Effects of Fano resonances on the interlayer coupling in magnetic multilayers

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Exchange couplings in (001) fcc Co/Cu/Co multilayers with various thicknesses of the Co layer are examined in a realistic tight-binding model. Many sharp features (known as Fano resonances) in the reflection amplitude as a function of energy are found, which do not exist in a one-band model. With a simplified two-band tight-binding model, the effects of Fano resonances can be calculated accurately, and they are found to play an important role in determining the magnetic-layer thickness dependence of the interlayer coupling. [S0163-1829(96)01242-8]

I. INTRODUCTION

Since the discovery of the magnetic interlayer coupling in metallic multilayers,[1,2] much research has been done to understand this phenomenon. Among many theoretical studies, a recent approach based on the reflection amplitude provides a physically transparent picture.[3,4] Due to the spin splitting in the magnetic layer, electrons with different spins in the spacer layer are confined differently. Thus, the interlayer coupling can be expressed with the spin asymmetry of reflection amplitudes. This picture is also consistent with spin polarized photoemission experiments.[5,6] For thick spacer layers, the coupling strength can be estimated from reflection amplitudes at the extremal points and the Fermi level.[7] When the magnetic layer has finite thickness, the reflection amplitudes vary as functions of magnetic-layer thickness due to the quantum interference inside the magnetic layer. Thus, the interlayer coupling is expected to show magnetic-layer thickness dependence.[8–10] This prediction was experimentally confirmed later.[11,12] However, those theoretical studies on the magnetic-layer thickness dependence are limited to free-electron-like or one-band models. There have been realistic calculations for the interlayer coupling, but they are either focused on the spacer-layer thickness dependence[13,14] or limited to thin magnetic layers.[15] In a one-band model, the reflection amplitude oscillates as a function of the magnetic-layer thickness and the period is determined from the spanning wave vector of the magnetic material. When there are multiple bands in the magnetic layer, the Fano resonance[16] can occur and the reflection amplitude is affected greatly. In this paper, we explore the case in which there is more than one transmitted wave vector in the magnetic layer. We will show that the effects of Fano resonance are significant for the magnetic-layer thickness dependence.

This paper is organized as follows. In Sec. II, we calculate reflection amplitudes for (001) Co/Cu/Co multilayer with finite Co layer thickness. We show that the Fano resonances[16] will occur in a realistic multiband model, while they do not exist in a one-band model. In Sec. III, we present a two-band model calculation in order to demonstrate the effects of the Fano resonance on the interlayer coupling. A discussion is presented in Sec. IV.

II. FANO RESONANCE IN (001) Co/Cu/Co MULTILAYERS

We shall consider the dependence on the magnetic-layer thickness for the exchange coupling in a magnetic-multilayer system which consists of two magnetic layers (Co) of equal thickness, L, separated by a layer of nonmagnetic material (Cu) with thickness D, and spanked between two semi-infinite slabs of the nonmagnetic material (Cu). The interlayer coupling J is defined as the total energy difference between the ferromagnetic and antiferromagnetic configuration, viz.

$$J=(\Omega_{\mathrm{F}}-\Omega_{\mathrm{AF}})/2S, \tag{1}$$

where Ω is the grand canonical potential and S is the area of the multilayer. J can be expressed in terms of r^+ and r^- which denote reflection amplitudes for the majority and minority spin, respectively, for an electron incident from the middle nonmagnetic (Cu) layer into the magnetic material (Co) on either side. A crucial factor for determining J is the spin asymmetry of the reflection amplitudes $\Delta r=(r^+-r^-)/2$. When there is only one reflected wave in the spacer, the interlayer coupling is approximately given by[3,4,7]

$$J=-\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}_\parallel}\int d\varepsilon f(\varepsilon)2|\Delta r|^2 e^{i(q_z D+\phi)}, \tag{2}$$

where q_z is the perpendicular component of the scattering vector, $\mathbf{k}_\parallel$ is the wave vector parallel to the plane, ε is the electron energy, f is the Fermi-Dirac distribution, and ϕ is the net phase factor due to the reflection from both interfaces. For a large spacer thickness D and semi-infinite magnetic layers, the asymptotic behavior of the interlayer coupling can be obtained analytically. If Δr is a smooth function of ε, then using the stationary phase approximation, one obtains at zero temperature

$$J=\mathrm{Im}\frac{\hbar v_z\kappa}{4\pi^2D^2}|\Delta r|^2 e^{i(q_F D+\phi+\phi_0)}, \tag{3}$$

where v_z is the average group velocity, κ is the average radius of curvature, and q_F is the spanning wave vector at the Fermi surface. Quantities Δr and ϕ are also evaluated at the Fermi level. The other phase factor ϕ_0 is determined by

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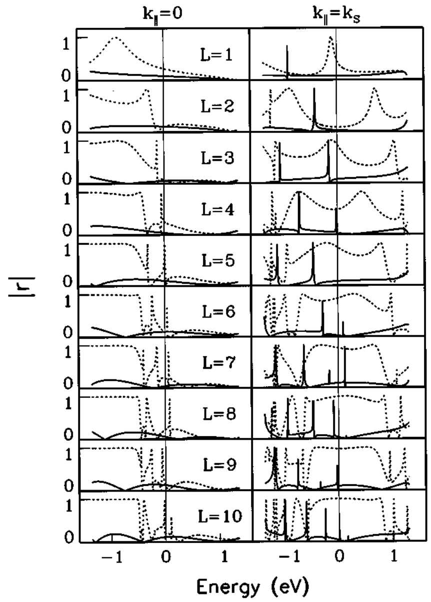

