Theory of the exchange interaction and magnetoresistance in metallic magnetic superlattices

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A common approach is proposed for describing the magnetoresistance and the oscillations in the exchange interaction between magnetic layers separated by nonmagnetic interlayers.

The magnetic interaction between two ferromagnetic layers separated by a nonmagnetic metallic interlayer which is thin (5–30 atomic layers) and the magnetic interaction in superlattices made of alternating magnetic and nonmagnetic materials have recently attracted considerable interest.[1]

Experiments based on the electron microscopy with polarization analysis,[2] spin-polarized low-energy electron diffraction,[3] and other methods[4–7] have shown that the magnitude of the exchange interaction oscillates (changing sign) as a function of the number of layers in the nonmagnetic interlayer. Oscillations with periods from several atomic layers to a single atomic layer, depending on the particular materials, have been observed.[2,5] Analysis of several experiments[8] leads to the conclusion that there is a biquadratic exchange between ferromagnetic layers.

In addition, a giant magnetoresistance in the direction perpendicular to the layers is observed in systems of this sort in an external magnetic field.[1,9]

Several theoretical studies have been carried out,[10–14] but we have not yet reached a complete understanding of the effects. In the present letter we wish to propose a common approach for describing them. Along this approach, the oscillations of the exchange interaction, including the appearance of a biquadratic exchange, and the magnetoresistance can be described in a common way.

An RKKY interaction is known to arise between transition metal ions in a metallic matrix as a result of a polarization of conduction electrons.[15] In the case at hand, an interaction between ferromagnetic layers arises because of a polarization of the electrons in the interlayer. This polarization arises because spin-polarized electrons tunnel out of the ferromagnetic layers. In order to determine that relative orientation of the magnetizations in the ferromagnetic layers which is most favorable from the energy standpoint, we need to find the energy of the system as a function of the number of layers and the orientation of the magnetizations. This can be done conveniently in the following way. We assume that we begin with three noninteracting subsystems (Fig. 1), and there is no tunneling between layers. To go over to a real system we need to allow an overlap of subsystems (Fig. 1). We describe this overlap by means of the Hamiltonian

$$\hat{H}_{int}=\hat{T}\hat{c}_{\alpha}^{+}\hat{c}_{a}+\hat{c}_{a}^{+}\hat{c}_{\alpha}\hat{T}^{+}+\hat{T}'\hat{c}_{\beta}^{+}\hat{c}_{b}+\hat{c}_{b}^{+}\hat{c}_{\beta}\hat{T}'^{+}, \tag{1}$$

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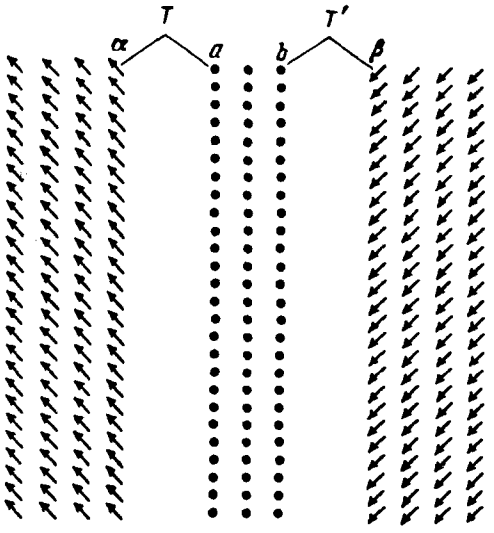

FIG. 1.

where $\hat{c}_i=\{c_{ink\sigma}\}$, $i=\alpha$, β, a, b (Fig. 1) are the outermost atomic layers in the corresponding subsystems; $\mathbf{k}$ is the quasimomentum along the layer; σ is a spin index; the index n specifies the type of orbital and its position at the lattice sites; and $\hat{T}$, $\hat{T}'$ are spin-diagonal matrices of overlap integrals (tunneling does not alter the orientation of a spin). After the subsystems are brought into close contact with each other, the change in the energy is given by the standard thermodynamic formula[16]

