Magnetic multilayers: A detailed analysis of continuum versus discrete treatments

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Magnetic multilayers: A detailed analysis of continuum versus discrete treatments

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A critical comparison is made between discrete and continuum treatments put forward to determine the magnetic ordering of exchange coupled superlattices. In particular, our interest is focused on the spatial patterns adopted by the coupling between ferromagnetic layers across the nonmagnetic spacers. We find that for values of the spacer electron Fermi wavevector $k_F > \pi/a$, where a is the lattice parameter, the continuum model breaks down. This gives rise to interesting interference effects, which emerge in the discrete three-dimensional treatment, but which are missed in a continuum pseudo one-dimensional approximation. The experimental evidence is discussed, and an analytic derivation of the critical k_F value is also given.

The development of new preparation techniques has led to the production of a wide variety of high quality multilayers systems. In particular, the magnetic properties of metallic multilayers, obtained intercalating ferromagnetic and non-magnetic metals (spacers), have lately attracted the attention of experimentalists[1] and theorists[2] alike. This interest is easy to understand in view of the appealing basic problems they pose, as well as their technological applications in the magnetic recording industry.

It has been observed that the coupling between the magnetic layers may oscillate from ferromagnetic to antiferromagnetic, depending mainly on the thicknesses of the spacer. It has also been observed that an applied magnetic field can induce big changes in the electrical resistivity of the system. This effect, denominated giant magnetoresistance, was first observed in Fe/Cr multilayer systems by Baibich *et al.*[3] The periodicity, phase, and magnitude of the oscillations vary, depending on the multilayer constituents and their spatial arrangement.

Early experimental results,[1,3] revealed oscillation periods of the order of 10–20 (Å). More recently, in well controlled experiments, Unguris *et al.*[4] found both long and short wavelength oscillations of the coupling, when the quality of the interface was varied. With sharp interfaces short wavelengths were observed, of around two atomic layers, similar to those obtained when a Rudermann-Kittel-Kasuya-Yosida (RKKY) type of interaction[5] is assumed to be responsible for the coupling of the magnetic layers.

On the theoretical front Yafet[6] investigated these systems in 1987, comparing results obtained for one- (1-D) and three-dimensional (3-D) geometries. He assumed that an RKKY interaction couples the magnetic moments of the magnetic layers adjacent to the interfaces, separated by the non-magnetic spacer. More recently Edwards and Mathon[7] proposed a Hubbard model based theory, and found out that it leads to answers which are quite close to those obtained from a plain Ruderman–Kittel treatment. In turn, Baltenspeger and Helman[8] provided a quantitative comparison between the Hubbard and RKKY results, on the basis of a pseudo 1-D treatment. Similar procedures have also been implemented by Coehoorn,[9] and by Chappert and Rennard.[10]

In this communication we show that, quite often, it is necessary to go one step further and implement a full 3-D calculation, because of significant deviations of the pseudo 1-D results, relative to the exact ones.

To carry out our calculations we consider a sandwich consisting of two ferromagnetic slabs, separated by N atomic layers of a nonmagnetic spacer. The ferromagnetic metal atoms on the first slab carry a magnetic moment $\mathbf{S}_1$. The nonmagnetic metal conduction electrons are polarized by the magnetic moments, giving rise to spatial oscillations of the spacer magnetization. The magnetic moments of the surface magnetic layer across the spacer, $\mathbf{S}_2$, feel the effect of the spin polarization and, depending on the thickness of the spacer, align ferromagnetically or antiferromagnetically, relative to the magnetization of the first slab.

The RKKY interaction energy between a magnetic moment $\mathbf{S}_1$ on the interface of the magnetic slab and the spacer, with all the magnetic moments on the opposite magnetic interface $\mathbf{S}_2$, with x denoting the distance between the two magnetic slabs, is given by

$$I(x) = -\frac{J^2 m^*}{2^5 \pi^3 \hbar^2} k_F^4 V^2 \times \sum_r \left(\frac{\sin(2k_F r) - 2k_F r \cos(2k_F r)}{(2k_F r)^4} \right) \mathbf{S}_1 \cdot \mathbf{S}_2, \quad (1)$$

where r is the distance between two magnetic moments on opposite magnetic slabs, J the exchange interaction between magnetic and conduction electrons, V the volume of the spacer unit cell, k_F its Fermi wavevector, and $|\mathbf{S}_i|$ the magnitude of the localized magnetic moments.