FIG. 1. Reflection amplitudes as functions of energy at extremal points for (001) Cu/Co/Cu systems. The left panel is for $\mathbf{k}_\|=0$ (long period) and the right is for $\mathbf{k}_\|=\mathbf{k}_S$ (short period). L is the thickness of Co layers. Solid and dotted curves are for majority and minority spins, respectively. The Fermi level is zero.

the shape of the Fermi surface at the extremal point: $\phi_0=0$, $\pi/2$, and π for maxima, saddle points, and minima, respectively.

In a free-electron-like model, the reflection amplitude for the finite magnetic layer with thickness L is

$$r=r_\infty \frac{1-e^{2ik'_zL}}{1-r_\infty^2 e^{2ik'_zL}}, \tag{4}$$

where r_∞ is the reflection amplitude for the semi-infinite magnetic layer and k'_z is the z-component wave vector in the magnetic layer. When $|r_\infty|$ is small, we have

$$r=r_\infty+r_{\rm osc} \tag{5}$$

with $r_{\rm osc}=-r_\infty(1-r_\infty^2)e^{2ik'_zL}$. Note that the function is oscillatory in L due to the Fabry-Pérot interference effect of the finite-thickness slab of the magnetic material.

First, we calculate the reflection amplitudes at extremal points for (001) fcc Co/Cu/Co multilayers using a realistic tight-binding (TB) model with s, p^3, and d^5 orbitals. The TB parameters are given in Ref. 7 and the Fermi level is taken to be zero. For the (001) orientation, there are two different kinds of extremal points. We denote them by $\mathbf{k}_\|=0$ (belly) and $\mathbf{k}_\|=\mathbf{k}_S$ (neck). The corresponding spanning vectors give rise to a long and short oscillation period, respectively. Theoretically, it was shown that the shorter period has a much bigger coupling strength due to the large magnitude of spin asymmetry of reflection amplitudes.[3,7,17] Our method for calculating reflection amplitudes is similar to that described in the appendix of Ref. 7 with some modifications to make it applicable for a trilayer system including a finite-thickness magnetic layer.

Figure 1 displays the reflection amplitudes as functions of

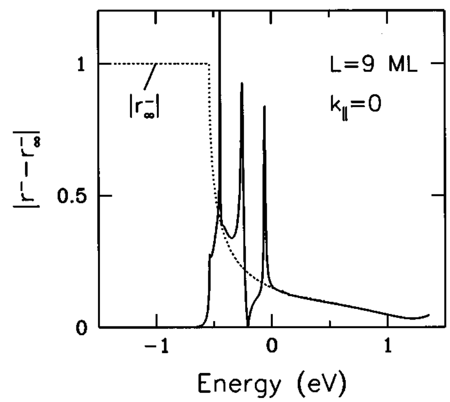

FIG. 2. $|r^- - r_\infty^-|$ as a function of energy at extremal points $\mathbf{k}_\|=0$ for (001) Cu/Co/Cu systems. The thickness of Co layer is taken as $L=9$. The dotted curve is $|r_\infty^-|$ for comparison.

energy at $\mathbf{k}_\|=0$ (left panel) and $\mathbf{k}_\|=\mathbf{k}_S$ (right panel) for different Co layer thicknesses (L's). The solid curve is for $|r^+|$ and dotted for $|r^-|$. $|r^+|$ for $\mathbf{k}_\|=0$ exhibits oscillatory behavior as a function of energy, which can be explained by the Fabry-Pérot effect since k'_z is a function of energy for a given $\mathbf{k}_\|$ [see Eq. (4)]. The striking result is that $|r^-|$ for $\mathbf{k}_\|=0$ and $|r^+|$ for $\mathbf{k}_\|=\mathbf{k}_S$ exhibit sharp asymmetric peaks. This is due to the Fano resonance[16] which occurs when a discrete state interacts with a continuum. This effect is quite common in the resonant-tunneling spectra[18,19] for materials with multiple bands and it has been observed experimentally.[20] The origin for such Fano resonance is better illustrated by examining the bulk band structures of Cu and Co at $\mathbf{k}_\|=0$ as shown in Fig. 2 of Ref. 7. In this case, the majority-spin band of Co is similar to the Cu band and there is only one possible transmitted wave vector (with real k'_z) near the Fermi level. As a consequence, $|r^+|$ shows a simple Fabry-Pérot oscillation as a function of energy. On the other hand, there are two possible k'_z states of the Δ_1 band near the Fermi level for the Co minority-spin electron. The portion of the band with smaller k'_z will be quantized due to the strong confinement effect from the nonmagnetic materials on both sides of the finite magnetic layer. A strong confinement exists for this portion of band in Co, because it has mostly d character (although it is connected to the s-band portion at larger k'_z), while the corresponding band in Cu near the Fermi level has predominantly s character. The mismatch in character leads to large reflection amplitude for electron to go from Co to Cu and a strong confinement results. The other portion of band (with larger k'_z) will not be quantized because it has mostly s character. The quantized states from the portion of the Co minority band with smaller k'_z will interfere with the continuum states of the other portion of the band with larger k'_z giving rise to Fano resonances in the transmission or reflection spectra for an incident electron from the Cu layer. Such Fano resonances for finite Co layer thicknesses do not appear in a one-band model which cannot include the hybridization of the s and d bands. We have also calculated $|r^-|$ versus $\mathbf{k}_\|$ at $E=E_F$ and found it to be a rather smooth function around $\mathbf{k}_\|=0$ even when the Fano resonance peak coincides with the Fermi level. At $\mathbf{k}_\|=\mathbf{k}_S$, the $|r^+|$ spectrum exhibits Fano resonances because there are again two possible transmitted wave vectors for the Co minority spin, with one portion of the band being quantized via quantum confinement. As the thickness of the magnetic layer L increases, more sharp peaks appear and the linewidth of the peaks becomes smaller, corresponding to more quantum confined states in the magnetic layer. In Fig. 2, we plot $|r^- - r_\infty^-|$ as a function of energy for $\mathbf{k}_\parallel = 0$ and $L = 9$ monolayers (ML's). Within a free-electron-like model, $|r^- - r_\infty^-|$ is almost the same as $|r_\infty^-|$ for small $|r_\infty^-|$ in Eq. (5). This relation holds well for energies slightly above the Fermi level where there is only one transmitted wave.[21] In contrast, where there are two possible transmitted waves (near and below the Fermi level), $|r^- - r_\infty^-|$ deviates significantly from $|r_\infty^-|$. In this energy range we can define $r_{\rm Fano}$, the contribution from the Fano resonance effect which does not exist in a one-band model, as

