Magnetization of ferromagnetic-antiferromagnetic double layers

A. Moschel,* K. D. Usadel, and A. Hucht
Theoretische Tieftemperaturphysik, Universität Duisburg, Lotharstrasse 1, 4100 Duisburg 1, Germany
(Received 3 December 1992)

Using a Green-function method the spin-wave excitation spectrum and the sublattice magnetizations of a system consisting of a ferro- and an antiferromagnetic layer are calculated. Both ferro- and antiferromagnetic interlayer couplings are considered. It is shown that in the extreme quantum case $S=\frac{1}{2}$ considered here interesting quantum effects appear at low temperatures.

I. INTRODUCTION

Layered magnetic systems have been a subject of growing interest in recent years. In particular the research has been focused on systems such as superlattices[1-7] and multilayers.[8-11] Very interesting effects are found in superlattices that are formed from two ferromagnetic materials which are coupled antiferromagnetically at the interface[2-5] or which are formed from alternating layers of ferromagnetic and antiferromagnetic materials[6,7] where spins are frustrated at the interface. In the presence of a magnetic field these systems show many different phases and interesting canting transitions occur.

Another important effect was found by Diep[1,11] in superlattices consisting of two antiferromagnetic layers with different interactions in the layers and between the layers, respectively. At low temperatures a surprising crossover between the layer magnetizations is observed which is explained as due to quantum fluctuations. A similar effect has been found in an antiferromagnetic film.[11]

In this paper we want to investigate a system consisting of a ferromagnetic and an antiferromagnetic layer with a simple square structure which are coupled ferro- or antiferromagnetically. The motivation for an investigation of this system is that it is one of the simplest models in which frustrated spins exist without an applied magnetic field (Fig. 1). Note that in the model of Hinchey and Mills[6,7] frustration at the interface arises due to an applied magnetic field. The model considered is of special interest since in this double-layer system every second spin in one of the layers is frustrated in the Néel ground state. As we will show this frustration leads to unusual quantum effects in the sublattice magnetizations as well as to interesting spin-canting transitions for strong interlayer coupling. From an experimental point of view a double-layer system might be oversimplified. However, the local magnetization at interfaces between ferro- and antiferromagnetic layers in multilayers resembles that of a double layer so that our model calculation can shed some light on these more complicated situations. Our calculation shows that in case the layers are coupled antiferromagnetically the sublattice magnetizations at low temperatures develop a surprising crossover which is due to quantum fluctuations. If the two layers are coupled ferromagnetically the system behaves similar to a classical system. These results hold for not too large interlayer coupling. If, on the other hand, the coupling between the two layers gets too strong the spin-wave calculations starting from a Néel-type ground state breaks down which signals a reconstruction of the ground state. Within a self-consistent mean-field calculation for a simpler four-spin cluster we show that there exist a canting transition with a variety of different local spin configurations as function of interlayer coupling.

In Sec. II we describe the model and give a short outline of the Green-function formalism for layered systems used in this paper. In Sec. III we present and discuss the results of the spin-wave calculations and the results of a self-consistent mean-field calculation for the canted spin configuration.

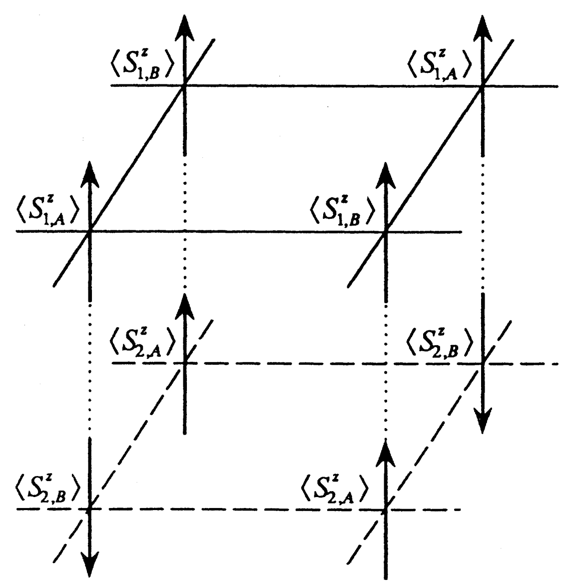

FIG. 1. A possible ground-state configuration for not too large interplane exchange and low temperatures for the double-layer system. A solid line means a (J^1,D^1) coupling, a dashed line a (J^2,D^2) coupling, and a pointed line a (J^z,D^z) coupling.