$$\delta E=\int_0^1 \frac{dg}{g}\langle \hat{H}_{\text{int}}\rangle, \tag{2}$$

where we have introduced the dimensionless tunneling–interaction constant $\hat{T}(g)=g\hat{T}$, $\hat{T}'(g)=g\hat{T}'$ ($g=0$ for the noninteracting subsystems, and $g=1$ for the subsystems in close contact). The average in (2) is over the state of the system, in which the tunneling interaction is taken into account. Direct substitution of (1) into (2) yields

$$\delta E=\int_0^1 \frac{dg}{g}\int \frac{d\epsilon d\mathbf{k}}{(2\pi)^3}$$

$$\mathrm{Tr}\{\hat{T}\hat{G}^+_{\alpha a}(\epsilon\mathbf{k},g)+\hat{G}^+_{a\alpha}(\epsilon\mathbf{k},g)\hat{T}^+ +\hat{T}'\hat{G}^+_{\beta b}(\epsilon\mathbf{k},g)+\hat{G}^+_{b\beta}(\epsilon\mathbf{k},g)\hat{T}'^+\}\,, \tag{3}$$

where the Tr (the trace) is over the indices of the orbitals and the spin indices, and G^+ is the Keldysh Green's function[17]

$$\hat{G}^+(\epsilon\mathbf{k},g)=i\langle \hat{c}^+_\alpha \hat{c}_a\rangle. \tag{4}$$

The Green's function in (3) can be expressed in terms of the Green's functions of the noninteracting subsystems. The latter functions contain complete information on the electron density, the local magnetization, and so forth. We assume that they are known. The Green' s function can be written in the form

$$\hat{\mathbf{G}}^{\pm}=\frac{\hat{\mathbf{I}}}{\hat{\mathbf{I}}-g\hat{\mathbf{g}}^{R}\hat{\mathbf{T}}}\,\hat{\mathbf{g}}^{\pm}\frac{\hat{\mathbf{I}}}{\hat{\mathbf{I}}-g\hat{\mathbf{T}}^{+}\hat{\mathbf{g}}^{A}},$$

$$\hat{\mathbf{g}}=\begin{pmatrix}\hat{g}_{11} & \hat{g}_{12}\\ \hat{g}_{21} & \hat{g}_{22}\end{pmatrix},\quad \hat{g}_{11}=\begin{pmatrix}\hat{g}_{\alpha\alpha} & 0\\ 0 & \hat{g}_{aa}\end{pmatrix},\quad \hat{\mathbf{g}}_{12}=\begin{pmatrix}0 & 0\\ \hat{g}_{ab} & 0\end{pmatrix},$$

$$\hat{\mathbf{g}}_{21}=\begin{pmatrix}0 & \hat{g}_{ba}\\ 0 & 0\end{pmatrix},\quad \hat{\mathbf{g}}_{22}=\begin{pmatrix}\hat{g}_{bb} & 0\\ 0 & \hat{g}_{\beta\beta}\end{pmatrix},$$

$$\hat{\mathbf{T}}=\begin{pmatrix}\hat{T} & 0\\ 0 & \hat{T}\end{pmatrix},\quad \hat{T}=\begin{pmatrix}0 & \hat{T}\\ \hat{T}^{+} & 0\end{pmatrix},\quad \hat{T}=\begin{pmatrix}0 & \hat{T}'\\ \hat{T}'^{+} & 0\end{pmatrix}. \tag{5}$$

Here R and A specify the retarded and advanced Green's functions, and the $\pm$ specifies Keldysh Green's functions. The final expression for the energy is

$$\delta E=\int_0^1 dg\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\hat{\mathbf{T}}\hat{\mathbf{G}}^{+}+\hat{\mathbf{G}}^{+}\hat{\mathbf{T}}^{+}\}\,. \tag{6}$$

The result has thus been expressed in terms of the Green's functions for the noninteracting layers. This method gives us an expression for the change in the energy of the system which is exact (in any order in T, T').

