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LETTER TO THE EDITOR

The nature and validity of the RKKY limit of exchange coupling in magnetic trilayers

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Abstract. The effects on the exchange coupling in magnetic trilayers due to the presence of a spin-independent potential well are investigated. It is shown that within the RKKY theory no bias or extra periods of oscillation associated with the depth of the well are found, contrary to what has been claimed in recent works. The range of validity of the RKKY theory is also discussed.

Metallic magnetic multilayers are systems composed of alternating ultrathin layers of magnetic and non-magnetic metallic materials. They exhibit exchange coupling between magnetic layers across a non-magnetic spacer. Such a coupling oscillates between ferromagnetic and antiferromagnetic and its strength decays as the spacer layer thickness is varied [1, 2, 3].

Basically, two mechanisms have been proposed for explaining the oscillatory coupling in multilayers. Edwards *et al* [4, 5] have related the phenomenon to the existence of quantum wells for electrons (or holes) with both spin orientations propagating through the multilayer structure, which result from the exchange interaction inside the magnetic layers. The existence of those quantum wells was recently confirmed by photoemission experiments [6]. According to the model proposed by Edwards *et al*, the observed oscillation in the coupling results from quantum interference effects inside the well and bears a formal analogy to the de Haas–van Alphen effect. The other proposed mechanism for the coupling in multilayers is due to Bruno and Chappert [7] and is based on an extension of the RKKY theory to the particular geometry of the system. In their approach the coupling arises from the polarization of magnetic carriers in the spacer, as in the ordinary RKKY theory for the coupling between localized magnetic moments in a non-magnetic host.

The formal connection between the two theories was recently made explicit by d'Albuquerque e Castro *et al* [8]. In their work, model-independent closed form expressions are derived for the coupling, as well as for the bilinear and biquadratic terms, and it is shown that the full confinement and the RKKY-like theories correspond to limiting cases in which the exchange interaction inside the magnetic layers is very strong and very weak, respectively. Another important point made by d'Albuquerque e Castro *et al* is that in the usual RKKY-like theories the difference between the non-magnetic parts of the potentials in the spacer and in the magnetic layers are neglected, which may lead to significant errors in the amplitude and phase of the coupling.

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Both the quantum well and RKKY-like theories relate the period of oscillation of the coupling to the extremal points of the spacer Fermi surface in the direction perpendicular to the layers. However, in a recent paper by Jones *et al* [9] the question of other possible sources for the period of oscillation is discussed and it is claimed that the oscillation period is determined by the depth of the quantum well formed by the magnetic and spacer layers rather than by the dimensions of the spacer Fermi surface. In addition those authors claim that such effects can generate a bias in the coupling, producing a preferred ferromagnetic coupling. In recent calculations Muñoz and Pérez-Díaz [10] have also found periods in the coupling not related to the spacer Fermi surface, which they claim are associated with the confined states in the quantum well.

In this communication we present results for the coupling for cases in which the quantum well due to the difference in the potentials of the spacer and the magnetic layers give rise to bound states for carriers with both spin directions. Those are just the situations considered by Jones *et al* and Muñoz and Pérez-Díaz. We have found that, provided the contributions to the coupling coming from singularities associated with the presence of the bound states are properly dealt with, no extra period nor any bias are obtained. We therefore conclude that the features observed by Jones *et al* and by Muñoz and Pérez-Díaz are spurious.

We consider trilayer systems described by the one-band tight-binding model with nearest-neighbour hopping, t , on a simple cubic lattice. The layers are displaced perpendicularly to the (100) direction and the site energies are chosen equal to $6|t|$ in the spacer and $6|t| + V$ in the magnetic material. Such a choice of parameters places the bottom of the spacer band at the origin of the energies. For sufficiently small values of the potential barrier V and of the Fermi energy E_F , the Fermi surfaces of both the spacer and magnetic materials are nearly spherical. Therefore the effective mass approximation can be safely applied to both materials, and the present model becomes equivalent to the electron gas model. We follow Jones *et al* and introduce a local exchange interaction V_{ex} only in the magnetic atomic layers next to the spacer. We label these two layers 0 and n , so that the number of atomic layers in the spacer is equal to $N = n - 1$. The restriction of the local exchange interaction to just one atomic layer in the magnetic material would have to be lifted if we were to study the dependence of the coupling on the magnetic layer thickness. A recent thorough investigation of such a dependence [11] has shown that as far as the behaviour of the coupling as a function of the spacer thickness is concerned, changes in the magnetic layer thickness just leads to changes in the phase and amplitude of the coupling, keeping the period of oscillation unchanged. Therefore, for the purpose of the present work the restriction of V_{ex} to just one monolayer in the magnetic material does not pose any limitation on the validity of our final conclusions.

