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Multiband coupling effect on density of states and tunneling conductance spectra of ferromagnetic material

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ABSTRACT

The electronic density of states (DOS) of ferromagnetic materials are theoretically studied within a two-band approach in one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) systems. In the two-band approximation, s-band and d-band coupling were considered. It has been found that if the coupling vanishes, the two bands can cross at some points in the energy spectra. When the coupling between bands is present, a gap is opened up at the corresponding point, thereby avoiding crossovers. The size of the gap depends on the size of the coupling strength. For any dimensionality, the DOS with no coupling behaves like a one-band model. When presenting the coupling strength, there is a change in the slope in the DOS, corresponding to those crossing points. In particular, this change is most prominent when the coupling strength is small and it almost disappears when the coupling strength is strong. With a large coupling strength, the energy band is extended. Finally, the measurable tunneling conductance spectra of a metal/ferromagnet junction within this approximation were clearly analyzed.

1. Introduction

The electronic density of states (DOS), of some novel materials, such as the $YBa_2Cu_3O_{7-\delta}$ (YBCO) family of high temperature superconductors, can be directly measured from real experiments with multiple energy scales [1–5]. This kind of material shows a coupling between bands in the DOS called chain–plan coupling. Many studies show interesting features due to the coupling, for example, the satellite features and the splitting peak of the main superconducting gap [6–9]. Thus, the band structure coupling in the material is piquant.

Currently, one of the most important materials is a ferromagnetic material and its family. This is because this kind of material can cause Giant Magnetoresistance (GMR) to occur in the junctions between ferromagnets and normal metals [10–12]. The application of this resistance is used in a new field called spin electronic or spintronics [13–15], which combines the concepts of electronic transport and spin physics. The main idea of this field is to produce a quantum state to contain information in quantum computing technology. The frontiers of spintronics have been pushed more and more towards the nanoscale; in particular, by attaching macroscopic leads to small quantum dots. However, the understanding of the band structure of the ferromagnetic material is still lacking: especially for new kinds of ferromagnet that can be found in experiments, for example, ferromagnetic semimetal [16], ferromagnetic semiconductor [17,18], ferromagnetic graphene [19], and ferromagnet with spin–orbit interaction. All of these materials can affect the efficiency of GMR in the tunnel junctions.

In a classic ferromagnet, like iron or nickel, the band structure calculations show that there is a hybridization region between different bands of the ferromagnet near the Fermi level, and this is referred to as s–d band mixing [20–22]. That is, one comes from the 3d band and another comes from the 4 s band. Especially, these two bands are occupied by valence electrons that directly reflect the physical properties of the material. In previous work, it was found that the electronic properties of ferromagnetic material was affected by s–d band coupling [23]. Thus, the band structure coupling in this material is interesting and plays a crucial role in determining the physical properties of this material.

In this work, we calculate the DOS of a ferromagnetic material within a two-band coupling approximation. The approach taken was phenomenological for a coupling strength between the bands in the material. In Section 2, we develop a model Hamiltonian for a ferromagnet within two-band coupling. We focused on the DOS of the ferromagnet with the s-band and d-band mixing via the coupling strength. Finally, for comparison, we calculate the DOS for both, with and without coupling strength. The results of these calculations were discussed in Section 3, and the last section is a summary of the work.

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2. Model and formulation

2.1. s–d band coupling Hamiltonian

From the band structure calculations of the ferromagnetic material, hybridization regions between the s band and d band near the Fermi level were identified. In principle, this scenario is caused by a mixing or overlap of the electronic wave functions of the electron with spin-σ from both bands. Due to this, the paper considered the kinetic energy of valence electrons with spin-σ from both bands (the s band and d band) via the coupling strength t to capture the essential effect of this coupling on the DOS. Due to there being four energy bands, d-band with spin-up or spin-down and s-band with spin-up or spin-down, the Hamiltonian of the coupling system is a 4×4 matrix as given by

$$H_{FM} = \begin{bmatrix} H_{\uparrow}^{d} & 0 & t & 0 \\ 0 & H_{\downarrow}^{d} & 0 & t \\ t & 0 & H_{\uparrow}^{s} & 0 \\ 0 & t & 0 & H_{\downarrow}^{s} \end{bmatrix}, \tag{1}$$

or

$$H_{FM} = \begin{bmatrix} H_0 - E_{ex}^{d} & 0 & t & 0 \\ 0 & H_0 + E_{ex}^{d} & 0 & t \\ t & 0 & H_0 - E_{ex}^{s} & 0 \\ 0 & t & 0 & H_0 + E_{ex}^{s} \end{bmatrix}, \tag{2}$$

where $H_0 \equiv -(\hbar^2/2m_{d(s)}^{*})\nabla^2 - \mu$ is the single particle Hamiltonian of the d (s) band, μ is the chemical potential, and ∇^2 represents $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ in cartesian coordinates. The electron effective mass of the d band and s band are represented by m_d^* and m_s^*, respectively. These two effective masses are different as can be seen in the band structure calculations. However, the electron effective mass of different spin bands in the same energy band are approximately assumed to be equal. That is $m_{s\uparrow}^{*} = m_{s\downarrow}^{*} \equiv m_s^{*}$ and $m_{d\uparrow}^{*} = m_{d\downarrow}^{*} \equiv m_d^{*}$. This is because the slope of the energy dispersion of electrons with spin-up and spin-down in either the s or d bands from the band structure calculations have almost the same value. $\mp E_{ex}^{d(s)}$ refers to the exchange energy of the d(s)-band dispersion with spin-up (-) and spin-down (+), respectively. In reality, it was also found from the band structure calculations that the exchange energy of the s-band (E_{ex}^{s}) and d-band (E_{ex}^{d}) dispersions are different values, so the two parameters were set to be different in this work. The matrix element, t, represents the s-band and d-band coupling with the same spin direction for the ferromagnet. However, the matrix element of the coupling between the spin-up and spin-down sub band from different energy bands is neglected as a way of reducing the number of fitting parameters in our model.