To derive analytic expressions for the coupling energy it is usual to integrate over the magnetic layer,[6,8] instead of adding the contribution of every individual magnetic moment, to obtain

$$I(\xi) = -\frac{J^2 m^*}{2^7 \pi^2 \hbar^2 A} k_F^2 V^2 \left(\frac{\sin\xi}{\xi^2} - \frac{\cos\xi}{\xi} - si(\xi) \right), \quad (2)$$

where $\xi = 2k_F x$, A is the area of the two-dimensional unit cell, and $si(\xi)$ is the usual sine integral.[11] This expression

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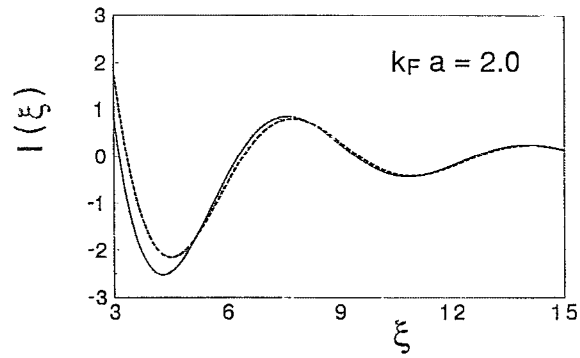

FIG. 1. Interaction energy $I(\xi)$ vs ξ for $k_F=1$ (Å^{-1}), in units of $m^*J^2S_1S_2/2^5\pi^3\hbar^2$. The dashed line gives the continuum pseudo 1-D approximation, while the continuous line is the large distance asymptotic limit.

was derived both by Yafet,[6] and by Baltensperger and Helman.[8] In the large distance limit $k_Fx \gg 1$, Eq. 2 reduces to

$$I(\xi)=-\frac{J^2m^*}{2^6\pi^2\hbar^2A}\,k_F^2V^2\frac{\sin\xi}{\xi^2}. \tag{3}$$

The dashed line in Fig. 1 illustrates the behavior of the coupling energy given by Eq. (2), while the continuous line is the large distance approximation, supplied by Eq. (3). The sign is chosen such that $I(\xi) > 0$ implies ferromagnetic coupling. As observed, for $\xi > 11$ the limiting form constitutes a very good approximation to $I(\xi)$. For transition metals k_F is typically of the order of 1–2 (Å^{-1}) and the lattice parameter a is of the order of 3–4 (Å), so that values of $\xi=2k_Fx<6$ are unphysical. Thus, the limiting form can be used most of the time.

We now proceed with a proper discrete 3-D treatment of the RKKY interaction, as given by Eq. (1). The results, which were obtained numerically, are given in Figs. 2 and 3. They illustrate the exchange coupling, for a simple cubic structure, in units of $m^*J^2S_1S_2/2^5\pi^3\hbar^2$, both for the continuum model of Eq. (3), and for the discrete one [Eq. (1)]. Adopting the typical values[12] for the above parameters $J/A\approx 1$ (eV/cm^2) and $S_i=1$, we obtain $m^*J^2S_1S_2/2^5\pi^3\hbar^2\approx 2$ (erg cm^{-2}). The results displayed in Figs. 2 and 3 imply a maximum coupling energy of the order of 1 (erg cm^{-2}), across a spacer 3 monolayers thick, in good agreement with experimental results.[1,3,4]

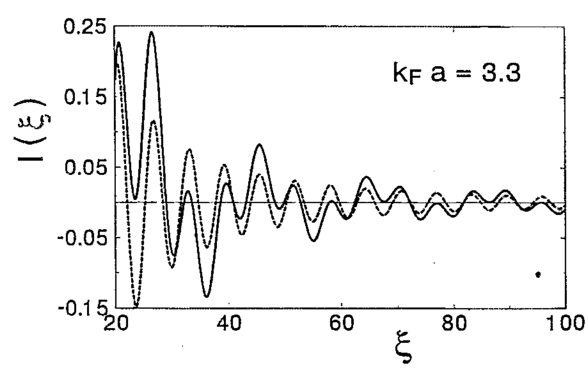

FIG. 2. $I(\xi)$ vs ξ, for $k_F=1.1$ (Å^{-1}), in units of $m^*J^2S_1S_2/2^5\pi^3\hbar^2$. The solid line corresponds to the exchange coupling $I(\xi)$ for the discrete 3-D calculation. The dotted line illustrates the coupling for the pseudo 1-D treatment.

