Conductance through a Magnetic Domain Wall in Double Exchange System

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The conductance through a magnetic domain wall is calculated for the double exchange system as a function of energy and the width of the domain wall. It is shown that when the carrier density is low enough, the blockade is almost complete even for the smoothly varying spin configuration, i.e., large width of the domain wall. This result is applied to the manganese oxides.

KEYWORD: double exchange system, doped Mott insulator, La$_{1-x}$Sr$_x$MnO$_3$

Recently intensive studies have been focused on the colossal magnetoresistance (CMR) in double exchange systems, e.g., manganese oxide La$_{1-x}$Sr$_x$MnO$_3$. The conduction electrons in $e_g$ orbitals are moving in the background of the $t_{2g}$ spin configuration, and the basic mechanisms of this phenomenon is that the coherent transfer of electrons is enhanced when the external magnetic field forces the spins to align. In these materials, the $t_{2g}$ spin is localized, and the Hund coupling $2g$ is so strong that the spin of the $e_g$ electrons obey that of the $t_{2g}$ spins at each site. Then the carrier becomes essentially spinless, and the hopping $t_{ij}$ between the two sites is determined by the relative orientation of the two localized spins.

$$t_{ij} = t \left( \cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} + e^{-i(\phi_i - \phi_j)} \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} \right),$$

where the direction of the localized spin at site $i$ is represented by the polar coordinates $\theta_i$ and $\phi_i$. The amplitude $|t_{ij}|$ is given by $t \cos(\theta_i/2)$ with $\theta_i$ being the angle between the two spins. The phase of $t_{ij}$, on the other hand, constitutes the gauge field discussed intensively in the context of RVB theories. In this paper we focus on the amplitude of $t_{ij}$ considering the magnetic domain wall. When the spins are inverted between two layers, i.e., $\theta_i = \pi$. The hopping $t_{ij} = 0$ and the conductance is zero through that domain wall. However this idealistic situation is rather difficult to realize, because the width of the magnetic domain wall $L$ is determined by the competition between the exchange interaction and the magnetic anisotropy energy. Recent neutron scattering experiment has revealed the spin wave dispersion in LaMnO$_3$, where the spin align ferromagnetically within the plane while antiferromagnetically ordered between planes. They observed the gap in the spin wave dispersion, from which they estimated the anisotropy energy $\Delta = g \mu_B H_A = 0.61 \pm 0.11$ meV which is about 1/20 of the exchange coupling $8JS = 13.36 \pm 0.18$ meV within the layer. A rough estimate of the domain wall width $L$ is given by $L \sim \sqrt{8JS/\Delta} \sim 5$ because $L$ is determined by the balance between the elastic energy $8JS \cdot L(1/L^2)$ and the anisotropy energy $\Delta \cdot L$. We then have to consider the conductance through a finite-width domain wall.

In this paper we study the conductance through a magnetic domain wall as a function of its width $L$ and the energy of the incoming carrier. The model we employ is the one-dimensional tight-binding Hamiltonian.

