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Letter to the Editor

# Dipolar interaction and its interplay with interface roughness

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**Abstract**

We present a comparison of the strength of the classical dipolar interaction, relative to quantum-mechanical coupling mechanisms like RKKY and complete confinement, between two ferromagnetic films separated by a paramagnetic spacer. The classical dipolar coupling, which vanishes if the two interfaces are perfectly continuous and flat, builds up strength as the interface roughness grows for several models of interface topography. These numerical estimates, carried out for a Co/Cu/Co trilayer show that, in the presence of substantial surface roughness, the dipole–dipole interaction strength is comparable, and at times even larger, than those obtained using other well established mechanisms. These results are also in qualitative agreement with experimental measurements in a variety of multilayer systems. Thus, for rough interfaces, the dipolar interaction cannot be ignored.

The precise description of the interlayer coupling in ferromagnetic (FM)–paramagnetic (PM) multilayer structures is still a subject of interest [1,2]. In many cases the magnetic layers order magnetically, even when separated by spacers ten or more monolayers thick. The approaches that have been published rest on the assumption that the magnetic coupling is due to indirect exchange, carried from one magnetic layer to the next by the system conduction electrons. Several descriptions, and calculations, based on this idea, but starting from different perspectives, have been put forward. Bruno and Chappert [3] implemented a calculation based on the RKKY mechanism [4], including effects due to Fermi surface nesting. Shi et al. [5] obtain RKKY and superexchange coupling, from the Anderson model mixing of local and conduction electron states. Edwards et al. [6] assume complete confinement of majority spins within the magnetic layers. Stiles [7] developed a model based solely on the Fermi surface topology of the spacer material, in which the extremal spanning vectors play an important role, just as in Ref. [3]. Linear and biquadratic terms have also been studied [8]. In the appropriate limits these different approaches have been shown to be equivalent [9]. In spite of the diversity in their quantum mechanical treatments, all of them yield similar interlayer coupling strengths, which reach a maximum energy of a few tenths of an erg/cm$^2$ in good agreement with experiments [1,2]. On the other hand, it is taken for granted that the classical dipolar electromagnetic interaction is of negligible magnitude when compared to these quantum mechanical alternatives [1,2,10]. The only exceptions to this viewpoint, to the best of our knowledge, are: (i) a

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paper by Demokritov et al. [11] where the contribution of the magnetic-dipole field, between a rough and a planar interface to the 90° alignment biquadratic interlayer coupling mechanism of Slonczewski [8], is proposed and estimated. This coupling energy is of the order of 0.01 erg/cm$^2$ for iron films separated by a spacer of 1 nm thickness; and (ii) a contribution by Hill et al. [12] in which the dipolar coupling strength was estimated in the framework of a continuum model calculation, to conclude that correlated roughness can explain trends in the experimental results.

Here we perform a critical comparison of the coupling, evaluating the RKKY and dipolar mechanisms in a variety of realistic situations which include structural disorder. With increasing interfacial roughness, the RKKY coupling decreases considerably, while the dipolar coupling grows. For certain models of interface roughness, the lower bound of the dipolar interaction is larger than the RKKY coupling, of the same order of magnitude as the experimentally observed values, and may exhibit a change of sign with increasing separator thickness.

Due to the similar results obtained from all the quantum mechanical treatments, the qualitative conclusions obtained here for the RKKY coupling may be extended to the other quantum mechanical treatments of the coupling mechanisms. These results imply that dipolar coupling, together with atomic level quantitative structural determination of interfacial structure, must be important ingredients of experimental and theoretical studies geared towards the understanding of coupling mechanisms in magnetic superlattices. Moreover, these results can contribute to the understanding, of the experimentally observed, non-oscillatory coupling behavior [13,14].