For a spin-polarized system, the Green's functions can be written

$$\hat{g}^{R,A}_{\alpha\alpha,\beta\beta}=\hat{g}^{NR,A}_{\alpha\alpha,\beta\beta}+(\vec{\sigma}\mathbf{m}_{\alpha,\beta})\hat{g}^{SR,A}_{\alpha\alpha,\beta\beta}$$

$$\hat{g}^{\pm R,A}_{\alpha\alpha,\beta\beta}=2\pi i\hat{\rho}^{N}_{\alpha\alpha,\beta\beta}+(\vec{\sigma}\mathbf{m}_{\alpha,\beta})\hat{\rho}^{S}_{\alpha\alpha,\beta\beta})\begin{cases}f(\epsilon)\\ f(\epsilon)-1\end{cases}, \tag{7}$$

$$\hat{\rho}^{N,S}_{\alpha\alpha,\beta\beta}=-\frac{1}{\pi}\{\hat{g}^{N,SR}_{\alpha\alpha,\beta\beta}\},$$

where $\mathbf{m}_\alpha$, $\mathbf{m}_\beta$ are unit vectors along the magnetizations in layers α and β; $\hat{\rho}^N$, $\hat{\rho}^S$ are the spin-independent and spin-dependent parts of the state density; $f(\epsilon)$ is a Fermi distribution;

$$\mathbf{M}_{\alpha,\beta}=\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\vec{\sigma}\hat{g}^{+}_{\alpha\alpha,\beta\beta}\}=\mathbf{m}_{\alpha\beta}\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\hat{\rho}^{S}_{\alpha\alpha,\beta\beta}\}f(\epsilon)$$

is the magnetization; and

$$\rho_{\alpha,\beta}=\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\hat{g}^{+}_{\alpha\alpha,\beta\beta}\}=\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\hat{\rho}^{N}_{\alpha\alpha,\beta\beta}\}f(\epsilon) \tag{8}$$

is the charge density. It follows from (5)–(7) that δE is a complex function of the magnetizations in the ferromagnetic layers. An expansion of the denominator in expression (5) for $\hat{\mathbf{G}}^{\pm}$ leads to a power series with various powers of the magnetizations in δE:

$$\delta E = (\text{const} + \mathbf{m}_\alpha^2 + \mathbf{m}_\beta^2 + J(\mathbf{m}_\alpha \mathbf{m}_\beta) + (\mathbf{m}_\alpha \mathbf{m}_\beta)^2 + \ldots). \tag{9}$$

The last term describes biquadratic exchange. This term arises in a more natural way along our approach than in Ref. 8. All the constants in (9) can be expressed in terms of microscopic characteristics of the layers. For the exchange-interaction constant $J(N)$ we find

$$\begin{aligned} J(N) = \frac{1}{4} \int \frac{d\epsilon d\mathbf{k}}{(2\pi)^3} f(\epsilon) \mathrm{Tr}\{ & \hat{T} \hat{\rho}_{\alpha\alpha}^S \hat{T}^+ \mathrm{Re}\{\hat{g}_{ab}^R \hat{T}' \hat{g}_{\beta\beta}^{SR} \hat{T}'^+ \hat{g}_{ba}^R\} \\ & + \hat{T}' \hat{\rho}_{\beta\beta}^S \hat{T}'^+ \hat{g}_{ba}^R \hat{T} \mathrm{Re}\{\hat{g}_{\alpha\alpha}^{SR}\} \hat{T}^+ \hat{g}_{ab}^A + \hat{T} \hat{\rho}_{ab} \hat{T}' \hat{g}_{\beta\beta}^{SA} \hat{T}'^+ \hat{g}_{ab}^A \hat{T}^+ \mathrm{Re}\{\hat{g}_{\alpha\alpha}^{SR}\} \\ & + \hat{T}' \rho_{ab} \hat{T} \mathrm{Re}\{\hat{g}_{\alpha\alpha}^{SR}\} \hat{T}^+ \hat{g}_{ab}^R \hat{T}'^+ \hat{g}_{\beta\beta}^{SR} + \begin{matrix} a \to b, & \alpha \to \beta, & T \to T' \\ b \to a, & \beta \to \alpha, & T' \to T \end{matrix} \Big\}. \end{aligned} \tag{10}$$

Information on the number of layers and the electronic structure of the interlayer is embodied in the Green's function $\hat{g}_{ab}$, which describes the propagation of an electron from one end of an interlayer to the other. An expression for $\hat{g}_{ab}$ (and the others) can be derived from band theory. To demonstrate the oscillatory behavior of $J(N)$, we calculate $\hat{g}_{ab}$ for a finite one-dimension interlayer (chains in the strong-coupling method with an overlap integral $t/2$) of length N. The oscillatory part of $J(N)$ satisfies the proportionality

$$J(N) \propto \int_0^{\epsilon_F} \mathrm{Im}\{[(\epsilon + i(t^2 - \epsilon^2)^{1/2})/t]^N\} d\epsilon \propto t \sin(N\epsilon_F/t)/N, \tag{11}$$

where ϵ_F is the Fermi energy in the interlayer. We wish to stress that this formula serves only as an illustration. It is important to note that the oscillation period is determined by the details of the electronic structure. Even in the simplest example, this period depends on the width of the band (t) and the Fermi energy; it can vary over a broad range. The decrease in $1/N$ also reflects the properties of the particular one-dimensional model.