$$H = -\sum_i t_i C_i^\dagger C_{i+1} + h.c. \quad (2)$$

where $t_i = t_{i,i+1}$ is given by $t_i = t \cos(\pi/2L)$ for $0 \leq i \leq L$ while $t_i = t$ for other $i$. One may worry about the degeneracy of $e_g$ orbitals, which is especially important when one consider the density of carriers. The basic observation is that the carrier number is the density of the holes doped to the Mott insulator. This is controlled by the Sr concentration $x$ in La$_{1-x}$Sr$_x$MnO$_3$. For $x = 0$ the system is a Mott insulator in the sense that the $e_g$ orbitals for each Mn ion is singly occupied. This is because the strong on-site Coulomb interaction prohibits the double occupancy of $e_g$ orbitals for each site. This constraint is treated by introducing the rotating coordinates with the isospin $\vec{T}_i$ for the orbital degrees of freedom together with the usual spin $\vec{S}_i$. The repulsive on-site interaction between the electrons in the $e_g$ orbitals is treated by introducing the Stratonovich-Hubbard variables $\vec{\phi}_{Ti}$ and $\vec{\phi}_{Si}$ corresponding to $\vec{T}_i$ and $\vec{S}_i$, respectively. Then the $e_g$ electrons $d_{\gamma\alpha}^i, d_{\gamma\alpha}^i$ ( $\alpha$: spin index, $\gamma$: orbital index ) are coupled with these fields as $\sum_\alpha \vec{\phi}_{Ti} \cdot d_{\gamma\alpha}^i \vec{\phi}_{Si} \cdot d_{\gamma\alpha}^i$ and $\sum_\alpha \vec{\phi}_{Si} \cdot d_{\gamma\alpha}^i \vec{\phi}_{Ti} \cdot d_{\gamma\alpha}^i$. In the rotating frame the transformed electrons are feeling both the $\vec{\phi}_{T}$ and $\vec{\phi}_{S}$ fields in the $+z$ direction, and hence the density of states are split into four. The lowest one corresponds to $\uparrow$ both for the spin and isospin, which is fully occupied for $x = 0$. The spin- and orbital-less operator $C^\dagger, C$ appearing in eq.(2) is the hole operator in this lowest bunch of the density of states, and their density is the Sr concentration $x$. Then in reality the effective hopping integral $t_{ij}$ depends also
on the isospin $\vec{T}$ as well as the spin $\vec{S}$. For the magnetic domain wall we have to determine also the spatial variation of the isospin. In this paper, however, we neglect this orbital degrees of freedom. We only mention that the conductance $G$ should be reduced if one consider this factor, and $G$ obtained in this paper gives the upper bound.

We calculate the transmission coefficients of the system by using the transfer matrix method and the conductance by the Landauer formula. By using a one-particle state which is written as $|\Psi\rangle = \sum_{i=1}^N \psi_i C_i^\dagger |0\rangle$, where $\psi_i$ are complex coefficients, the corresponding Schrödinger equation, $H|\Psi\rangle = E|\Psi\rangle$, where $E$ is the energy eigenvalue, is

$$-t_{i+1}\psi_{i+1} - t_{i-1}\psi_{i-1} = E\psi_i.$$

This equation can be written as

$$\Psi_{i+1} = M_i \Psi_i,$$

where

$$\Psi_i = \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}, \quad M_i = \begin{pmatrix} -E/t_{i+1} & -t_{i-1}/t_{i+1} \\ 1 & 0 \end{pmatrix}. \tag{5}$$

These matrices describes the propagation of a plane wave and their two eigenstates are corresponding to the left- and right-going solutions, $\bar{\psi}_i(\pm)$ and $\bar{\psi}_i(-)$, respectively. Any state can be represented by a linear combination of them as

$$\psi_i = (\bar{\psi}_i(+), \bar{\psi}_i(-)) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \tag{6}$$

where $c_1$ and $c_2$ are the expansion coefficients. When the domain wall locates between the 0-th and $L$-th sites, the transfer matrix

$$M = \prod_{i=-1}^L M_i, \tag{7}$$

relates the incoming and outgoing amplitudes as

$$\begin{pmatrix} t \\ r' \end{pmatrix}_{L+1} = M \begin{pmatrix} 1 \\ r \end{pmatrix}_{-1}, \tag{8}$$

where $(t, r')$, and $(1, r)$, are the expansion coefficients describing the wave amplitudes on the left and right ferromagnetically ordered regions, respectively. To obtain the reflection and transmission amplitudes, $(r$ and $t$, respectively,) we solve the coupled equation under the restriction $r' = 0$. By using the Landauer formula, the conductance is obtained as

$$G = \frac{e^2}{\hbar} T,$$\tag{9}

where $T = t^* t$ is the transmission coefficient. Since the analytical form as a function of $E$ and $L$ is tedious to write down, we only show the results in Fig. 2, where the conductance is shown as a function of the energy $E$ for $L = 2, 3, 5, \text{ and } 10$.