By solving the eigenvalue problem, one can obtain the eigenvalues of the mixing system as given by

$$\lambda_{mix-\uparrow}^{d}(k_{mix}) = \frac{\xi_{\uparrow}^{d}(k) + \xi_{\uparrow}^{s}(k)}{2} + \sqrt{\left|\frac{\xi_{\uparrow}^{d}(k) - \xi_{\uparrow}^{s}(k)}{2}\right|^2 + t^2}, \tag{3}$$

$$\lambda_{mix-\downarrow}^{d}(k_{mix}) = \frac{\xi_{\downarrow}^{d}(k) + \xi_{\downarrow}^{s}(k)}{2} + \sqrt{\left|\frac{\xi_{\downarrow}^{d}(k) - \xi_{\downarrow}^{s}(k)}{2}\right|^2 + t^2}, \tag{4}$$

$$\lambda_{mix-\uparrow}^{s}(k_{mix}) = \frac{\xi_{\uparrow}^{d}(k) + \xi_{\uparrow}^{s}(k)}{2} - \sqrt{\left|\frac{\xi_{\uparrow}^{d}(k) - \xi_{\uparrow}^{s}(k)}{2}\right|^2 + t^2}, \tag{5}$$

$$\lambda_{mix-\downarrow}^{s}(k_{mix}) = \frac{\xi_{\downarrow}^{d}(k) + \xi_{\downarrow}^{s}(k)}{2} - \sqrt{\left|\frac{\xi_{\downarrow}^{d}(k) - \xi_{\downarrow}^{s}(k)}{2}\right|^2 + t^2}, \tag{6}$$

where

$$\xi_{\uparrow}^{d}(k) = \frac{\hbar^2 k^2}{2m_d^{*}} - E_{ex}^{d} - \mu, \tag{7}$$

$$\xi_{\downarrow}^{d}(k) = \frac{\hbar^2 k^2}{2m_d^{*}} + E_{ex}^{d} - \mu, \tag{8}$$

$$\xi_{\uparrow}^{s}(k) = \frac{\hbar^2 k^2}{2m_s^{*}} - E_{ex}^{s} - \mu, \tag{9}$$

$$\xi_{\downarrow}^{s}(k) = \frac{\hbar^2 k^2}{2m_s^{*}} + E_{ex}^{s} - \mu. \tag{10}$$

The subscription *mix* in Eqs. (2)–(6) refers to the system of hybridization (s–d mixing); so, these four equations are for the four mixing bands. However, we still superscript either *d* or *s* in those equations because we would like to remind the reader that these four mixing bands can become the energy bands in the normal case when the coupling strength t in the expressions is absent ($t = 0$).

3. Results and discussion

3.1. Energy dispersion relations

To understand the physical meaning of DOS of ferromagnet within a two band model, we first look more closely at the energy dispersion relations of electrons for each band of the s–d band coupling system based on a simple free electron approach. In Fig. 1, the energy dispersion relations of the four mixing bands are plotted in the cases where (a) t=0, (b) t = 0.05 eV, and (c) t = 0.2 eV. Obviously, Fig. 1(a) with no coupling shows the two kinds of crossing points between energy bands as indicated by the solid and dashed arrows. That is, the crossing points between the same spin direction but different energy bands are indicated by the solid arrows; while, the dashed arrows indicate the crossing points between the bands with the opposite spin directions. When the coupling strength t is presented in the calculation, the dispersion relations are shown in Fig. 1(b) and (c). In this figure, the crossing points in the first case are affected by the coupling strength t, and opened up as a gap; whereas the crossing points in the second case still cross. This is also an expected result of the model because it only considers the coupling strength between the bands of the first kind of crossing point as mentioned in the text above. Particularly, the size of these avoiding crossing points or gaps depends on the size of t as depicted in Fig. 1(c). The last feature identified in the energy dispersion relations is for the energy band extension due to a large coupling strength (t = 0.2 eV). Furthermore, this gap region will be important in the DOS in the next section.

3.2. Density of states: DOS

In this section, we show the density of states of the electrons of the ferromagnet within a two-band model. By definition [24], the DOS is defined by

$$\rho_{mix-\sigma}^{D}(\lambda) = \left(\frac{L}{2\pi}\right)^{D} \int_{-\infty}^{\infty} d\mathbf{k}_{mix}\, \delta[\lambda - \lambda_{mix-\sigma}^{d(s)}(\mathbf{k})], \tag{11}$$

where index D refers to the dimensions of the system. $d\mathbf{k}_{mix}$ is for dk_{mix}^{x} in a 1D system, $dk_{mix}^{x}dk_{mix}^{y}$ in a 2D system, and $dk_{mix}^{x}dk_{mix}^{y}dk_{mix}^{z}$