transmission coefficient in terms of Green's function matrix elements which are derived by using the transfer matrix method.

2. The model and formalism

In this section, we obtain an analytical formalism for the spin-dependent transport of ferromagnetic nanowires. Suppose a magnetic

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chain is divided into three different regions, i.e., $\alpha = L, W, R$. Each region is explained by the following Hamiltonian:

$$\mathbf{H}_\alpha = \sum_i (\varepsilon_\alpha I - \vec{h}_\alpha \cdot \vec{\sigma})\mathbf{C}_i^\dagger \mathbf{C}_i + \beta_\alpha \sum_i \mathbf{C}_i^\dagger \mathbf{C}_{i+1} + h.c., \tag{1}$$

where $i = -\infty, \ldots, 0$ stands for the L, $i = 1, \ldots, N$ identifies W and $i = N+1, \ldots, \infty$ distinguishes the R region. Here, I is the unit matrix, ε_α and β_α are the spin-independent on-site and hopping energies of region α, respectively, and the term $\vec{h}_\alpha \cdot \vec{\sigma}$ describes the interaction of electron spin with the magnetic field of atoms in region α. In the spherical coordinates, $\vec{h}_\alpha$ is specified by the amplitude h_α (the spin flip parameter), polar angle θ_α and azimuthal angle ϕ_α; and $\vec{\sigma}$ is the Pauli spin operator having components of $(\sigma_x, \sigma_y, \sigma_z)$. Furthermore, $\mathbf{C}_i^\dagger$ and $\mathbf{C}_i$, respectively, are the row and column vectors of creation and annihilation operators with $c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger$ and $c_{i\uparrow}, c_{i\downarrow}$ elements. The Hamiltonian for the left (right) contact reads

$$\mathbf{H}_{WL(R)} = \mathbf{H}_{L(R)W} = \beta_{WL(R)} \mathbf{C}_{0(N)}^\dagger \mathbf{C}_{1(N+1)} + h.c., \tag{2}$$

where $\beta_{WL(R)}$ is the spin-independent hopping integral between the left (right) lead and the center wire. In Fig. 1, we show that this magnetic chain can be regarded as a ladder network with on-site energies of $\varepsilon_\alpha \pm h_\alpha \cos\theta_\alpha$ and hopping parameter of $-h_\alpha \sin\theta_\alpha \exp(-\imath\phi_\alpha)$. Now, we can follow the presented formalism in Appendix A by introducing the following block matrices in Eq. (A.1):

$$\mathbf{H}_{i,i} = \begin{pmatrix} \varepsilon_W - h_W \cos\theta_W & -h_W \sin\theta_W e^{-\imath\phi_W} \\ -h_W \sin\theta_W e^{\imath\phi_W} & \varepsilon_W + h_W \cos\theta_W \end{pmatrix}, \tag{3a}$$

$$\mathbf{H}_{i,i+1} = \mathbf{H}_{i+1,i} = \beta_W I; \quad i = 2, \ldots, N-1. \tag{3b}$$

This means all the atoms are the same except the first and last ones in the center wire that is for these tow atoms, the magnetic and tight-binding parameters can be different. In this paper, we assume that this difference exists just in their magnetic moments. So, we represent the magnetic moment vector of the first (last) site by $h_{W1(N)}$, $\theta_{W1(N)}$ and $\phi_{W1(N)}$ components. By substituting Eqs. (3) in Eqs. (A.4), and after simplification, we derive the following analytic formula for the system transfer matrix:

$$(\mathbf{P}_i)^{N-2} = \begin{pmatrix} f_N^+ & g_N^+ & -f_{N-1}^+ & -g_{N-1}^+ \\ g_N^- & f_N^- & -g_{N-1}^- & -f_{N-1}^- \\ f_{N-1}^+ & g_{N-1}^+ & -f_{N-2}^+ & -g_{N-2}^+ \\ g_{N-1}^- & f_{N-1}^- & -g_{N-2}^- & -f_{N-2}^- \end{pmatrix}, \tag{4}$$

in which

$$f_n^\pm = \cos^2(\theta_W/2) D_n^\pm + \sin^2(\theta_W/2) D_n^\mp, \tag{5a}$$

$$g_n^\pm = \tfrac{1}{2} e^{\mp\imath\phi_W} \sin\theta_W (D_n^+ - D_n^-), \tag{5b}$$

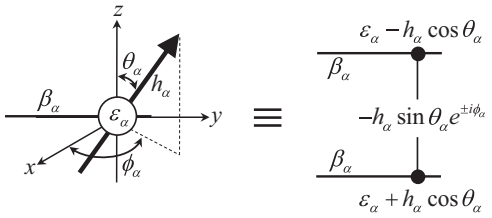

Fig. 1. In the system $\alpha = W, L, R$, each atom with on-site energy ε_α and magnetic moment $\vec{h}_\alpha$, specified by $(h_\alpha, \theta_\alpha, \phi_\alpha)$ in spherical coordinates, corresponds to an effective ladder unit cell with $\varepsilon_\alpha \pm h_\alpha \cos\theta_\alpha$ and $-h_\alpha \sin\theta_\alpha e^{\pm\imath\phi_\alpha}$ tight-binding parameters.