$$r_{\rm Fano} = r - (r_\infty + r_{\rm osc}), \tag{6}$$

where $r_{\rm osc}$ is given in Eq. (5) for the larger k_z' in Co.

The Co layer dependence of reflection amplitudes at the two extremal points at the Fermi level is shown in Fig. 3. Filled squares are for $|r^+|$ and open circles are for $|r^-|$. At $\mathbf{k}_\parallel = 0$ [Fig. 3(a)], $|r^+|$ shows a simple Fabry-Pérot oscillation with a period given by the spanning wave vector of the majority electron in Co as expressed in Eq. (4). On the other hand, $|r^-|$ is rather irregular due to the Fano resonances and no well-defined periods can be found. At $\mathbf{k}_\parallel = \mathbf{k}_S$ [Fig. 3(b)], despite the presence of Fano resonances, $|r^+|$ appears oscillatory except at $L = 15$ and 26 ML. This is because the Fano resonance peaks are so sharp that they rarely hit the Fermi level, when $|r^+|$ is plotted as a function of energy (see Fig. 1). $|r^-|$ fluctuates due to the tunneling effect for thin Co layers and it reaches one when the Co layer is sufficiently thick. Since the interlayer coupling is obtained by integrating $|\Delta r|^2$ [see Eq. (2)], it is instructive to plot $|\Delta r|$ versus Co layer thickness at the two extremal points at the Fermi level as shown in Fig. 4. At $\mathbf{k}_\parallel = 0$ (filled squares), the variation of Δr is dominated by r^- and the Fano resonance plays a significant role. At $\mathbf{k}_\parallel = \mathbf{k}_S$ (open circles), the fluctuation of Δr is mainly due to r^- for thin Co layers (say, L is less than 10 ML) and r^+ for thick Co layer, which are affected by the tunneling and the Fano resonance, respectively.

In general, when $|\Delta r|$ is large at the extremal point and the Fermi level, the corresponding interlayer coupling is strong.[7] However, when $|\Delta r|$ is very large due to the Fano resonance peak, the situation is much more complicated. In this case, $|\Delta r|$ is not a smooth function around the Fermi level and the assumption used to obtain Eq. (3) cannot be applied. In order to calculate the interlayer exchange coupling, $|\Delta r|^2 e^{i(q_z D + \phi)}$ needs to be integrated over E and the linewidth of the peak ΔE is a crucial factor for the coupling strength. ΔE changes as a function of L and $\hbar v_z / \Delta E$ is of the order of 100 Å for thin Co layers ($\Delta E \sim 0.1$ eV). Consider the case that $|\Delta r|$ is sharply peaked near the Fermi level due to the Fano resonance. For $D \gg \hbar v_z / \Delta E$, $|\Delta r|$ varies rather smoothly compared with $e^{i q_z D}$ and the coupling strength will be much larger than the semi-infinite magnetic-layer case. When D is less than $\hbar v_z / \Delta E$, the Fano resonance peak at the Fermi level will give rise to fluctuation of the coupling strength roughly proportional to ΔE. Considering the deviation of $|r - r_\infty|$ from $|r_\infty|$ in Fig. 2, we expect that the fluctuation of the coupling strength is large enough to be detected even for small D. We expect the contribution of the Fano resonance is much smaller for $\mathbf{k}_\parallel = \mathbf{k}_S$ than for $\mathbf{k}_\parallel = 0$ because the peaks are very sharp at $\mathbf{k}_\parallel = \mathbf{k}_S$ in Fig. 1. As L increases, the Fano resonance peaks become sharper and their contribution to the interlayer coupling will be smaller. A quantitative analysis seems possible only by performing accurate integration as described in Eq. (2) or a total energy calculation with full band structures with the use of an extremely fine mesh in the $\mathbf{k}_\parallel$ space. Such a calculation with Co/Cu/Co systems requires too much computational effort. Instead, we will take a simpler yet realistic model and investigate how the Fano resonances affect the interlayer coupling in the next section.