II. THEORY

We consider a model consisting of two layers with a square structure. In the first layer the exchange interactions are ferromagnetic while in the second layer they are antiferromagnetic. The interplane interaction between the two layers can be either ferromagnetic or antiferromagnetic, respectively. The Hamiltonian reads

$$\mathcal{H}=-2\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j-2\sum_{\langle i,j\rangle} D_{ij}S_i^zS_j^z\ , \tag{1}$$

where the sums are over distinct pairs of nearest-neighbor spins only and $\mathbf{S}_i$ denotes spin operators. $J_{ij}(D_{ij})$ is equal to $J^1(D^1)$ if both spins are in the first layer, equal to $J^2(D^2)$ if both spins are in the second layer, and equal to $J^z(D^z)$ if one spin is in the first and the other spin in the second layer. J^1 and D^1 are both positive corresponding to ferromagnetical ordering along the z axis which is assumed to be perpendicular to the layers while J^2 and D^2 are both negative corresponding to antiferromagnetic ordering along the z axis. The interplane exchange J^z and D^z may have both signs. A configuration of spin-expectation values in one of the degenerated ground states for not too large interplane exchange is shown in Fig. 1. It is convenient to introduce two sublattices (A and B) corresponding to up and down magnetizations in the antiferromagnetically ordered layer. Note that due to the interplane exchange $\langle S_{2,A}^z\rangle$ is not the opposite of $\langle S_{2,B}^z\rangle$ and that a certain A-B structure is also introduced in the ferromagnetic layer in the sense that $\langle S_{1,A}^z\rangle$ is not equal to $\langle S_{1,B}^z\rangle$.

Following Zubarev[12] we define four double-time Green functions $\langle\langle S_i^+(t);S_j^-(t')\rangle\rangle$, where $S_i^{\pm}$ are the usual spin lowering and raising operators and we restrict ourselves to $S=\frac{1}{2}$. These Green functions are denoted by $G_{ij}(t,t')$ if i and j belong to the same sublattice and $F_{ij}(t,t')$ if i and j belong to different sublattices. After writing down the equations of motion for the Green functions $G_{ij}(t,t')$ and $F_{ij}(t,t')$ we get higher-order Green functions which are decoupled by the so-called Tyablikov decoupling scheme

$$\langle\langle S_i^zS_l^+(t);S_j^-(t')\rangle\rangle=\langle S_i^z\rangle\langle\langle S_l^+(t);S_j^-(t')\rangle\rangle\ . \tag{2}$$

In the following we assume that the expectation values $\langle S_i^z\rangle$ are equal at equivalent sites in the sublattices, i.e., in the following we have to deal with the four order parameters:

$$|\langle S_{i,v}^z\rangle|\equiv m_i^v\ , \tag{3}$$

where $i=1,2$ denote layer indices while $v=A,B$ denote the two sublattices. We now introduce for the Green functions $G_{ij}(t,t')$ and $F_{ij}(t,t')$ a two-dimensional Fourier transform, which emphasize the layered structure of the system

$$E_{ij}(t,t')=\frac{1}{2\pi}\int\int dk_x dk_y\int d\omega\, E_{nm}(k_x,k_y)e^{-i\omega(t-t')}e^{i\mathbf{k}_{\parallel}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\ , \tag{4}$$

where $E_{ij}(t,t')$ stands for one of the four Green functions. $\mathbf{k}_{\parallel}=(k_x,k_y)$ is a two-dimensional wave vector and the indices m and n represent the z component (first or second layer) of the positions of the spins at the lattice sites $\mathbf{r}_i$ or $\mathbf{r}_j$. Inserting (4) in the equation of motion for the Green functions we obtain for each sublattice magnetization $m_i^v(i=1,2;v=A,B)$ a set of equations of the following form:

$$\underline{M}^v\cdot\mathbf{E}_i^v=\mathbf{u}_i^v\ . \tag{5}$$

The matrix $\underline{M}^v$ $(v=A,B)$ and the vectors $\mathbf{E}_i^v$ $(i=1,2)$ and $\mathbf{u}_i^v$ are given as

$$\underline{M}^A=\begin{bmatrix}\omega-A_1^B & B_1^A & 0 & C_1^A\\ B_1^B & \omega-A_1^A & C_1^B & 0\\ 0 & C_2^A & \omega-A_2^B & B_2^A\\ C_2^B & 0 & B_2^B & \omega-A_2^A\end{bmatrix}\ , \tag{6}$$