The change in the thermodynamical potential Ω at $T = 0$ due to a rotation by an angle θ of the magnetization in one of the magnetic layers relative to that in the other layer is given by [8]

$$\Delta\Omega(\theta) = \frac{1}{\pi} \sum_{q_{\parallel}} \int_{-\infty}^{E_F} d\omega \operatorname{Im} \ln \{1 - 2V_{ex}^2 (\cos \theta - 1) G_{n0}^{\uparrow}(\omega, q_{\parallel}) G_{0n}^{\downarrow}(\omega, q_{\parallel})\} \quad (1)$$

where $G_{0n}^{\sigma}(\omega, q_{\parallel})$ is the off-diagonal matrix element between sites 0 and n of the retarded Green's function for an electron with spin σ in the ferromagnetic $\theta = 0$ configuration of the system. Here the summation over q_{\parallel} is restricted to the two-dimensional Brillouin zone. It is worth stressing that the Green's function G^{σ} properly takes into account the presence of the potential well and, consequently, exhibits poles at the corresponding bound states energies. Those poles lie on the real axis. However, because the integrand in equation (1) is analytic in the upper-half of the complex energy plane, the integration over the energy ω

can be performed along a straight line joining the points $E_F + i\infty$ and E_F , thereby avoiding the singularities.

The expansion of the integrand in equation(1) in powers of $\cos(\theta)$ [8] enables us to introduce the bilinear J_1 and intrinsic biquadratic J_2 coefficients, in terms of which the expression for $\Delta\Omega$ reads,

$$\Delta\Omega(\theta) = \Delta\Omega_0 - J_1 \cos\theta - J_2 \cos^2\theta \quad (2)$$

It is found that higher order terms than $\cos^2\theta$ are negligible so that

$$J_1 = \Delta\Omega(\pi)/2 \quad (3)$$

Here we are interested in those situations in which the local exchange interaction V_{ex} is small and the coupling can be calculated by perturbation theory in that parameter. It is then straightforward to show that to lowest order in V_{ex} the bilinear coefficient is given by [8]

$$J_1^{\text{RKKY}} = \frac{1}{\pi} \sum_{q_{\parallel}} \int_{-\infty}^{E_F} d\omega \text{Im}\{2V_{\text{ex}}^2 G_{n0}^0(\omega, q_{\parallel}) G_{0n}^0(\omega, q_{\parallel})\} \quad (4)$$

where the Green's functions are now calculated for $V_{\text{ex}} = 0$. This is just the second-order perturbation theory or RKKY result for the coupling.

Using the above expression we evaluated J_1^{RKKY} for the trilayer system as a function of the spacer thickness N , for fixed values of E_F and V_{ex} , but for different well barriers V . For the systems under consideration it is possible to derive analytical expressions for the off-diagonal Green's function elements $G_{n0}^0(\omega, q_{\parallel})$ and $G_{0n}^0(\omega, q_{\parallel})$ for an arbitrary value of n [12]. Those expressions can be analytically continued to non-integer n , which permits us to consider continuous variations of the spacer thickness. We set $E_F = |t|$, which gives rise to a period of oscillation of exactly three atomic layers, and $V_{\text{ex}} = 0.04|t|$. In all cases, the calculated values of J_1^{RKKY} (diamonds) are compared, following equation (3), with $\Delta\Omega(\pi)/2$ (solid circles), the latter quantity being calculated from the full expression (1).

Figure 1(a) shows results for the case in which $V = 0$ (no potential well). As expected the coupling oscillates about zero (no bias) and with a well defined period of three atomic layers. However, in contrast with what was found by Jones *et al* and Muñoz and Perez-Díaz, those features are not changed when non-zero values of V are considered. We have performed calculations for V equal to $0.3E_F$, $0.6E_F$, and $0.9E_F$. Results are shown in figure 1(b), (c) and (d), respectively. The only noticeable changes in the curves are in the phase and in the amplitude of oscillations. We have observed, however, that because of the singular behaviour of the integrand along the real energy axis, spurious features, such as bias and extra period, can be easily obtained when the contributions from the singularities are not properly taken into account. We have explicitly verified this point by evaluating the energy integration also along the real axis. It should be stressed that numerical problems may occur even when $V = 0$. In such a case, for each q_{\parallel} , the integrand in equation (4) has a pole right at the bottom of the band. In all cases, if the contribution from poles is not treated properly, a bias in the coupling is obtained. This point was already noticed by Yafet [13] in the case of the RKKY interaction for the one-dimensional electron gas with $V = 0$. It is interesting to notice that for the value of V_{ex} considered above, the second order perturbation result J_1^{RKKY} for the coupling agrees well with the full calculation $\Delta\Omega(\pi)/2$. For higher values of this parameter, however, the second order perturbation theory does not provide a satisfactory description of the coupling and full calculations have to be performed. This point is illustrated in figure 2 which shows results of both J_1^{RKKY} (diamonds) and full