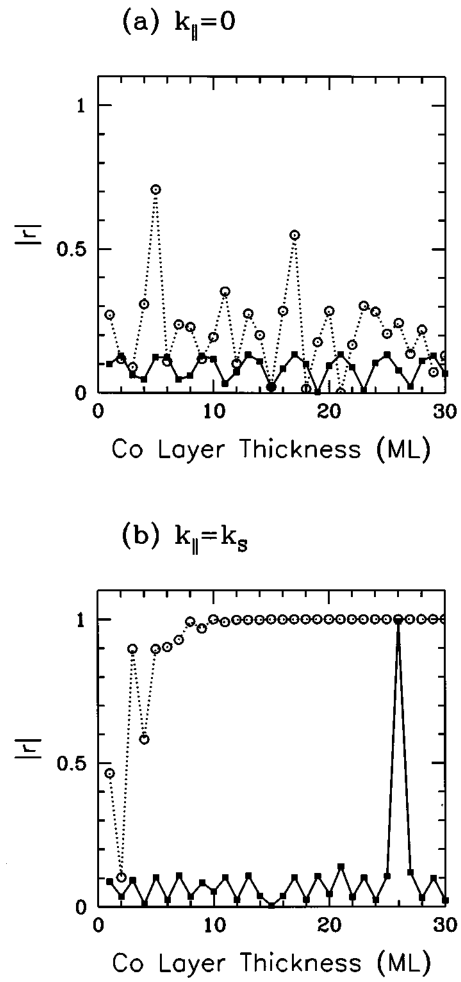

FIG. 3. Reflection amplitudes as functions of L (the thickness of Co layer) at extremal points and the Fermi level for (001) Cu/Co/Cu systems. (a) $\mathbf{k}_\parallel = 0$ (long period) (b) $\mathbf{k}_\parallel = \mathbf{k}_S$ (short period). Solid and dotted curves are for the majority and minority spins, respectively.

III. MODEL CALCULATION

In order to investigate the effect of the Fano resonance quantitatively, we perform a two-band model calculation. For simplicity, we take a simple cubic lattice with lattice constant c. In the k_z direction, the band dispersion is ob-

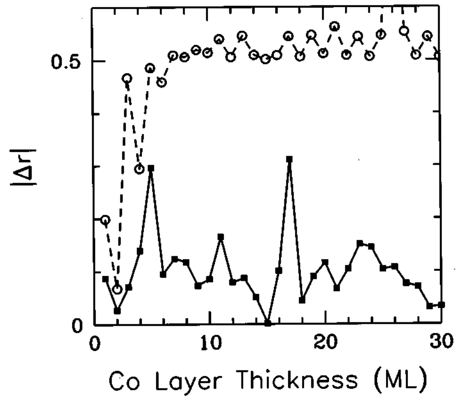

FIG. 4. Spin asymmetry of reflection amplitudes as a function of L (the thickness of Co layer) at extremal points and the Fermi level for (001) Cu/Co/Cu systems. Solid rectangles are for $\mathbf{k}_{\parallel}=0$ (long period) and open circles are for $\mathbf{k}_{\parallel}=\mathbf{k}_S$ (short period).

tained with a nearest-neighbor tight-binding model, while in the $\mathbf{k}_{\parallel}$ direction a parabolic band is assumed. The band structures in this model are obtained from the eigenvalues of the matrix

$$\begin{pmatrix} E_s+2t_s\cos k_z c+\dfrac{\hbar^2k_{\parallel}^2}{2m^*} & 2V_{sd}\cos k_z c \\ 2V_{sd}\cos k_z c & E_d+2t_d\cos k_z c+\dfrac{\hbar^2k_{\parallel}^2}{2m^*} \end{pmatrix}, \quad (7)$$

where E_s (E_d) is the on-site energy for an s-like (d-like) orbital, t_s (t_d) is the nearest-neighbor interaction between s (d) orbitals, V_{sd} is interaction between s and d orbitals, and m^* is the effective mass to the $\mathbf{k}_{\parallel}$ direction. The spin splitting of the magnetic material is given by the difference in E_d while the other parameters are the same. Our model band structures for the bulk magnetic material are shown in Fig. 5. We take $E_s=-2.85$ eV, $E_d=-9.35$ eV, $t_s=-3.2$ eV, $t_d=0.16$ eV, and $V_{sd}=2.0$ eV for the majority-spin band.