$$\mathbf{E}_i^A=\begin{bmatrix}G_{1i}^{AA}\\ F_{1i}^{BA}\\ G_{2i}^{AA}\\ F_{2i}^{BA}\end{bmatrix}\ ,\quad \mathbf{u}_i^A=\begin{bmatrix}2m_1^A\delta_{1i}\\ 0\\ 2m_2^A\delta_{2i}\\ 0\end{bmatrix}\ , \tag{7}$$

with

$$\begin{aligned}A_1^v&=8(J^1+D^1)m_1^v+2(J^z+D^z)m_2^v\ ,\\ A_2^v&=8(J^2+D^2)m_2^v+2(J^z+D^z)m_1^v\ ,\end{aligned} \tag{8}$$

$$B_i^v=2J^i\gamma m_i^v\ ,\quad C_i^v=2J^zm_i^v\ , \tag{9}$$

and $\gamma=4[\cos(k_x/2)\cos(k_y/2)]$.

The matrix $\underline{M}^B$ and the vectors $\mathbf{E}_i^B$ and $\mathbf{u}_i^B$ are obtained from $\underline{M}^A$, $\mathbf{E}_i^A$, and $\mathbf{u}_i^A$ by replacing A and B and vice versa. To solve the four sets of equations we need another set of equations which connects the Green functions with the layer magnetizations. Using the spectral theorem which relates the correlation function $\langle S_i^-S_j^+\rangle$ with the Green functions and considering that for $S=\frac{1}{2}$ we can write for the sublattice magnetizations

$$m_i^v=\langle S_{i,v}^z\rangle=\tfrac{1}{2}-\langle S_{i,v}^-S_{i,v}^+\rangle \tag{10}$$

we get

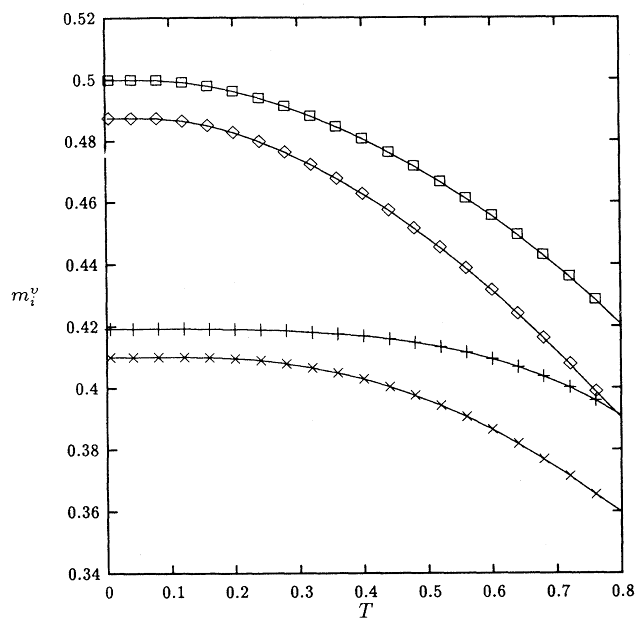

FIG. 2. Sublattice magnetizations m_1^A ($\Diamond$), m_1^B ($\square$), m_2^A (+), and m_2^B ($\times$) with $J^2=-1$, $J^z=+0.7$, $D^1=0.1$, $D^2=-0.1$, and $D^z=0.0$ (all quantities in units of J^1).

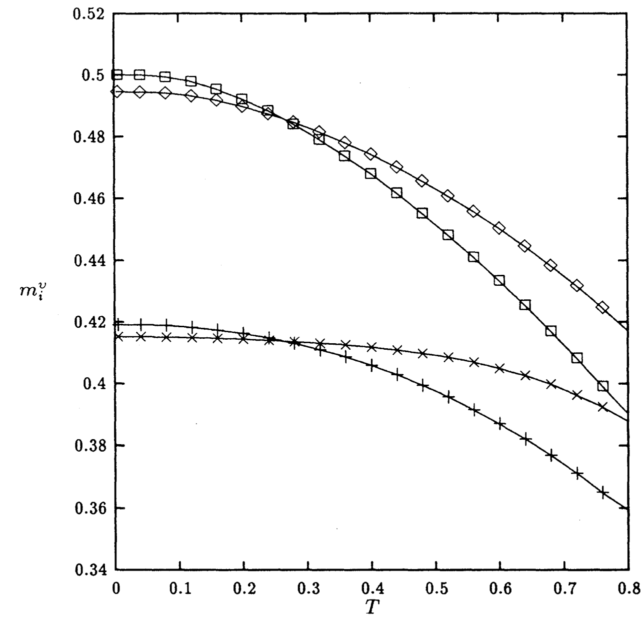

FIG. 3. Sublattice magnetizations m_1^A ($\Diamond$), m_1^B ($\square$), m_2^A (+), and m_2^B ($\times$) with $J^2=-1$, $J^z=-0.7$, $D^1=0.1$, $D^2=-0.1$, and $D^z=0.0$ (all quantities in units of J^1).

