Elementary excitations and thermodynamical properties of ultrathin magnetic films

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We study the elementary excitations for a multilayer of spins represented by a Heisenberg ferromagnet with nearest-neighbor and next-nearest-neighbor exchange. In addition to the bulk modes, and the usual monotonic surface ones characterized by an exponential decay of the amplitude of the spin fluctuations, we find for opportune conditions other localized modes that present a π phase variation when passing from a layer to the adjacent one. Furthermore we show that the surface-plane magnetization is much more affected by the surface modes in a film than in a semi-infinite system. Also the effects of surface single-ion anisotropies and of dipolar interactions are investigated using the Green's-function method. Some analytical expressions are obtained for the energy of the lowest mode of the multilayer, which makes it possible to find the dependence on the number of layers N. Finally, we derive a formal expression for the magnetization profile which is valid for systems with a nondiagonal quadratic boson Hamiltonian.

I. INTRODUCTION

Much attention has been given in recent years to the development of, and the research on, ultrathin magnetic films of a few layers thickness.[1] The theoretical interest for these systems is due mainly to two reasons. First, in the single monolayer limit they are the best realization of a two-dimensional (2D) Heisenberg model with weak anisotropies for which a nonperturbative treatment must be used in order to explain the experimental results.[2] Second, for more than one layer the absence of translational invariance in the normal direction to the film implies a very peculiar behavior, which can be experimentally observed. The clearest evidence is obtained by means of conversion electron Mössbauer spectroscopy[3] measuring the magnetization profile, from which it results that the surface magnetization is smaller than the inner one.

In order to understand the properties of these systems it is necessary to determine the elementary excitations that, of course, in the normal direction to the film have a standing wave character. Usually this problem has been investigated using a classical continuum approach developed in the micromagnetic theory, which gives the correct results for thick films and for sufficiently long wavelength excitations.[4,5] However, in order to study the properties of very thin films and to obtain an accurate definition of the excitations character as well as their complete dispersion curve in the whole Brillouin zone, a discrete approach is necessary.[6] In particular, under favorable circumstances, localized surface modes are present, and their nature is completely determined only in a discrete approach. It is well known that in the semi-infinite limit, for the (100) surface of a simple-cubic lattice, the inclusion of next-nearest-neighbor (NNN) interaction, J_2, in addition to the nearest-neighbor (NN) one, J_1, leads to the excitation of a surface spin wave, even though its presence does not influence the magnetization profile.[7] In this paper we show that for ultrathin films it is possible to have different numbers and types of localized modes as a function of three parameters: the ratio J_1/J_2, the number of layers N, and the 2D wave vector $\mathbf{k}_{\parallel}$. Concerning this problem, the main result of our analysis is the prediction, for sufficiently high wave vectors, of oscillating surface magnons in addition to the usual monotonic surface ones. While both of them are characterized by an exponential decay of the amplitude of the spin fluctuations, the oscillating ones present a π phase variation when passing from a layer to the adjacent one. Clearly such oscillating modes can only be obtained within a microscopic approach, not limited to the low-k region. It is worthwhile to note that the surface modes always have the lowest energies with respect to the volume modes, and consequently they are very important for the thermodynamics. For this we have extended the expression for the surface mode to generic N. Furthermore, contrary to the semi-infinite case, the presence of the localized surface modes determines a much smaller surface magnetization. A detailed study of these modes in the case of films was, to our knowledge, still lacking.

Moreover, the case $J_2 \neq 0$ appears physically interesting: e.g., for epitaxial thin films of bcc Fe/Au(100), the NNN interaction is only responsible for the long-range order observed at room temperature in the monolayer limit.[8]

The general analysis of the properties of the films is further complicated because, contrary to the usual 3D systems, it is fundamental to consider the role of the dipolar interaction. The ground-state configuration is determined by the competition between the uniaxial surface anisotropy,[9] which favors a spin alignment perpendicular to the film, and the dipolar interaction, which forces the spins to lie in the film plane. The latter, for an isotropic model, gives a modification of the spin-wave frequency for low wave vectors, $\omega \propto k^{1/2}$, leading to a spontaneous magnetization.[10] In the case of a thin film with N layers (see Yafet, Kwo, and Gyorgy[11]) being based upon the long-range character of the dipolar interaction, it is suggested that each plane should equally contribute to the linear term in the k-dependent dipolar sums, leading to $\omega \propto (Nk)^{(1/2)}$.

In this paper we also present the results, obtained within a Green's function formalism, for the spin-wave spectrum and a formal expression for the magnetization in the presence of a dipolar interaction including the effect of a surface magnetocrystalline single-ion anisotropy always present in real systems. Also in this case we are able to obtain an analytical expression for the frequency of the acoustic mode of the multilayer, a property that could easily be investigated experimentally, e.g., by Brillouin light scattering or ferromagnetic resonance. In the appropriate limit we recover not only the results of Yafet, Kwo, and Gyorgy,[11] but also the expression of the Damon-Eshbach magnetostatic theory.[4] The results of the spectrum will be reported, for completeness sake, in a very concise way because they have already been presented elsewhere.[12] It should be mentioned that similar results have been independently obtained by Erickson and Mills,[13,14] using the method of the equation of motion for the spin operators.