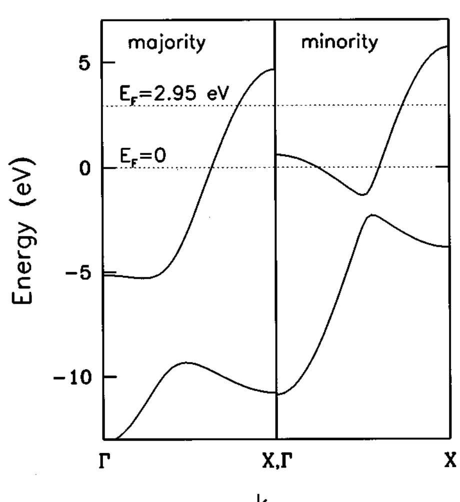

FIG. 5. Model band structures for the magnetic material at $\mathbf{k}_{\parallel}=0$. Parabolic dispersion in the in-plane direction is assumed.

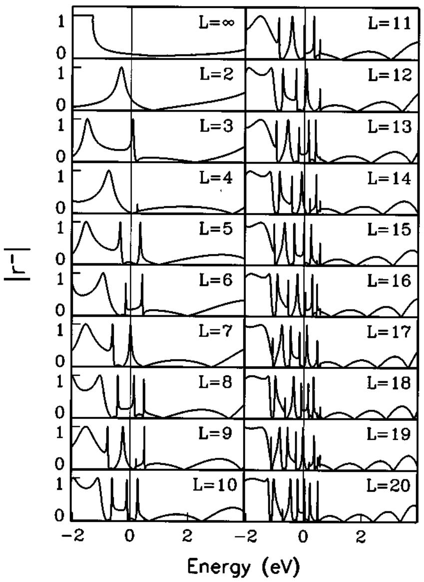

FIG. 6. Reflection amplitudes as functions of energy at $\mathbf{k}_{\parallel}=0$ for the (001) orientation model system. L is the thickness of the magnetic layer.

For the minority spin, we take $E_d=-1.35$ eV. The effective mass is same as the bare electron mass. Comparing Fig. 5 with Fig. 1(a) of Ref. 7, we see that the features of the Δ_1 band near the Fermi level are reproduced nicely here in this simple model. For convenience, the band structure for the spacer material (Cu) is taken to be same as the majority-spin band of the magnetic material (Co), since the small difference between them will not cause qualitative change in the results. Thus, we always have $r^+=0$ in this model, while in the full tight-binding model we get a finite but small r^+ near the Fermi level (see Fig. 3 of Ref. 7). We will consider two cases with the Fermi level $E_F=0$ and 2.95 eV. The $E_F=0$ case is close to the realistic situation. Note that there are two transmitted waves in the minority-spin band which is similar to the situation for (001) Co/Cu/Co at $\mathbf{k}_{\parallel}=0$. On the other hand the $E_F=2.95$ eV case is similar to a free-electron-like model near the Fermi level, which allows us to examine the behavior of exchange coupling when the Fano resonance effect becomes negligible. We plot $|r^-|$ as a function of energy at $\mathbf{k}_{\parallel}=0$ in Fig. 6, which resembles $|r^-|$ at $\mathbf{k}_{\parallel}=0$ for the (001) Co/Cu/Co system (Fig. 1). As expected, we see the Fano resonance peaks around $E=0$ and only simple Fabry-Pérot oscillations around $E=2.95$ eV. We also plot $|r^-|$ versus magnetic-layer thickness L for two different Fermi levels in Fig. 7. For $E_F=0$, $|r^-|$ varies rather irregularly due to the Fano resonance effect and it hits one for $L=7$ ML. For $E_F=2.95$ eV, a well-defined oscillation as a function of the magnetic-layer thickness is seen, and the period is related to the spanning wave vector of the magnetic material, just as expected from the free-electron model. In order to see how the Fano resonances affect the coupling strength, we evaluate the interlayer coupling J from Eq. (1) by performing a total energy calculation for superlattices within the above model. A slab method is used to determine superlattice states. In order to make sure that the number of particles is conserved, we use $\Delta\Omega$ rather than Ω (for the zero temperature),

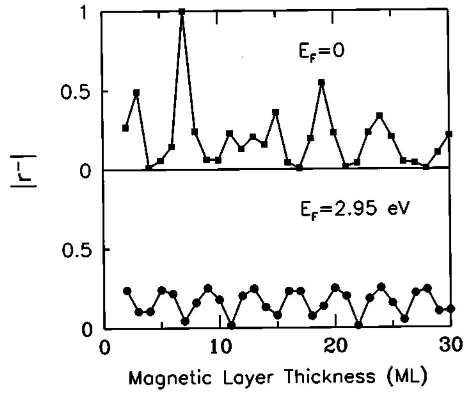

FIG. 7. Reflection amplitudes as functions of magnetic-layer thickness at $\mathbf{k}_\parallel = 0$ and the Fermi level for our model system. Upper panel is for $E_F = 0$ and lower is for $E_F = 2.95$ eV.

$$\Delta\Omega = \sum_{\mathbf{k}_\parallel} \sum_{n,q} [E_n(\mathbf{k}_\parallel, q) - E_F]\Theta[E_F - E_n(\mathbf{k}_\parallel, q)], \quad (8)$$

where n is the band index, q is the wave vector for the superlattice, and Θ is a Heaviside step function. Since the parabolic dispersion is assumed in the in-plane direction, the integration over $\mathbf{k}_\parallel$ is done analytically, which makes it possible to calculate J with great accuracy and efficiency.