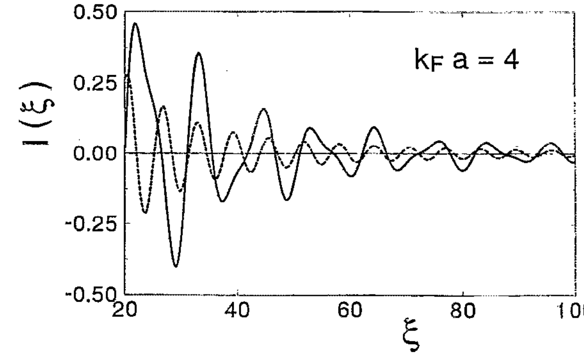

FIG. 3. Same as Fig. 2, but for $k_F=4/3$.

The computations were carried out for several values of $k_F a$. For $k_F a<\pi$ the results for $I(\xi)$ obtained from a discrete pseudo 1-D and from a full 3-D calculation are indistinguishable, and quite similar to those illustrated in Fig. 1. But, as $k_F a$ grows, a significant difference between the two calculations becomes apparent. While in a continuum 1-D approach $I(\xi)$ shows regular oscillations, these are severely modified when a discrete 3-D calculation is carried out, as illustrated in Figs. 2 and 3. We observe that the interaction has a rich structure, quite different from a simple damped periodic function. For $k_F a>\pi$ a severe pattern modification, due to the discrete character of the lattice, is observed. A derivation of the critical value $k_F^{\text{crit}}=\pi/a$ is given in the Appendix. Moreover, in Fig. 3 it is observed that these effects are so strong as to induce a breakdown in the periodicity, generated by the interference of the different terms that contribute to the summation in Eq. (1).

As far as experimental evidence for this effect we notice that, when the magnetic patterns of the Fe/Cr/Fe multilayer system (especially Fig. 3 of the paper of Unguris *et al.*[4]) are carefully examined, deviations from perfect periodicity are quite apparent. Further evidence in this direction can also be found in Ref. 13. Moreover, elements commonly used as spacers are copper, silver, and gold. If the ferromagnetic layers are made of a transition metal element (TM), then multilayer systems like TM/Cu/TM, TM/Ag/TM, and TM/Au/TM do satisfy the requirement that $k_F>k_F^{\text{crit}}=\pi/a$, and thus also are likely candidates for the observation of the above described interference patterns.

We have also estimated the magnitude of atomic finite size effects, that is, the consequences of considering magnetic moments which are spread out over a finite volume, rather than localized at the lattice site. Our calculations convinced us that finite size effects, in this instance, are quite negligible.