$$m_i^v=\frac{1}{2}-\lim_{\epsilon\to 0}\frac{1}{\pi^2}\int\int dk_x dk_y \int \frac{d\omega}{e^{\beta\omega}-1}\frac{i}{2\pi}[G_{ii}^{vv}(\omega+i\epsilon)-G_{ii}^{vv}(\omega-i\epsilon)] \ . \tag{11}$$

This equation can be recast into the following form:[1,11,13]

$$m_i^v=\frac{1}{2}-\frac{1}{2\pi}\int\int dk_x dk_y \sum_{l=1}^{4}\frac{a_i^v(\omega_k^l)}{e^{\beta\omega_k^l}-1} \tag{12}$$

with

$$a_i^v(\omega_k^l)=\frac{|\underline{N}^v(\omega_k^l)|}{\prod_{m\neq l}(\omega_k^l-\omega_k^m)} \ . \tag{13}$$

The frequencies ω_k^l can be obtained by solving $|\underline{M}^v(\omega)|=0$ where $|\underline{M}^v(\omega)|$ is the determinant of the matrix $\underline{M}^v(\omega)$ and $|\underline{N}^v(\omega_k^l)|$ is the determinant of the matrix $\underline{N}^v(\omega_k^l)$ obtained by replacing the first or third column of $\underline{M}^v(\omega)$ by the vector $\mathbf{u}_i^v$ and setting $\omega=\omega_k^l$.

The system of equations above has been solved numerically and the results are discussed in the next section.

III. RESULTS AND DISCUSSION

We have calculated the spin-wave spectra and the sublattice magnetizations for the double-layer system (Fig. 1) for the two cases of ferromagnetic and antiferromagnetic coupling between the two layers. Numerical results for the sublattice magnetizations for typical values of system parameters are shown in Figs. 2 and 3, and a characteristic spin-wave spectrum in case of an antiferromagnetically interlayer coupling is shown in Fig. 4.

In the case of ferromagnetic interlayer coupling the interaction between the spins in the A sublattice of the first layer and the B sublattice of the second layer are frustrated while this is not the case for the coupling of the other two sublattices. Due to this weaking of the net interac-

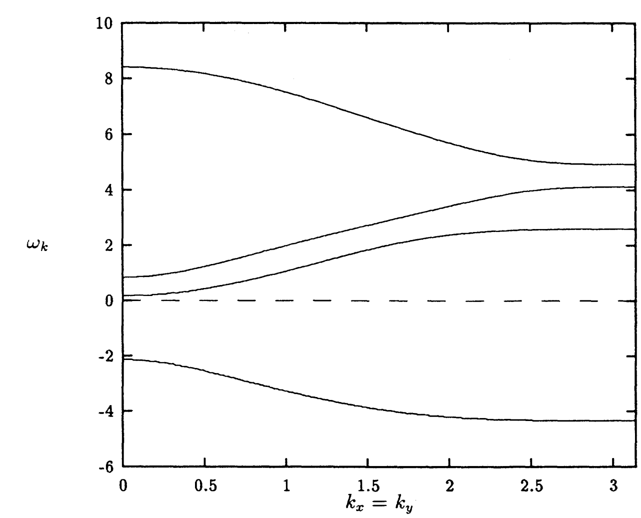

FIG. 4. Spin-wave spectrum with $J^2=-1$, $J^z=-0.7$, $D^1=0.1$, $D^2=-0.1$, and $D^z=0.0$ at $T=0.1$ (all quantities in units of J^1).