In order to obtain a greater comprehension of the properties of ultrathin films and to have the largest analytical development, we have studied a simple-cubic lattice. In particular, we solve exactly the case $N=2$, and we are able to extend the analytical expression for the acoustic mode to generic N. Furthermore, for thermodynamical properties such as the magnetization profile, we expect that the qualitative behavior does not depend on the details of the structure.

The paper is organized as follows. In Sec. II the investigated model is introduced. In Sec. III the results concerning the elementary excitations in a system with only NN and NNN exchange interactions are presented, while the pertinent prediction for the magnetization is shown in Sec. IV. The effects of the surface anisotropy and the dipolar interaction on the same quantities are reported in Sec. V. Finally in Sec. VI the conclusions are summarized.

II. THE MODEL

We want to describe a thin ferromagnetic film of thickness L consisting of N layers ($L=Na$, with a lattice constant) parallel to the (010) surface of a simple-cubic lattice assuming the following interaction Hamiltonian between spins localized at sites $\mathbf{i}$:

$$\mathcal{H}=-\frac{1}{2}\sum_{\mathbf{i}\neq\mathbf{j}} J(|\mathbf{i}-\mathbf{j}|)\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j}-g\mu_B H\sum_{\mathbf{i}} S_\mathbf{i}^z-\lambda\sum_{\mathbf{i}}{}'(S_\mathbf{i}^y)^2+\frac{1}{2}\frac{g^2\mu_B^2}{a^3}\sum_{\mathbf{i}\neq\mathbf{j}}\frac{a^3}{|\mathbf{i}-\mathbf{j}|^3}\left\{\mathbf{S}_\mathbf{i}\cdot\mathbf{S}_\mathbf{j}-3\frac{[\mathbf{S}_\mathbf{i}\cdot(\mathbf{i}-\mathbf{j})][\mathbf{S}_\mathbf{j}\cdot(\mathbf{i}-\mathbf{j})]}{|\mathbf{i}-\mathbf{j}|^2}\right\}, \quad (1)$$

where we have taken the y axis to be perpendicular to the surface, while in the xz plane—the film plane—we have translational invariance. For the exchange interaction $J(|\mathbf{i}-\mathbf{j}|)$ we assume

$$\begin{aligned} &J(|\mathbf{i}-\mathbf{j}|)=J_1 \quad \text{for } \mathbf{i} \text{ and } \mathbf{j} \text{ NN} \\ &J(|\mathbf{i}-\mathbf{j}|)=J_2 \quad \text{for } \mathbf{i} \text{ and } \mathbf{j} \text{ NNN} \qquad (2) \\ &J(|\mathbf{i}-\mathbf{j}|)=0 \quad \text{otherwise} \end{aligned}$$

with J_1, $J_2>0$. The single-ion surface anisotropy λ, which favors the alignment along the y axis, is assumed to act only on the surface spins [primed summation in Eq. (1)]. In the case, usually studied, of epitaxial thin films of transition metals, the strengths of the dipolar interaction $w=(g\mu_B)^2/a^3$ and the surface anisotropy λ are much smaller than the exchange interactions and consequently one can assume a collinear ground state. We define the following constants: $A=S\lambda(N)/N$ and $h=g\mu_B H$, where $\lambda(1)=\lambda$ and $\lambda(N)=2\lambda$ for $N\geq 2$. The total number of spins is $N_T=NN_\parallel$, where $N_\parallel$ is the number of spins in each plane.

The real systems usually investigated are generally transition metals or rare earths, and the use of a localized model can be questionable. However, as shown by Luchini and Heine this description is well justified, at least in the ordered phase.[15]

III. EXCHANGE INTERACTION ONLY: ELEMENTARY EXCITATIONS

A. Equation of motion

In this section we report the results for the elementary excitations in a system with Hamiltonian (1) but without surface anisotropy and dipolar interaction; e.g., $\lambda=w=0$. We begin studying this simplified model in order to have a better comprehension of the role of the exchange interactions.

Furthermore, a thermodynamical property as the magnetization is usually measured in a temperature region where it is mainly determined by the exchange constants because in the real systems we have λ, $w \ll J_i$. The presence of an external magnetic field is insignificant giving only a shift for the frequency.