In conclusion, for small values of $k_F a$ there is no dif-

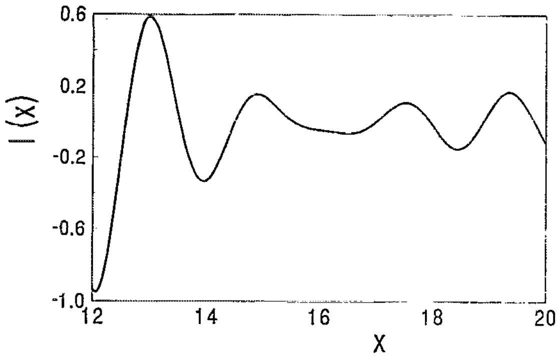

FIG. 4. $I(x)$, in arbitrary units, vs x (Å), for $k_F a=5.4$

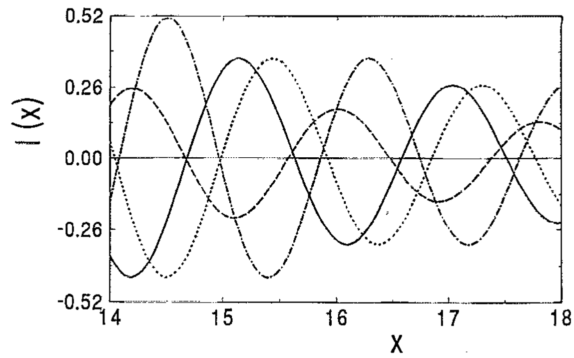

FIG. 5. Lower order contributions to $I(x)$, in arbitrary units, vs x (Å), for $k_F a=5.4$. The dot-dashed line corresponds to $\rho = 1$, the dashed line to the $\rho=\sqrt{2}$, the dotted line to $\rho=\sqrt{4}$, and the solid line to $\rho=\sqrt{5}$.

ference between the results of the 1-D and discrete 3-D treatments. However, for $k_F > k_F^{\text{crit}}$, considerable deviations do result, which are missed by pseudo 1-D continuum treatments. The magnitude of the effect is large enough and cannot always be ignored.

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APPENDIX: CRITICAL WAVEVECTOR

In this Appendix we derive the critical magnitude of the Fermi wavevector k_F^{crit}, for the onset of interference effects. Consider a magnetic moment $\mathbf{S}_1$ interacting with all the moments $\mathbf{S}_2$ on a yz–layer located a distance x away. The interaction strength $I(x)$ is given by Eq. (1), where $r=\sqrt{x^2+\rho^2}$ is the distance between $\mathbf{S}_1$ and $\mathbf{S}_2$, while $\rho=\sqrt{y^2+z^2}$.

On the other hand, the spherical Bessel function $j_1(u)=u^{-2}\sin u - u^{-1}\cos u$, and thus

$$I(x) \propto \sum_r \frac{j_1(2k_F r)}{r^2} . \tag{A1}$$

The function $j_1(u)$ has an infinite number of zeros, denoted by $z_{1,n}(u)$. The asymptotic form for their location is $u \rightarrow (n+\frac{1}{2})\pi$, for $n \gg 1$. It is observed that these zeros coincide with the zeros of the expression in the summation of Eq. (1).

In Fig. 4 we display the function $I(x)$ of Eq. (A1), generated by a magnetic moment $\mathbf{S}_1$ interacting with a square lattice magnetic layer, with nearest neighbor distance $a = 3$ (Å), for $k_F=1.8$ (Å^{-1}). It is noticed that $I(x)$ is far from being a periodic function, showing a peculiar pattern in the region $15<x<17$. This anomaly can be traced to the *simultaneous* pairwise cancelling of the lowest order contributions to the summation of Eq. (1), in the region of interest. In particular, as can be noticed in Fig. 5, an almost total cancelling of the nearest neighbor contributions develops between the pairs $\{\rho=\sqrt{1}, \rho=\sqrt{4}\}$, and $\{\rho=\sqrt{2}, \rho=\sqrt{5}\}$, for $15<x<17$. For this cancelling to occur

$$z_{1,n}(2k_F r') \approx z_{1,n+1}(2k_F r''), \tag{A2}$$

where $r'=\sqrt{\rho'^2+x^2}$ and $r''=\sqrt{\rho''^2+x^2}$. The vectors ρ' and ρ'' denote the position of a pair of nearest neighbors on the magnetic layer, and thus $\rho''^2=\rho'^2+a^2$. Consequently $r''^2-r'^2=\rho''^2-\rho'^2$. Since the peculiar interference patterns occur for $x \gg a$, we have $2r'(r''-r') \approx \rho''^2-\rho'^2$. Equation (A2), for two zeros to concur, is thus satisfied when both

$$2k_F r' = (n+\tfrac{1}{2})\pi \quad \text{and} \quad 2k_F r'' = (n+\tfrac{3}{2})\pi, \tag{A3}$$

which readily yields

$$\frac{\pi}{2k_F r'} = \frac{r''-r'}{r'}, \tag{A4}$$

so that $k_F(\rho''^2-\rho'^2) \approx \pi r'$, but $\rho''^2-\rho'^2=a^2$, and thus $k_F a^2 \approx \pi r'$. Due to the discreteness of the lattice $r' \geqslant a$, one finally obtains the for the critical k_F value:

$$k_F^{\text{crit}} a=\pi. \tag{A5}$$

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