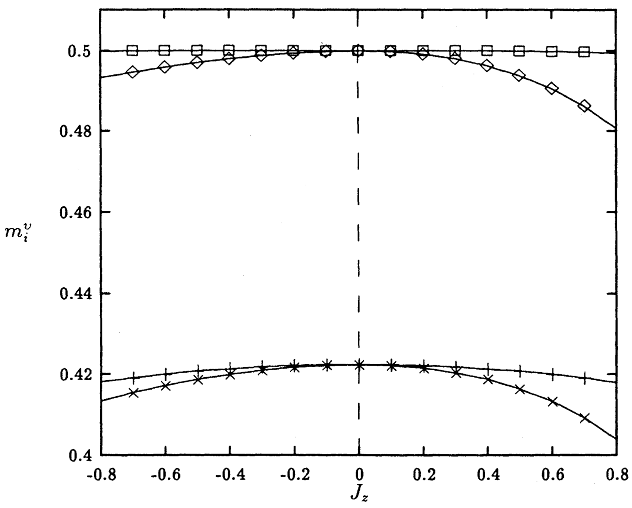

FIG. 5. Sublattice magnetizations m_1^A (◇), m_1^B (□), m_2^A (+), and m_2^B (×) with $J^2=-1$, $D^1=0.1$, $D^2=-0.1$, $D^z=-0.1$ if $J_z<0$ and $D_z=0.1$ if $J_z>0$ at $T=0$ (all quantities in units of J^1).

tion one would expect that the sublattice magnetization m_1^B should be larger than m_1^A and m_2^A larger than m_2^B. The result of our calculation is shown in Fig. 2 and it confirms this expectation.

In the case of antiferromagnetic interlayer coupling a similar argument would lead to the expectation that m_1^A should be larger than m_1^B and m_2^B larger than m_2^A. However, surprisingly this is not found at low temperatures. Figure 3 shows the result of our calculations. There is a clear crossover from the expected behavior obtained for high temperatures to a different behavior at low temperatures. This interesting effect has its origin in the quantum mechanics of spin operators. In the corresponding classical model ferro- and antiferromagnetic interlayer couplings lead to the same result since obviously these two cases can be transformed into each other by a gauge transformation $\mathbf{S}_i \to -\mathbf{S}_i$ of the spins in one of the layers, i.e., for classical spins Figs. 2 and 3 should coincide. For quantum spins, however, this is only the case for high temperatures.

A similar quantum effect has been found by Diep[1] in an antiferromagnetic superlattice. He investigated a superlattice with different antiferromagnetic couplings in the layers and between the layers. He found that at low temperatures the layer with the stronger coupling in the plane has a smaller magnetization than the layer with the weaker coupling in the plane. In ferromagnetic superlattices and in classical systems he did not find this behavior.

In Fig. 5 the dependence of the sublattice magnetizations on the interlayer coupling for $T=0$ is shown. The calculations are restricted to values of the interlayer coupling in the range $-08<J^z<0.8$ for reasons to be discussed later. Here we find that in the ground state the expectation values of $\langle S_{1,B}^z \rangle$ are nearly equal to $\frac{1}{2}$ for all values of J^z, and the sublattice magnetizations are not symmetric functions of J^z in contrast to a classical system.

These quantum effects observed in double-layer systems at low temperatures we found out are also present in a simpler four-spin cluster coupled to four external fields which are calculated self-consistently in a mean-field-like