We consider the magnetic-layer thickness dependence first. The interlayer coupling versus the magnetic-layer thickness L for a given spacer thickness D is plotted in Fig. 8. For both $E_F = 0$ and $E_F = 2.95$ eV, the amplitude of the fluctuation is comparable to that of asymptotic behavior obtained for large D and L with Eq. (5). For $E_F = 2.95$ eV [Fig. 8(b)], J oscillates in exactly the same way as $|r^-|$ shown in Fig. 7 as predicted by the simple free-electron model. For $E_F = 0$ [Fig. 8(a)], J is rather irregular especially for thinner magnetic layers (say, less than 15 ML). J can hardly be described by an oscillatory function with a fixed period. This is due to the Fano resonances effect. J for a thicker spacer layer ($D = 22$ ML) is quite different from J for thinner spacer layers ($D = 5$ ML or $D = 8$ ML). In the previous section, we argued that there are two length scales: D and $\hbar v_z / \Delta E$ for a given L. For small L, $D = 22$ ML is comparable to $\hbar v_z / \Delta E$. The peaks of J [Fig. 8(a)] do not always coincide with those of $|r^-|$ (Fig. 7, $E_F = 0$) since J is obtained from the integration of $|r^-|$.

In order to investigate the effect of the Fano resonance further, we plot in Fig. 9 the interlayer coupling as a function of the spacer thickness D (taking $E_F = 0$) for (a) $L = 4$ ML, (b) $L = 7$ ML, and (c) $L = 19$ ML. Also included for comparison is the asymptotic results for the case $L = \infty$ (dotted curve). From Fig. 7, we noted that $|r^-|$ is almost zero at $L = 4$ ML, and becomes large at $L = 7$ ML and $L = 19$ ML due to the Fano resonances. First of all, we see that the oscillation period of the interlayer coupling as a function of the spacer-layer thickness is not affected by Fano resonance at all. For $L = 4$ ML [Fig. 9(a)], the overall coupling strength is reduced due to small $|r^-|$. For $L = 7$ ML [Fig. 9(b)], $|r^-|$ is almost one and the interlayer coupling is stronger. The interlayer coupling for $L = 7$ ML is much stronger than that of $L = 4$ ML especially for the thick spacer layer. For

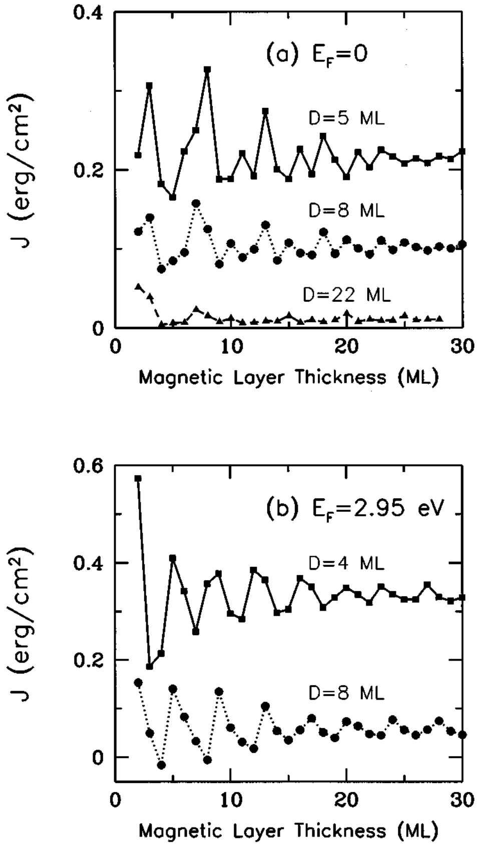

FIG. 8. Interlayer coupling as a function of magnetic-layer thickness for magnetic superlattices described in our two-band model. (a) $E_F = 0$. (b) $E_F = 2.95$ eV.

$L = 19$ ML [Fig. 9(c)], $|r^-|$ is big but the interlayer coupling appears very similar to the asymptotic behavior for $L = \infty$. This is because the Fano resonance peak at $E = 0$ for $L = 19$ ML is much sharper than that for $L = 7$ ML as shown in Fig. 6. As L further increases, the Fano resonance peaks become very sharp and J rapidly converges to the $L = \infty$ result.

IV. DISCUSSION

In the previous section, we have shown that the Fano resonances affect the interlayer coupling strength. When the interlayer coupling is plotted as a function of the spacer thickness, the effect is not very pronounced, because the change in coupling strength due to Fano resonances is comparable to or smaller than the amplitude of oscillation and it does not alter the oscillatory behavior. However, the effect shows up clearly in the magnetic-layer thickness dependence especially when the magnetic layer is thin. The fluctuation of the interlayer coupling as a function of magnetic-layer thickness cannot be explained by a simple free-electron model. However, since the interfaces in magnetic multilayers are quite rough, these fluctuation of the interlayer coupling due to the Fano resonances may be smeared out.