![Fig. 2. Conductance through a domain wall as a function of the energy $E$ for various domain wall width $L$.](image)

It is noted that the conductance $G$ is suppressed below a certain energy $\epsilon_c^{(L)}$ which depends on the domain wall width $L$. This means that the magnetic domain wall acts as a energy filter. This can be understood as follows. In the domain wall region, the hopping is reduced from $t$ to $t \cos(\pi/2L)$. Therefore if $L$ is large enough, we can consider the band structure in the domain wall region $(0 \leq x \leq L)$ where the band width is reduced by the factor $\cos(\pi/2L)$. The lower band edge is shifted upward to $\epsilon_{\min}^{(L)} = -2t \cos(\pi/2L)$ for $0 \leq x \leq L$, and the particle with energy less than $\epsilon_{\min}^{(L)}$ should tunnel though the potential barrier. Roughly $\epsilon_c^{(L)}$ coincides with $\epsilon_{\min}^{(L)}$. When one consider the 1D Schrödinger equation

$$-\frac{\hbar^2}{m} \frac{d^2 \psi}{dx^2} + V(x)\psi = \epsilon \psi \tag{10}$$

where $\frac{\hbar^2}{m} = t$, $\epsilon = E + 2t$, and the potential $V(x)$ being given by

$$V(x) = \begin{cases} V = 2t \left(1 - \frac{\cos \frac{x}{L}}{\cos \frac{\pi}{L}}\right) & 0 < x < L \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

Then the conductance $G_s(\epsilon)$ for this continuum model is obtained as

$$G_s(\epsilon) = \frac{\frac{V^2}{4x_0(V-\epsilon)} \sinh^2 \left(\frac{2x_0(V-\epsilon)}{\hbar^2}\right)}{\sqrt{\frac{2x_0(V-\epsilon)}{\hbar^2}}} \tag{12}$$

From eq.(12), it can be seen that $G_s(\epsilon) \sim \frac{e^2}{\hbar} L^2 \epsilon$ for $\epsilon \ll t/L^2$ and $G_s(\epsilon) \sim \frac{e^2}{\hbar} t^2$ for $\epsilon \gg t/L^2$. This behavior is seen in the large $L$ case, e.g., $L = 10$, in Fig. 2.
Now we discuss the possible application of our results to manganese oxides. As discussed above the undoped LaMnO$_3$ shows ferromagnetism within the layer while the moments align antiferromagnetically between the layers. Then the dilute hole carriers doped to it should be able to move freely within the plane. However the experiments show insulating behavior in La$_{1-x}$Sr$_x$MnO$_3$ for small $x$. One possible explanation is that the local Jahn-Teller distortion occurs around the carrier (Jahn-Teller polaron) and finally leads to the self-trapping. Another possibility is that each plane is divided into several magnetic domains, and the domain walls block the carriers. When the carrier concentration is $x$, the Fermi wavevector $k_F$ is $(4\pi x)^{1/2}$ assuming that the hopping between the layers is zero due to the antiferromagnetic ordering. Then the energy $\epsilon$ for the occupied states measured from the bottom of the band satisfies $\epsilon \leq tk_F^2 = 4\pi tx$ which should be compared with $\epsilon_c(L)$. Assuming $L = 5$, $\epsilon_c(L) + 2t$ can be read to be around 0.2t from Fig. 2. Then for $x < x_c = \frac{2t}{4\pi t} \cong 0.02$, domain walls block the carriers and the system will become insulator.

In summary we have studied the effect of a magnetic domain wall on the transport in the double exchange system. It is found that even a smoothly varying domain wall reflects the carriers when the carrier concentrations is low enough, and this might explain the insulating behavior of La$_{1-x}$Sr$_x$MnO$_3$ for small $x$. In 2 and 3D the curvature of the domain wall will affect the conductance, and its fluctuations generate the noise. This may explain the 1/f noise observed experimentally, but the detailed analysis in now in progress. We also propose that this sensitivity of the conductance to the magnetic domain wall in slightly doped Mott insulator will give a unique opportunity for the device made of strongly correlated electronic systems.

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