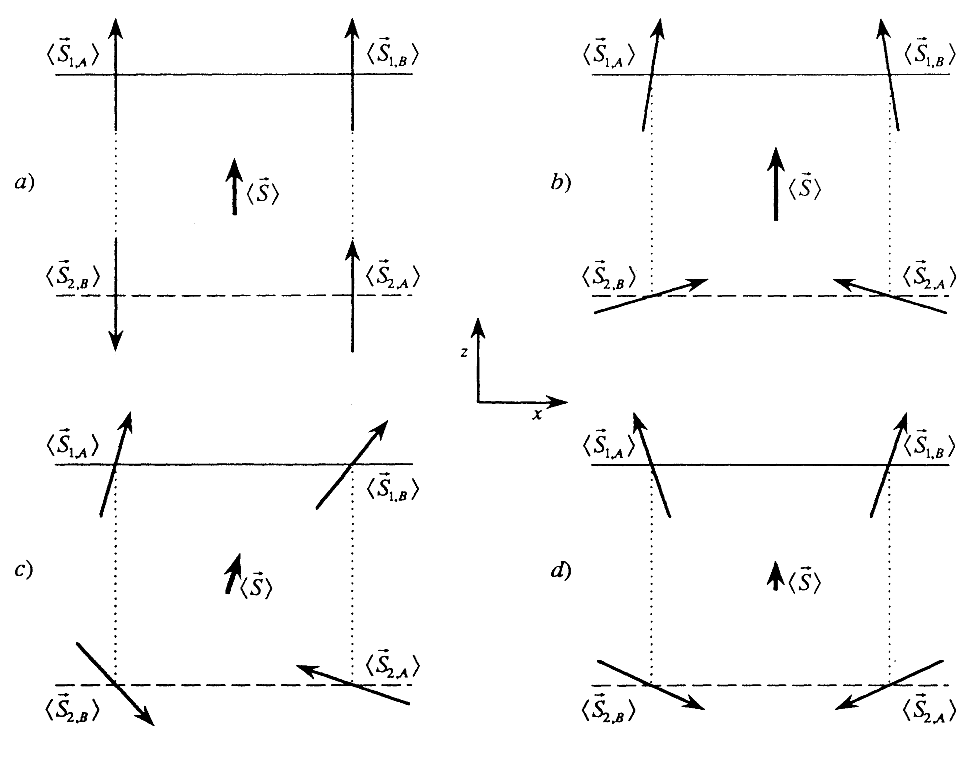

FIG. 6. Four-spin cluster considered in a mean-field-type calculation with $J^2=-1$, $D^1>0$, $D^2<0$, D^z and (a) $J_c^{\mathrm{F}}>J^z>J_{c_1}^{\mathrm{AF}}$, (b) $J^z>J_c^{\mathrm{F}}$, (c) $J^z<J_{c_1}^{\mathrm{AF}}$, and (d) $J^z<J_{c_2}^{\mathrm{AF}}$ (all quantities in units of J^1). Note that the total spin per site $\langle \mathbf{S} \rangle$ in (c) deviates from the z direction.

fashion (Fig. 6). In this calculation the eigenstates of the four-spin cluster in external fields are obtained exactly and the fields which approximate the interaction with all the other spins outside the cluster are determined self-consistently. The sublattice magnetizations obtained are in qualitative agreement with those from a spin-wave calculation. The advantage of this simpler approach is that some insight into the different behavior of the sublattice magnetizations as a function of the interlayer coupling can be gained. Analyzing the eigenstates of the four-spin cluster it can be seen that the spin $\mathbf{S}_{1,B}$ in Fig. 6(a) which corresponds to the B sublattice in the first layer in Fig. 1 indeed is practically fully polarized in the ground state. The reason is that in low-order perturbation theory there is a cancellation of those matrix elements leading to flips of this particular spin. This is independent of J^z for not too large J^z. Increasing J^z below a critical value $J_{c_1}^{\mathrm{AF}}$ in case of an antiferromagnetically coupling or above J_c^{F} in case of a ferromagnetically coupling there is a canting transition leading to $\langle S_j^x \rangle \neq 0$, see Figs. 6(b)–6(d) where three other characteristic spin arrangements with typical J^z values are shown. This is precisely the region where the decoupling scheme is expected to and indeed does break down, i.e., only inside the J^z region shown in Fig. 5 the spins are polarized in a Néel-type state and the Tyablikov decoupling used is applicable.

The J^z asymmetry in Fig. 5 corresponds to a similar asymmetry in the energy eigenstates of the four-spin cluster which has its origin in the quantum mechanics of spin operators. The details of the spin-canting transition mentioned above are very interesting to investigate. This problem is left for future research.

ACKNOWLEDGMENT

This work was supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 166.

*Electronic address: andreas@hal6000.uni-duisburg.de

[1] H. T. Diep, Phys. Rev. B **40**, 4818 (1989).
[2] R. E. Camley and D. R. Tilley, Phys. Rev. B **37**, 3413 (1988).
[3] J. G. LePage and R. E. Camley, Phys. Rev. B **40**, 9113 (1989).
[4] R. E. Camley, Phys. Rev. B **39**, 12 316 (1989).
[5] J. G. LePage and R. E. Camley, Phys. Rev. Lett. **65**, 1152 (1990).
[6] L. L. Hinchey and D. L. Mills, Phys. Rev. B **33**, 3329 (1986).
[7] L. L. Hinchey and D. L. Mills, Phys. Rev. B **34**, 1689 (1986).
[8] B. Hillebrands, Phys. Rev. B **41**, 530 (1990).
[9] K. Mika and P. Grünberg, Phys. Rev. B **31**, 4465 (1985).
[10] D. Schwenk, F. Fishman, and F. Schwabl, Phys. Rev. B **38**, 11 618 (1988).
[11] H. T. Diep, Phys. Rev. B **43**, 8509 (1991).
[12] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [Sov. Phys. Usp. **3**, 320 (1960)].
[13] D. T. Hung, J. C. S. Levy, and O. Nagai, Phys. Status Solidi B **93**, 351 (1979).