We also wish to stress that the actual expansion parameter is not the overlap itself, i.e., not the quantities T, T' (which are by no means small), but T/N (or T/N^2, in the three dimensional case). The correction to the energy is thus small, on the same order as T/N^2 (per unit surface area). The energy of the layers itself is $\sim T$, i.e., on the order of the bulk width of the band.

We turn now to a calculation of the conductivity of the system. Experiments on the magnetoresistance in the direction perpendicular to the layers reveal a clearly defined threshold in the strength of the external magnetic field.[9] The resistance remains essentially constant up to a certain field strength; then it changes abruptly, and later it becomes constant again as the field is increased further. This behavior results from a reversal in the orientation of the magnetizations in the ferromagnetic layers in the external magnetic field. Our problem is to find the abrupt change in the conduc-

tivity in terms of microscopic characteristics of the electronic spectrum of the system. For this purpose we must determine that component of the current which depends on the relative orientation of the magnetizations. In the tunneling-Hamiltonian method,[18] the current can be described by (in any order in the overlap)

$$I=ie\int\frac{d\epsilon d\mathbf{k}}{(2\pi)^3}\,\mathrm{Tr}\{\hat{\mathbf{T}}\hat{\mathbf{G}}^+-\hat{\mathbf{G}}^+\hat{\mathbf{T}}^+\}\,. \tag{12}$$

In calculating $\hat{\mathbf{G}}^{\pm}$ in this case we must use the Green's function in (5) and allow for the applied voltage. The spin-dependent component of the tunneling current (after an expansion of the denominator in the overlap and the retention of terms of up to second order) can be described by

$$I_S=I_1(\mathbf{m}_\alpha\mathbf{m}_\beta) \tag{13}$$

$$\begin{aligned}I_1=2e\int\frac{d\epsilon d\mathbf{k}}{2\pi}\,\mathrm{Tr}\{&\hat{T}\hat{\rho}^S_{\alpha\alpha}\hat{T}^+\hat{g}^R_{ab}\hat{T}'\hat{\rho}^S_{\beta\beta}\hat{T}'^+\hat{g}^A_{ba}[f_\alpha-f_\beta]\\&+\hat{T}\hat{\rho}^S_{\alpha\alpha}\hat{T}^+(\hat{\rho}_{ab}\hat{T}'\hat{g}^{SA}_{\beta\beta}\hat{T}'^+\hat{g}^A_{ba}+\hat{g}^R_{ab}\hat{T}'\hat{g}^{SR}_{\beta\beta}\hat{T}'^+\hat{\rho}^A_{ba})[f_\alpha-f_{ab}]\\&+\hat{T}'\hat{\rho}^S_{\beta\beta}\hat{T}'^+(\hat{\rho}_{ba}\hat{T}\hat{g}^{SA}_{\alpha\alpha}\hat{T}^+\hat{g}^A_{ab}+\hat{g}^R_{ba}\hat{T}\hat{g}^{SR}_{\alpha\alpha}\hat{T}^+\hat{\rho}^A_{ab})[f_\beta-f_{ab}]\},\end{aligned}$$

where f_α, f_β, and f_{ab} are the distribution functions in the left-hand layer, the right-hand layer, and the interlayer, respectively. The quantity I_1 determines the amplitude of the change in the current upon a change induced in the orientation of the magnetizations $\mathbf{m}_\alpha$ and $\mathbf{m}_\beta$ by the external magnetic field.

In summary, the approach proposed here makes it possible to describe the magnetoresistance and the exchange interaction between magnetic layers from a common standpoint. This approach can easily be generalized to the case with a spin-orbit interaction and thus to incorporate a magnetic anisotropy. This approach is also convenient for realistic numerical calculations.

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