where

$$D_n^\pm = \frac{\lambda_\pm^{n+1} - \lambda_\pm^{-n-1}}{\lambda_\pm - \lambda_\pm^{-1}},$$

with

$$\lambda_\pm = \xi_W^\pm + [(\xi_W^\pm)^2 - 1]^{1/2}.$$

Here, $\xi_W^\pm = (\varepsilon - \varepsilon_W \pm h_W)/2\beta_W$ are dimensionless parameters for the magnetic center wire. In order to get the total spin-dependent transmission coefficient, the self-energies of the center wire due to the existence of magnetic leads are needed. The left (right) self-energy can be calculated by the left (right) surface Green's function of the center wire. The result for a lead with arbitrary magnetic parameters, in the nearest neighbor tight-binding approach, gives

$$\mathbf{\Sigma}_\alpha = \begin{pmatrix} \Sigma_\alpha^+ & \Delta_\alpha^+ \\ \Delta_\alpha^- & \Sigma_\alpha^- \end{pmatrix}; \quad \alpha = L, R, \tag{6}$$

where

$$\Sigma_\alpha^\pm = \frac{\beta_{W\alpha}^2}{\beta_\alpha}\Big([(\xi_\alpha^\pm)^2 - 1]^{1/2} \cos^2(\theta_\alpha/2) + [(\xi_\alpha^\mp)^2 - 1]^{1/2} \sin^2(\theta_\alpha/2) + \frac{\varepsilon - \varepsilon_\alpha \pm h_\alpha \cos\theta_\alpha}{2\beta_\alpha} \Big),$$

$$\Delta_\alpha^\pm = \frac{\beta_{W\alpha}^2}{2\beta_\alpha} e^{\mp\imath\phi_\alpha} \Big([(\xi_\alpha^+)^2 - 1]^{1/2} - [(\xi_\alpha^-)^2 - 1]^{1/2} + \frac{h_\alpha}{\beta_\alpha} \Big) \sin\theta_\alpha,$$

in which $\xi_\alpha^\pm = (\varepsilon - \varepsilon_\alpha \pm h_\alpha)/2\beta_\alpha$ are dimensionless parameters for the lead $\alpha = L, R$. The relation $|\xi_\alpha^{+(-)}| \le 1$ determines the allowed energy range for the electron with spin up (down). The left (right) self-energy is related to the left (right) broadening matrix as

$$\mathbf{\Gamma}_{L(R)} = \imath(\mathbf{\Sigma}_{L(R)} - \mathbf{\Sigma}_{L(R)}^\dagger).$$

Finally, the system transmission coefficient, $T(\varepsilon)$, can be computed by the following formula:

$$T(\varepsilon) = \mathrm{tr}(\mathbf{\Gamma}_L \mathbf{G}_{N,1}^\dagger \mathbf{\Gamma}_R \mathbf{G}_{N,1}). \tag{7}$$

where $\mathbf{G}_{N,1}$ is the left-most block of the wire Green's function matrix and can be calculated by Eq. (A.3b). Now, all quantities in Eq. (7) are provided and one can evaluate the total transmission coefficient of magnetic junctions analytically.

By choosing the preferred direction of magnetic moments in the leads at the z direction, we can simplify the matter. This equivalents to the cases of $\theta_{L(R)} = 0$ and π corresponding to up and down directions of magnetic moments, respectively. Therefore, there are two transmission channels with energy bands of $\varepsilon = \varepsilon_{L(R)} \pm h_{L(R)} + 2\beta_{L(R)} \cos k_{L(R)} a_{L(R)}$, where $a_{L(R)}$ is the lattice constant and $k_{L(R)}$ is the electron wave-number of the left (right) lead. In these cases, four well-defined transmission coefficients can be introduced as follows [20,21]:

$$T^{\sigma\sigma'} = 4\,\mathrm{Im}\,\Sigma_L^\sigma\,\mathrm{Im}\,\Sigma_R^{\sigma'}\,|G_{N,1}^{\sigma\sigma'}|^2, \tag{8}$$

where $\sigma = \uparrow, \downarrow$ and the $\Sigma_{L(R)}^\sigma$ from Eq. (6) for two angles of $\theta_{L(R)} = 0$ and π, respectively, read

$$\Sigma_{L(R)}^{\uparrow(\downarrow)} = \Sigma_{L(R)}^{+(-)} = \frac{\beta_{WL(R)}^2}{\beta_{L(R)}} (\xi_{L(R)}^{+(-)} + [(\xi_{L(R)}^{+(-)})^2 - 1]^{1/2}).$$

Also, $G_{N,1}^{\sigma\sigma'}$ is the (i,j)th entry of $\mathbf{G}_{N,1}$ where $i(j) = 1, 2$ corresponds to $\sigma(\sigma') = \uparrow, \downarrow$. The total transmission coefficient is

$$T = \sum_{\sigma,\sigma'} T^{\sigma\sigma'} = \sum_\sigma T^\sigma, \tag{9}$$

where $T^\sigma = T^{\uparrow\sigma} + T^{\downarrow\sigma}$.

Without loss of generality and for the sake of simplicity, hereafter we take all on-site and hopping energies in the system