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1994 J. Phys.: Condens. Matter 6 1941

(http://iopscience.iop.org/0953-8984/6/10/012)

J. Phys.: Condens. Matter 6 (1994) 1941–1946. Printed in the UK

The interlayer exchange coupling in magnetic multilayers: the effect of the thickness of the ferromagnetic layer

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Received 17 August 1993

Abstract. In this work the effect of the ferromagnetic layer thickness on the interlayer exchange coupling in magnetic multilayers, which has rarely been considered so far, is investigated by employing the one-band tight-binding hole-confinement model. The numerical calculations for a simple cubic lattice show that although the oscillatory variation of coupling parameter J with the variation of non-magnetic layer thickness N has periods insensitive to the ferromagnetic layer thickness M, when M becomes smaller the amplitude and phase of such oscillations depend strongly on M, and J varies with M in an oscillatory-like fashion. Our theoretical results may be helpful in understanding the recent experimental data.

1. Introduction

During recent years, much attention has been paid to the interlayer exchange coupling in magnetic multilayers consisting of alternating magnetic and non-magnetic materials [1–14]. In a number of magnetic multilayers (including the sandwich as a particular case), it has been found experimentally that the interlayer coupling parameter J is an oscillatory function of the non-magnetic layer thickness N [3–5] with unexpectedly long period or two periods. A broad spectrum of theoretical approaches has been adopted to explain these peculiar phenomena, such as the first-principles method [6], the tight-binding total-energy calculation [7], the RKKY theory [8, 9], the tight-binding hole-confinement model [1], the free-electron model [10], etc. Great progress has been made towards understanding the origin of the oscillatory behaviour. It is clear now that the *aliasing* effect [11–13], i.e. the fact that J is sampled at discrete values of N, can shift the RKKY-like short-period oscillations to long-period ones, and, the two-period oscillations are attributed to the special structure of the Fermi surface.

It seems to be popularly accepted that the interlayer coupling is only a surface effect, insensitive to M. However, a few experiments with small M (about 5–10 monolayers), showed [2] that the effect of ferromagnetic layer thickness should not be negligible. Recently, Barnás [10] studied this effect theoretically, using a free-electron model. In our opinion, however, such a model may be not realistic for magnetic multilayers. In a more recent theoretical work [14], the effect of M was investigated by means of first-principles calculations for $M = 1, 3$ and N = 1,3,5,7 monolayers. The results showed that the function $J(N)$ for $M = 1$ monolayer is significantly different from that for $M = 3$ monolayers. Obviously, the first-principles calculation is difficult to carry out for larger M and N. In this paper, the effect of M on J is investigated by numerical calculations based on

0953-8984/94/101941+06$19.50

the one-band tight-binding hole-confinement model. The system considered is a sandwich consisting of two identical ferromagnetic metallic layers separated by one non-magnetic metallic layer with the same simple cubic lattice structure.

2. Model and improvements

The Hamiltonian in the one-band tight-binding hole-confinement model is [1]

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + \sum_{i} U_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $a_{i\sigma}(a_{i\sigma}^{+})$ is the operator annihilating (creating) an electron of spin σ on site i and $n_{i\sigma} = a_{i\sigma}^{+} a_{i\sigma}$. The hopping parameters t_{ij} are assumed to be the same in both metals and $U_i = \infty$ or 0 in the ferromagnetic or non-magnetic layer, respectively. The Hartree–Fock approach is exact for Hamiltonian (1) in this case [1]. Let the layers be perpendicular to the z axis. H can be divided into two terms:

$$H = H(\uparrow) + H(\downarrow) \tag{2}$$

where $H(\uparrow)$ $(H(\downarrow))$ is the Hamiltonian of electrons with spin $\uparrow$ $(\downarrow)$. In the case of ferromagnetic coupling between two ferromagnetic layers, we have

$$H(\uparrow) = h_{\uparrow}(2M + N) \qquad H(\downarrow) = h_{\downarrow}(N) \tag{3}$$

where

$$h_{\sigma}(N) = \sum_{\langle i,j\rangle} t_{ij} a_{i\sigma}^{+} a_{j\sigma} \tag{4}$$

is the Hamiltonian of electrons that have spin σ in the non-magnetic layer consisting of N monolayers, while in the case of antiferromagnetic coupling, (3) becomes

$$H(\uparrow) = h_{\uparrow}(M + N) \qquad H(\downarrow) = h_{\downarrow}(M + N). \tag{5}$$