To place the comparison on a firm quantitative basis we have carried out calculations of both the RKKY and the dipolar interaction for an FM/PM/FM trilayer. In these computations we added the contribution of each one of the atoms that participates in the exchange interaction, assuming a particular interface configuration, with a well defined rough structure which is correlated with the rough structure of the adjacent interface. This roughness correlation has been adopted in view of the experimental results [15], which show that certain deposition conditions lead to the formation of parabolic growth fronts, which in turn are crucial to several physical properties. In the calculation of the RKKY interaction only the magnetic interface atoms were considered. The reason for this is twofold: the interaction due to the deeper layers in the ferromagnet is screened and, for the parameter values we use, including these atoms in the computations decreases the interlayer RKKY coupling energy, thus magnifying the effects discussed below. The magnitude of the RKKY interaction, computed as described earlier [16,17] is in agreement with experimental [18] and theoretical [19] results for flat interfaces, found in the literature.

The dipolar energy, on the other hand, is calculated directly from first principles, i.e. using the textbook expression for the magnetic dipole–dipole interaction [20]. This interaction energy per unit area $E_{\mathrm{dip}}$, between the magnetic moments $\boldsymbol{m}_i$ and the magnetic moments $\boldsymbol{m}_j$ on the opposite interface across the spacer, is given by

$$E_{\mathrm{dip}} = \frac{2}{NA}\sum_{i,j}\frac{\boldsymbol{m}_i\cdot\boldsymbol{m}_j - 3(\boldsymbol{m}_i\cdot\hat{n})(\boldsymbol{m}_j\cdot\hat{n})}{r_{i,j}^3} \equiv I\,\mathrm{sign}(\boldsymbol{m}_i\cdot\boldsymbol{m}_j),$$

where $\hat{n}$ denotes a unit vector along the direction that connects the magnetic moments $\boldsymbol{m}_i$ and $\boldsymbol{m}_j$, $A$ is the area of the two-dimensional unit cell and $N$ the number of atoms in one flat interface (i.e. without roughness). The factor of 2 is due to the presence of two atoms per area $A = a^2$, on the 100 planes of the fcc structure. In both cases we write the interaction energy as $E \equiv I\,\mathrm{sign}(\boldsymbol{m}_i\cdot\boldsymbol{m}_j)$ with $I$ defined as the 'interaction coupling strength'. With this definition, positive coupling strength ($I > 0$) corresponds to antiferromagnetic order (i.e. $\boldsymbol{m}_i$ antiparallel to $\boldsymbol{m}_j$), whereas $I < 0$ implies ferromagnetic order (i.e. $\boldsymbol{m}_i$ parallel to $\boldsymbol{m}_j$).

The three dimensional system we investigate is illustrated in Fig. 1 and in the insets of Figs. 2–4. It has channels and plateaus along a direction parallel to the interface; the basic module, of length $d$, which is repeated periodically along the interface is the one shown in the insets. Along the direction orthogonal to the one illustrated, but also parallel to the interface, the system is translationally invariant. Note that the flat atomic planes in the ferromagnet do not contribute to the dipolar interactions. Therefore, only

the interface atoms of the ferromagnet were considered. The sums were calculated in one direction essentially to infinity (i.e. when the effect was smaller than the computer precision) and in the other direction periodic boundary conditions were maintained. In this fashion, an essentially infinite system is simulated. Obviously, the same sort of calculations can be carried out adopting periodic boundary conditions along the two directions on the interface. The latter procedure yields even bigger results, i.e. with a larger magnitude of the dipolar coupling, than the ones shown here.

The relevant parameters that characterize the interface roughness, illustrated in Fig. 1, are: the repeat unit of the roughness $d$, the number $n$ of PM spacer layers, the width $w$ of channels and their depth $h$, the width $L$ of the plateaus and their height, which is also made equal to $h$. Basically, we have investigated terraced interfacial structures, which seem plausible and consistent with fluctuations of thin film thickness, as experimentally observed and recently reported [15,21–23]. It should be pointed out, that the types of disorder present in metallic superlattices are hard to establish quantitatively, and in general only averages over some length scale (larger than the interatomic spacing) are obtained. On the other hand, in the models used to study coupling mechanisms the details of the local atomic arrangement play a crucial role.