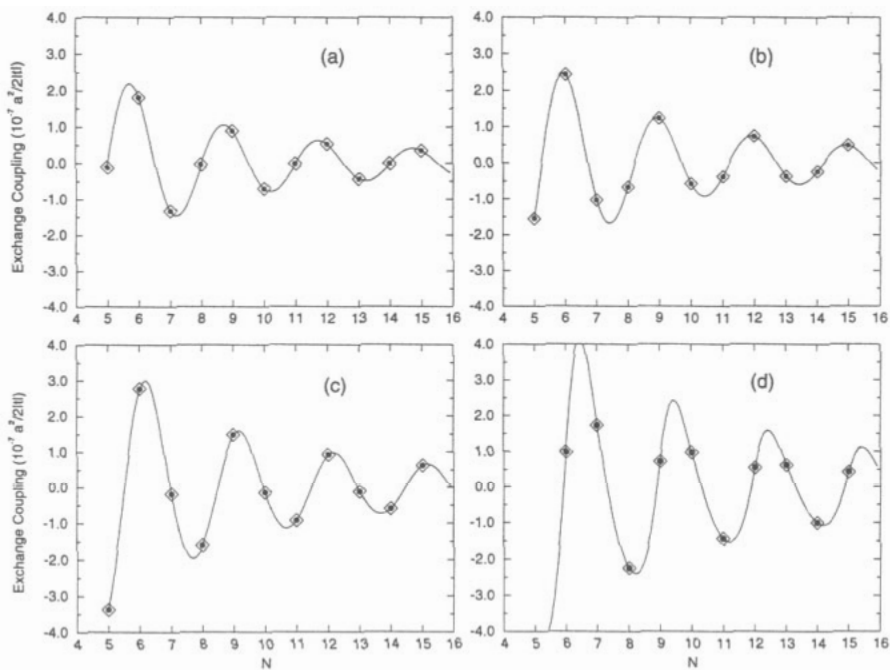


Figure 1. Exchange coupling as a function of spacer thickness for barrier heights $V = 0$ (a), $0.3E_F$ (b), $0.6E_F$ (c), and $0.9E_F$ (d). In each graph, results for J_1^{RKKY} are represented by diamonds and those for $\Delta\Omega(\pi)/2$ by solid circles. Full lines are for continuous values of n .

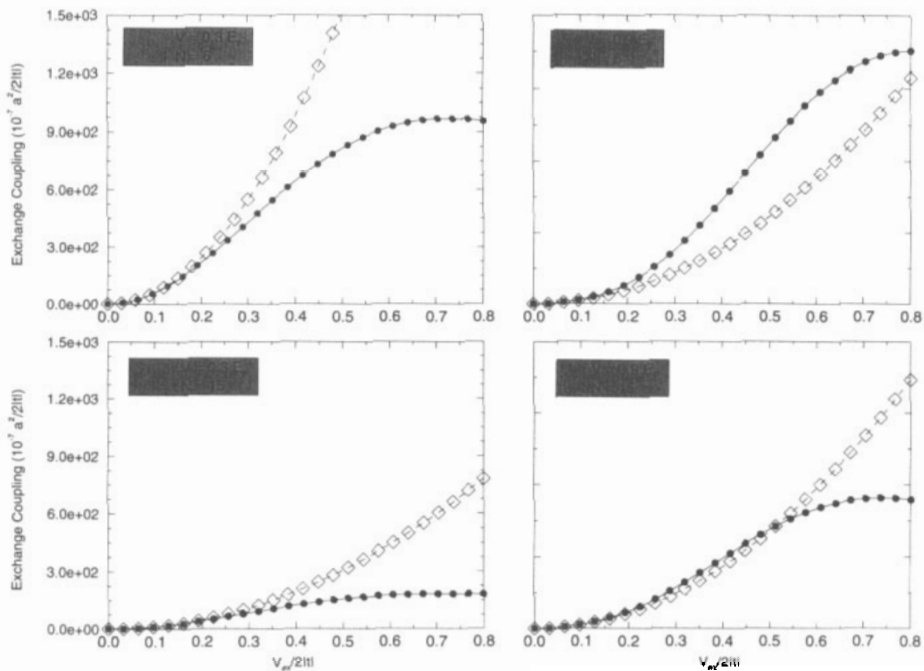


Figure 2. Exchange coupling as a function of the local exchange interaction V_{ex} for different heights of the well and spacer thicknesses. Results for J_1^{RKKY} are represented by diamonds and those for $\Delta\Omega(\pi)/2$ by solid circles.

calculation (solid circles) as functions of V_{ex} , for different values of V and N . We clearly see that for fixed E_F the range of applicability of the second order perturbation theory strongly depend on both N and V . In summary, we have shown that the inclusion of interface effects through a spin independent square well potential does not alter the period of oscillation of the RKKY bilinear coupling, as it was recently claimed. We have also checked that the appearance of a ferromagnetic bias is due to numerical inaccuracy in the calculation and does not reflect any real effect due to presence of bound states. Finally, we have explicitly shown the limited validity of the RKKY-like theories.

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