Now, the original problem has been converted into the simpler one in which only $h_{\sigma}(N)$ is concerned. In the following, we take $t_{ij} = t(t < 0)$ for i, j nearest neighbours and $t_{ij} = 0$ otherwise; the temperature is assumed to be zero ($T = 0$ K), and the energies are measured in unit of $2|t|$. The eigen-energies of $h_{\sigma}(N)$ are

$$\epsilon(k_x, k_y, r) = -\cos[r\pi/(N+1)] - \cos(k_x a) - \cos(k_y a) \qquad r = 1, 2, \ldots, N. \tag{6}$$

The number of electrons that occupy levels (6) up to the Fermi energy E_{F} is

$$n_{\mathrm{e}}(E_{\mathrm{F}}, N) = \sum_{r,k_x,k_y} \theta[E_{\mathrm{F}} - \epsilon(k_x, k_y, r)]. \tag{7}$$

The total energy of these electrons is given by

$$E(E_{\mathrm{F}}, N) = \sum_{r,k_x,k_y} \epsilon(k_x, k_y, r)\theta[E_{\mathrm{F}} - \epsilon(k_x, k_y, r)] \tag{8}$$

and the corresponding thermodynamic potential is

$$\Omega(E_F, N) = E(E_F, N) - E_F n_e(E_F, N). \tag{9}$$

When $M \to \infty$, the Fermi energy of the sandwich is equal to the bulk Fermi energy $\tilde{E}_F$ independent of whether the interlayer coupling is ferromagnetic or antiferromagnetic. Thus, the interlayer coupling parameter can be expressed as

$$J = [\Omega_{FM}(\tilde{E}_F) - \Omega_{AF}(\tilde{E}_F)]/S \tag{10}$$

where S is the area of the film, while $\Omega_{FM}(E_F)$ and $\Omega_{AF}(E_F)$ are the thermodynamic potentials for the ferromagnetic and antiferromagnetic couplings, respectively. Although (10) has been extensively utilized, it is no longer useful in the present work because in our case M is small and hence the variation of Fermi energy ($\sim O(1/M)$)is not negligible. The significant effect of M on J in the case of small M is in part due to the variation of E_F with M. Equations (2.2)–(2.12) of [1] are suitable only in the large-M limit. Hence in the following calculations we use the formula

$$J = [E^{(FM)}(E_F^{(FM)}) - E^{(AF)}(E_F^{(AF)})]/S. \tag{11}$$

Here,

$$E^{(FM)}(E_F^{(FM)}) = E(E_F^{(FM)}, 2M + N) + E(E_F^{(FM)}, N) \tag{12}$$

and

$$E^{(AF)}(E_F^{(AF)}) = 2E(E_F^{(AF)}, 2M + 2N) \tag{13}$$

are the total energies of electrons related to the ferromagnetic and antiferromagnetic interlayer coupling, respectively, and $E_F^{(FM)}$ and $E_F^{(AF)}$ stand for the corresponding Fermi energies determined by

$$n_e(E_F^{(FM)}, N) + n_e(E_F^{(FM)}, 2M + N) = N_e \tag{14}$$

and

$$2n_e(E_F^{(AF)}, M + N) = N_e \tag{15}$$

respectively, where N_e is the total number of electrons in the sandwich. The relation between N_e and the bulk Fermi energy $\tilde{E}_F$ is given by

$$N_e = 2(M + N) \lim_{L\to\infty} [n_e(\tilde{E}_F, L)/L]. \tag{16}$$

The bulk Fermi energy $\tilde{E}_F$ is the only adjustable parameter in our calculations. The summation over k_x, k_y in equations (7) and (8) can be converted into an integral with respect to energy $\epsilon = -\cos(k_x a) - \cos(k_y a)$:

$$n_e(E_F, N) = \sum_r \int d\epsilon N_{2D}(\epsilon)\theta\left[E_F - \epsilon + \cos\left(\frac{r\pi}{N+1}\right)\right] \tag{17}$$

$$E(E_F, N) = \sum_r \int d\epsilon N_{2D}(\epsilon)\left[\epsilon - \cos\left(\frac{r\pi}{N+1}\right)\right]\theta\left[E_F - \epsilon + \cos\left(\frac{r\pi}{N+1}\right)\right] \tag{18}$$

where $N_{2D}(\epsilon)$ denotes the two-dimensional density of states, for $-2 < \epsilon < 0$,

$$N_{2D}(\epsilon) = -\frac{S}{\pi^2 a^2} \int_1^{-\epsilon-1} \frac{dx}{\sqrt{(1-x^2)[1-(\epsilon+x)^2]}}. \tag{19}$$