The physical parameters we adopted correspond to a Co/Cu/Co trilayer, grown along the 100 face, with an fcc lattice parameter $a = 3.6$ Å and a magnetic moment $|\boldsymbol{m}_k| = 1.76\mu_B$ (Bohr magnetons) for Co [24]. The magnetic moments are assumed to be

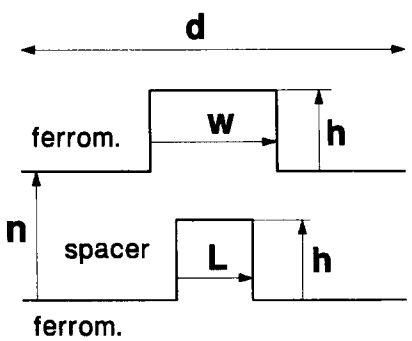


Fig. 1. Illustration of the spatial parameters that characterize the system: $n$, $h$, $L$, $w$ and $d$.

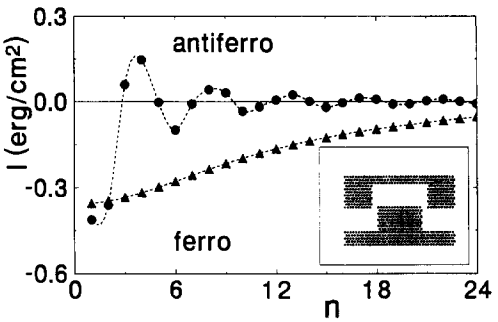


Fig. 2. Interaction coupling strength $I$ versus the number $n$ of PM spacer layers, with $h = 8$, $L = 16$, $w = 20$ and $d = 40$ (in units of $a/2 = 1.8$ Å), for RKKY (circles) and dipolar (triangles) coupling. The inset depicts the structure of the plateaus and channels of the interface for $n = 7$ and illustrates the meaning of $h$, $L$, $w$ and $d$.

parallel to the principal interface and along the 100-direction (i.e. in plane anisotropy). For the dipole–dipole interaction this completely specifies the system. To evaluate the RKKY interaction energy the additional parameters used are $k_F = 1.36$ Å$^{-1}$ for the Fermi wavevector and $J = 1$ eV [19,25,26] for the exchange interaction between magnetic moments. It should be mentioned that the estimates for the value of $J$ vary from 0.1 to 2.0 eV [19,25,26], therefore the comparative importance of the dipolar coupling maybe even larger.

As mentioned above, for an ideal (perfectly flat) interface the dipolar interaction is zero for all values of $n$, while the RKKY coupling strength reaches a maximum of several tenths of an erg/cm$^2$ consistent with experimental values reported in the literature [2,13,14,18]. These values are provided as a reference, to establish a baseline of comparison for the rough interfaces.

Fig. 2 shows the RKKY and the dipolar magnetic exchange coupling strengths for a terraced surface, as a function of spacer thickness $n$, for $h = 8$, $w = 20$, $L = 16$ and $d = 40$, in units of $a/2 = 1.8$ Å. The inset corresponds to a value of $n = 7$. While for $n = 1$ both the dipolar and the RKKY coupling strengths are of the order of 0.3 eV, as $n$ grows the former becomes larger than the RKKY strength. Experimental measurements in Fe/Au/Fe (Fig. 4, Ref. [13]) and in Fe/Cr/Fe (Fig. 5, Ref. [14]) systems have shown large ferromagnetic and antiferromagnetic coupling, respectively. In these measurements the oscillatory coupling is superimposed on a

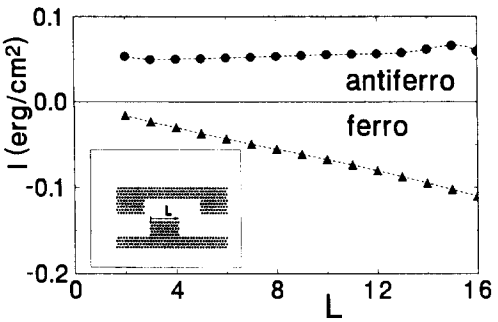


Fig. 3. Interaction coupling strength $I$ versus $L$, for $n = 7$, $h = 5$, $d = 40$ and $w = 20$, for RKKY (circles) and dipolar (triangles) coupling. The inset, which corresponds to $L = 11$, depicts the structure of the periodic plateaus and valleys of the interface and illustrates the meaning of $L$, $n$, $h$, $w$ and $d$.