In Ref. 22, Castro *et al.* have shown that quasiperiodic oscillations of the interlayer coupling can be obtained when the difference in Fermi surfaces for majority and minority spin in the magnetic material are considered. Although this

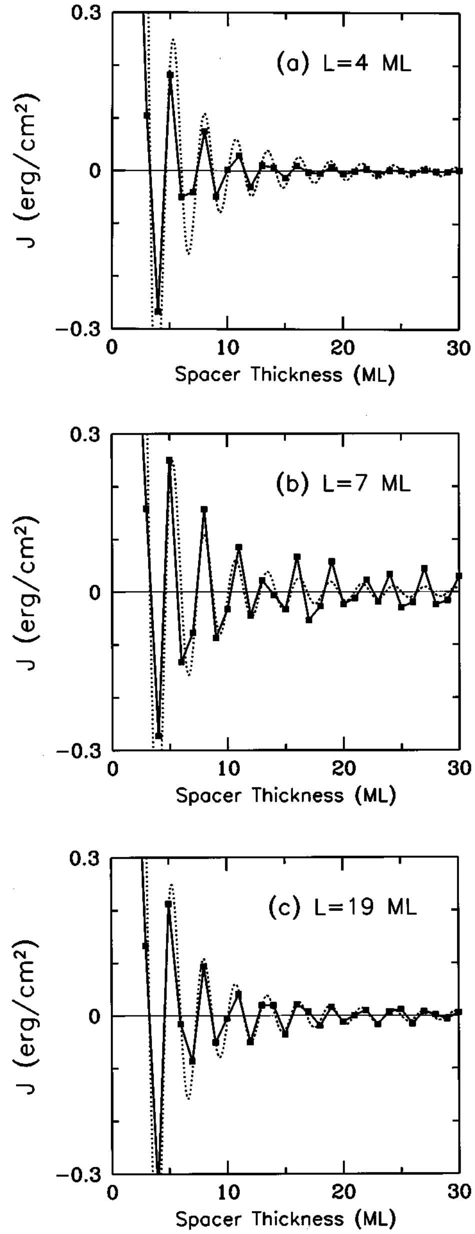

FIG. 9. Interlayer coupling as a function of spacer thickness for magnetic superlattices described in our two-band model with $E_F=0$. (a) $L=4$ ML, (b) $L=7$ ML, (c) $L=19$ ML. The dotted curve is the asymptotic behavior for $L=\infty$.

quasiperiodicity may look similar to the effect discussed in this paper, the origin is totally different because Fano resonances do not occur in their model. This can be seen easily since they used a one-band TB model for each spin of the magnetic material and electrons with different spins do not mix. Thus, in their model, there is only one possible transmitted wave in the magnetic layer for any incident wave from the spacer and there is no Fano resonance as explained in Secs. II and III. The quasiperiodic oscillations in Ref. 22 can be explained also with reflection amplitudes. In their model, when $|r_\infty^+|$ and $|r_\infty^-|$ are small, the reflection amplitude r^+ and r^- for a finite magnetic layer can be expressed as $r^+=r_\infty^+-r_\infty^+[1-(r_\infty^+)^2]e^{iq_z'^+L}$ and $r^-=r_\infty^- - r_\infty^-[1-(r_\infty^-)^2]e^{iq_z'^-L}$, where $q_z'^+$ and $q_z'^-$ are the z components of the scattering wave vector in the magnetic layer for majority and minority spin, respectively. Then, the spin-asymmetry reflection amplitude is

$$(\Delta r)^2=\frac{(r_\infty^+-r_\infty^-)^2}{4}-\frac{(r_\infty^+-r_\infty^-)r_\infty^+}{2}e^{iq_z'^+L}+\frac{(r_\infty^+-r_\infty^-)r_\infty^-}{2}e^{iq_z'^-L}, \qquad (9)$$

while higher order terms in the reflection amplitudes and more rapidly oscillating terms are neglected. The interlayer coupling can be obtained by inserting the above equation into Eq. (2). Therefore, the interlayer coupling as a function of the magnetic-layer thickness is a superposition of two smoothly oscillating functions with different periods. The superposition of two different periods gives rise to a beating effect, which is the origin of the quasiperiod of Ref. 22. Especially when the difference of two periods is large and one period is very short as in the figures of Ref. 22, the result may look rather irregular. This is partly due to the aliasing effect. Note that still the result can be expressed by the sum of two sinusoidal functions. Now, we consider under what circumstances this quasiperiod will show up experimentally. First, both $|r_\infty^+|$ and $|r_\infty^-|$ should be big enough. If one of them is much smaller than the other, only one period will dominate and the beating effect will not be observed. Thus, the quasiperiod can be detected only when r_∞^+ and r_∞^- both have large magnitudes and they are almost out of phase, a condition not easily satisfied. For most cases of strong interlayer coupling, the reflection is big for one spin and small for the other. Also if a total reflection occurs for one spin, there is no magnetic layer thickness dependence for this spin unless the magnetic layer is thin enough for the tunneling to occur. Moreover, one period needs to be much different from the other. If they are close, the overall period will be given by the average of the two periods and the beating effect will not show up unless the interlayer coupling is measured up to a very thick magnetic layer. As an example, we consider (001) Co/Cu/Co systems. At $\mathbf{k}_\parallel=0$, $|r_\infty^+|$ is smaller than $|r_\infty^-|$ (Refs. 3 and 7) and two periods are very close. At $\mathbf{k}_\parallel=\mathbf{k}_S$, a total reflection occurs for minority spin and the magnetic-layer thickness dependence will be dominated only by r^+ unless the magnetic layer is extremely thin. Therefore, we do not expect the quasiperiodic oscillation discussed in Ref. 22 to show up in (001) Co/Cu/Co systems.