Therefore, for $-3 < E_F < -1$, we have

$$n_e(E_F, N) = \frac{S}{\pi^2 a^2} \sum_{r=1}^{j_F} \tilde{n}_e\left[E_F + \cos\left(\frac{r\pi}{N+1}\right)\right] \tag{20}$$

$$E(E_F, N) = -\frac{S}{\pi^2 a^2} \sum_{r=1}^{j_F} \left\{4\tilde{E}\left[E_F + \cos\left(\frac{r\pi}{N+1}\right)\right] + \cos\left(\frac{r\pi}{N+1}\right)\tilde{n}_e\left[E_F + \cos\left(\frac{r\pi}{N+1}\right)\right]\right\} \tag{21}$$

where

$$j_F = \min\left\{N, \mathrm{int}\left[\frac{N+1}{\pi}\cos^{-1}(-E_F - 2)\right]\right\} \tag{22}$$

$$\tilde{n}_e(\epsilon) = \int_0^{\cos^{-1}(-\epsilon-1)} \cos^{-1}(-\epsilon - \cos x)\,dx \tag{23}$$

$$\tilde{E}(\epsilon) = \int_0^{1+\epsilon/2} \ln\left[\frac{4x^2 + 4 - \epsilon^2 + \sqrt{(4x^2+4-\epsilon^2)^2 - 64x^2}}{8x}\right] dx. \tag{24}$$

Table 1. The variation of λ (the oscillation period of J as a function of N), in monolayers with $\tilde{E}_F$ (in $2|t|$) when $M = 5$ monolayers

$\tilde{E}_F$	−1.05	−1.1	−1.2	−1.3	−1.4	−1.5	−1.6	−1.7	−1.8	−1.9
λ	11	7	5	4	4	3	3–2	3–2	3–2	2
$\tilde{E}_F$	−2.0	−2.1	−2.2	−2.3	−2.4	−2.5	−2.6	−2.7	−2.8	−2.9
λ	2	2	2	2–3	3–2	3	3–4	4	5	7

3. Results and discussion

In table 1, the calculated oscillation period λ of $J(N)$ versus the relative bulk Fermi energy $\tilde{E}_F$ is given for $M = 5$. Here and in the following the thicknesses, such as M, N, and λ, are all in the units of monolayers. This result agrees qualitatively with $\lambda \sim \pi/\cos^{-1}|2 + \tilde{E}_F|$ of [1] for $M = \infty$, implying that the period of $J(N)$ is insensitive to M. However, when M is small, the phase and amplitude of $J(N)$ are clearly M dependent. The variations of J with N corresponding to $M = 5, 10$, and 200 obtained by us are shown in figure 1, for $\tilde{E}_F = -1.05, -2.9$, and -2.6. Our results show that by fixing $N = N_0$, $J(M, N_0)$ behaves like damping oscillations of M around $J(\infty, N_0)$. Independent of whether the coupling $J(\infty, N_0)$ is ferromagnetic or antiferromagnetic, the interlayer coupling $J(M, N_0)$

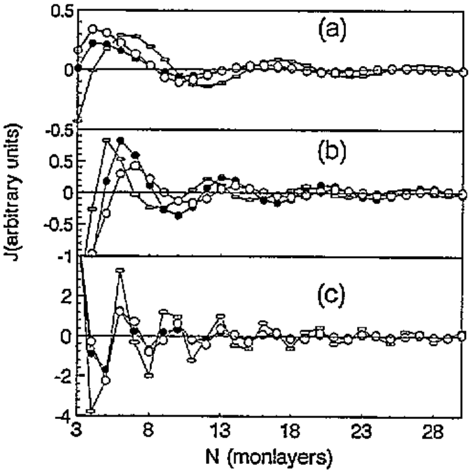

Figure 1. Exchange couplings $J(N)$: $M = 200$ (open circles), 10 (solid circles) and 5 (rectangles). The lines are guides for the eye. (a) $E_F = -1.05$; (b) $E_F = -2.9$; (c) $E_F = -2.6$.