large, smoothly varying, contribution which is either ferro- or antiferromagnetic. This coupling is in qualitative agreement with the calculations presented here (see also the discussion after Fig. 4). An alternative explanation, based on the Anderson model [5], yields superexchange which results in a smoothly varying antiferromagnetic coupling.

The dependence of $I$ as a function of $L$, with $n = 7$, $h = 5$, $d = 40$ and $w = 20$, is also interesting (see Fig. 3). For these values of the parameters the dipolar strength increases faster, and becomes larger, than the RKKY strength, with growing $n$. We point out that even for $h = 2$, coupling strengths as large as 0.05 erg/cm$^2$ are obtained, so this is a non negligible effect even for almost perfect interfaces.

Fig. 4 shows the dependence of $I$ as a function of $n$, for $h = 8$, $d = 20$, $L = 4$ and $w = 8$, and also gives a very large value of the dipolar coupling strength (of $\sim 0.3$ erg/cm$^2$), comparable to the RKKY coupling strength. On the other hand, the dipolar coupling is ferromagnetic for small $n$, is considerably enhanced and changes sign at $n \approx 20$, all of which can easily be understood from naive expectations. The interaction along the vertical direction, together with lateral interactions, may give rise to this sign reversal. While this geometry may seem somewhat artificial, it is consistent with experimental observations [22,23].

With the parameters used here, the implication is that the PM layers have an impurity concentration of FM atoms of $\sim 10\%$ on the average. For instance, grain boundary diffusion may give rise to unexpected topographies. The local arrangement of atoms, together with the customary assumption that the intralayer coupling is much stronger than the interlayer coupling, is what gives rise to this unusual behavior. The latter assumption is of course central to all treatments of the problem. All in all, the RKKY interaction is smeared out due to the variation in the relative orientations of the spins, whereas the dipolar interaction is reinforced by roughness effects.

In conclusion, a simple model calculation was carried out to estimate and compare the magnitudes of the dipolar and RKKY interaction strength between magnetic layers separated by a non-magnetic spacer. Special attention was given to the interplay of coupling strength and interface roughness, since surface defects depress the strength of the RKKY interaction, while enhancing the dipolar one.

The results of our model computation show that, in the presence of interface roughness, the dipolar interaction energy is of the same order of magnitude as the one calculated via RKKY. Since these are in good agreement with experimentally observed values and the smooth dependence of the coupling observed in some systems, the dipolar interaction must be included as a possible coupling mechanism, for multilayer systems with rough interfaces. Moreover, these results imply that quantitative structural studies at the atomic level are essential for a meaningful and complete comparison of experiment and theory of magnetic coupling in these systems.

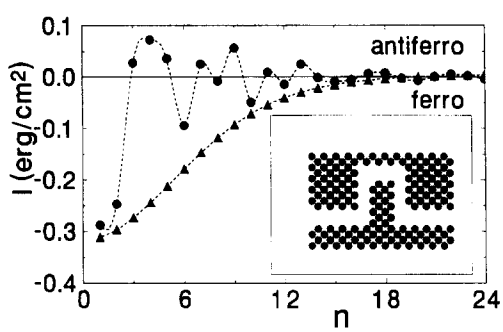


Fig. 4. Interaction coupling strength $I$ versus $n$, for $h = 8$, $L = 4$ $w = 8$, and $d = 20$, for RKKY (circles) and dipolar (triangles) coupling. The inset depicts the structure of the periodic plateaush) and valleys of the interface, for $n = 3$, and illustrates the meaning of $h$, $L$, $w$ and $d$.

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