Unlike the quasiperiod in Ref. 22, the contribution from the Fano resonance cannot be expressed by an oscillatory function with a period. It can be further illustrated by examining the (001) Co/Cu/Co $\mathbf{k}_\parallel=0$ case in Sec. II and also our model in Sec. III. For minority spin only, there are two possible transmitted waves (corresponding to two different points on the Fermi surface). However, r^- cannot be expressed as a sum of two oscillating functions. If r^- could be expressed in this way, $|r^- - r_\infty^-|$ in Fig. 2 would be almost the same as $|r_\infty^-|$ since the transmission to the band with smaller k_z' is negligible. Instead, it was expressed as $r^-=r_\infty^- - r_\infty^-[1-(r_\infty^-)^2]e^{iq_z'L}+r_{\rm Fano}$ in Eq. (6), where q_z' is twice of the larger k_z' and $r_{\rm Fano}$ mainly consists of sharp peaks. As pointed out already in Sec. II, this is because the portion of band with smaller k_z' has mostly d character while the incident wave has predominantly sp character. This portion of band plays a negligible role for the semi-infinite magnetic layer. For the finite magnetic layer, this portion is quantized and interacts with the continuum states of the other portion of the band with larger k_z'. This gives rise to sharp peaks known as Fano resonances, instead of another periodic function. In the cases we are considering, the Fano resonance happens only for minority spin and the spin-asymmetry reflection amplitude is given in a form similar to Eq. (9):

$$(\Delta r)^2 = \frac{(r_\infty^+ - r_\infty^-)^2}{4} - \frac{(r_\infty^+ - r_\infty^-) r_\infty^+}{2} e^{iq_z'^+ L} + \frac{(r_\infty^+ - r_\infty^-) r_\infty^-}{2} e^{iq_z'^- L} - \frac{r_\infty^+ - r_\infty^-}{2} r_{\text{Fano}}^- . \quad (10)$$

In Sec. II, it is shown that r_{Fano}^- consists of sharp peaks and is not periodic. The contribution of Fano resonances to the interlayer coupling is considerable when the peaks hit the Fermi level at the extremal points and the linewidth is big. The peaks are rather sharp and they hit the Fermi level in an almost random fashion. Thus, the contribution as a function of magnetic-layer thickness is pretty much irregular and it cannot be expressed in an analytical form. As the magnetic-layer thickness increases, the linewidth decreases rapidly as shown in Figs. 1 and 6. We expect that the Fano resonance effect can show up for relatively thin magnetic layers and it will disappear for thick magnetic layers. However, the magnetic layers treated in experiments are considered to be thin enough for the Fano resonance effect to be detected. Even when there are multiple bands, if the other wave vectors are forbidden due to different symmetry, or if the other bands are immersed below the Fermi level, there is only one possible transmitted wave at the Fermi level in the magnetic layer for each spin. If this happens for the both spins, there is no Fano resonance and the situation will be qualitatively the same as that of Ref. 22.

There are few experiments available on the magnetic-layer thickness dependence of the interlayer coupling. In Ref. 11, the interlayer coupling in the fcc (001) Co/Cu/Co multilayers was measured as a function of Co thickness up to about 20 Å. The coupling strength for fcc (001) Co/Cu/Co multilayers greatly depends on the sample quality.[23,24] The interlayer coupling measured in Ref. 11 is still much weaker than theoretically predicted one[7,14] and it is not clear which spanning vector dominates the experimental data. In Sec. II, the fluctuation of $|\Delta r|$ with respect to the Co layer is dominated by the Fano resonance effect at $\mathbf{k}_\parallel = 0$ and by the tunnelling effect for thin Co layers at $\mathbf{k}_\parallel = \mathbf{k}_S$. In Ref. 11, when the Co layer is thicker than 10 Å, the interlayer coupling fluctuates rather irregularly. This may be due to the Fano resonances. On the other hand, fluctuation at thin Co layers may be due to the tunneling. For a quantitative comparison, an accurate full band calculation seems necessary for the (001) Co/Cu/Co multilayers.

In contrast, well-defined oscillations were observed in Fe/Au/Fe multilayers[25] when the interlayer coupling was measured as a function of the Fe thickness. The Fermi surface of Au is very similar to that of Cu. At the Fermi level and $\mathbf{k}_\parallel = 0$, there is only one band for Au. Since bands with the same symmetry (Δ_1) are not available for Fe majority spin and there is one for Fe minority spin around the Fermi level at $\mathbf{k}_\parallel = 0$, strong interlayer coupling is expected for the corresponding extremal vector of Au. This extremal vector gives rise to a long period. Considering the short period is easily suppressed by the interface roughness, we expect that the interlayer coupling versus Au layer in Fe/Au/Fe will be dominated by the long period. Since there is only one possible transmitted wave for the Fe minority spin at the Fermi level and $\mathbf{k}_\parallel = 0$, no Fano resonance effect exists for this extremal point. Thus, a well defined oscillatory behaviour as a function of the magnetic-layer thickness is expected, which accounts for the experimental observation.

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