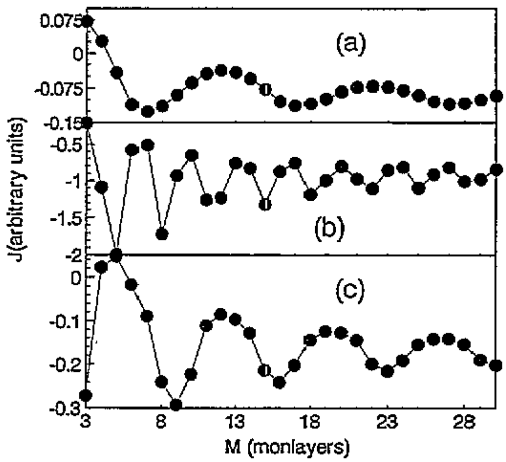

Figure 2. The exchange coupling J as a function of M. The line is only a guide for the eye. (a) $E_F = -1.05, N = 10$; (b) $E_F = -2.6, N = 8$; (c) $E_F = -2.9, N = 11$.

Table 2. J_1 and J_2 (the first and second peaks of J as a function of N, in arbitrary units) as well as N_1 and N_2 (the thicknesses of the non-magnetic layer corresponding to J_1 and J_2, respectively, in monolayers) for different $\tilde{E}_F$ (in $2|t|$).

		M						
		4	5	6	7	8	9	10
$\tilde{E}_F = -1.2$	J_1	− 1.3	− 0.7	− 0.9	− 1.5	− 1.8	− 1.3	− 1
	J_2	− 0.4	− 0.1	− 0.2	− 0.5	− 0.6	− 0.3	− 0.2
	N_1	5	5	5	5	5	5	5
	N_2	9	10	10	10	10	10	10
$\tilde{E}_F = -2.8$	J_1	− 0.5	− 0.3	− 1.1	− 1.3	− 0.8	− 0.5	− 0.5
	J_2	− 0.14	− 0.08	− 0.5	− 0.6	− 0.4	− 0.1	− 0.1
	N_1	6	7	7	7	6	7	7
	N_2	11	12	12	12	11	12	12
$\tilde{E}_F = -2.9$	J_1	− 0.56	− 0.24	− 0.11	− 0.09	− 0.24	− 0.34	− 0.36
	J_2	− 0.23	− 0.11	− 0.03	− 0.02	− 0.10	− 0.14	− 0.16
	N_1	9	8	9	10	11	10	10
	N_2	16	15	16	18	18	17	17

may be ferromagnetic, antiferromagnetic, or even zero depending on the thickness of the ferromagnetic layer, provided that $J(\infty, N_0)$ is not far from zero. An example of our results is illustrated in figure 2. It can be seen that the oscillation period of $J(M)$ with N fixed is roughly the same as that of $J(N)$ with M fixed. In table 2, the dependences of the first and second peak values, J_1 and J_2 respectively, of $J(N)$ on M are given for $\tilde{E}_F = -1.2, -2.8$, and -2.9. Here, N_1 and N_2 are the thicknesses of the non-magnetic layer corresponding to J_1 and J_2, respectively. These results show once more that the amplitude of $J(N)$ is sensitive to M. The recent experimental data [2] manifested that J oscillates with M, which can be considered as supporting our theoretical results.

4. Summary

Based on the one-band tight-binding hole-confinement model [1] in which it is assumed that the exchange split is large enough in ferromagnetic layers, we have investigated the effect of the ferromagnetic layer thickness M on the interlayer exchange coupling J in a magnetic sandwich for a simple cubic lattice structure at $T = 0$. Numerical results show that when M is small (about 5–10 monolayers) the phase and amplitude of oscillations of J as a function of N are sensitive to M, but not so for the oscillation period. In addition, J varies in an oscillatory-like fashion with M and the oscillation period of J as a function of M with N fixed is roughly the same as that of N with M fixed. Some recent experimental data support qualitatively our theoretical results.

Acknowledgments

This work was supported by the National Foundation for Natural Sciences in China and the State Key Laboratory of Magnetism, Institute of Physics, Chinese Academy of Sciences. We are grateful to Dr Min Li and Dr Ming-Lang Yan for helpful discussions.

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