We assume the magnetization to lie along the z direction in the xz plane parallel to the surfaces, and we linearize the Heisenberg equations of motion for the transversal components S^x and S^y of the spin operators in the free-spin-wave approximation. Owing to the translational invariance in the xz plane $S_l^{x,y} \equiv S^{x,y}(\mathbf{l},t)$ has a plane-wave-like dependence on $\mathbf{l}_\parallel \equiv (l_x, l_z)$:

$$S^{x,y}(\mathbf{l},t)=\mathcal{S}^{x,y}(l_y,\mathbf{k}_\parallel)\exp[i\omega t - i\mathbf{l}_\parallel\cdot\mathbf{k}_\parallel] ,$$

where $\mathbf{l}=(\mathbf{l}_\parallel,l_y)$ and $\mathbf{k}_\parallel=(k_x,k_z)$ with $-\pi/a \le k_x,k_z \le \pi/a$. From now on, for brevity's sake, we put $a=1$, $l_y=l$, and we omit the explicit $\mathbf{k}_\parallel$ dependence. Putting $\mathcal{S}^x(l)=S^x(l)$, $\mathcal{S}^y(l)=iS^y(l)$, taking into account that from the symmetry of the problem $S^x(l)=S^y(l)=S(l)$ we obtain

$$\omega S(l)=\sum_m \underline{A}(l,m)S(m) , \tag{3}$$

where

$$\underline{A}(l,m)=H^{\mathrm{eff}}(l)\delta_{l,m}-SJ(\mathbf{k}_\parallel;l-m) \tag{4}$$

is a real symmetric tridiagonal $(N\times N)$ matrix. We have introduced

$$H^{\mathrm{eff}}(l)=h+S\sum_{\mathbf{m}} J(|\mathbf{l}-\mathbf{m}|) , \tag{5}$$

$$J(\mathbf{k}_\parallel;l-m)=\sum_{\mathbf{m}_\parallel} J(|\mathbf{l}-\mathbf{m}|)\exp[i(\mathbf{l}_\parallel-\mathbf{m}_\parallel)\cdot\mathbf{k}_\parallel] . \tag{6}$$

For the effective field $H^{\mathrm{eff}}(l)$, we distinguish between a surface plane and an inner one; for the simple-cubic geometry one has

$$H^{\mathrm{eff}}(l)=\begin{cases} h+(5J_1+8J_2)S\equiv H_s, & l=1,N \quad (7\mathrm{a})\\ h+(6J_1+12J_2)S\equiv H_i, & l=2,\ldots,N-1 , \quad (7\mathrm{b})\end{cases}$$

while for the 2D Fourier transform of the exchange interaction we obtain

$$J(\mathbf{k}_\parallel,0)=4J_1\gamma_1+4J_2\gamma_2$$

and

$$J(\mathbf{k}_\parallel,1)=J_1+4J_2\gamma_1$$

with

$$\gamma_1=\tfrac{1}{2}[\cos k_x+\cos k_z] ,$$

$$\gamma_2=\cos k_x \cos k_z .$$

B. Eigenvalues and eigenvectors

The eigenvectors of the matrix $\underline{A}$ have defined parity

$$S(l)=\pm S(N+1-l), \quad l=1,2,\ldots,N , \tag{8}$$

i.e., they can be symmetric (+) or antisymmetric (−) with respect to the center of the film. From Eq. (3), with $l=2,\ldots,N-1$, we see that $S(l)$ must be of the form $S(l-1)+S(l+1)\propto S(l)$, which is satisfied if $S(l)=x^l$.

Requiring the eigenvector to have defined parity, if we introduce the variable $k_\perp$, through $x=e^{-ik_\perp}$, we have

$$S(l)=\exp[-ik_\perp(l-1)]\pm\exp[-ik_\perp(N-l)] , \tag{9}$$

$$\omega=H_i-J(\mathbf{k}_\parallel;0)-J(\mathbf{k}_\parallel;1)[e^{-ik_\perp}+e^{ik_\perp}] , \tag{10}$$

and imposing that $(x+x^{-1})$ be real, we obtain three different solutions: (a) $k_\perp=-i\alpha$ corresponding to monotonic (M) surface magnons, (b) $k_\perp=-i\alpha+\pi$ corresponding to oscillating (O) surface magnons, and (c) $k_\perp=\alpha$ corresponding to the usual bulk magnons. The value of α must be determined as a function of $\mathbf{k}_\parallel$ and the parameters (J_1,J_2,N) of the system, using the boundary condition given by the equation of motion for a surface spin. The latter can be written as

$$\mathcal{M}(\mathbf{k}_\parallel)=\mathcal{F}(k_\perp) , \tag{11}$$

where

$$\mathcal{M}(\mathbf{k}_\parallel)\equiv\frac{H_i-H_s}{J(\mathbf{k}_\parallel;1)}=\frac{J_1+4J_2}{J_1+4J_2\gamma_1}=\frac{J^*}{J_1+4J_2\gamma_1} , \tag{12}$$

$$\mathcal{F}(k_\perp)\equiv-\frac{S(2)}{S(1)}+(x+x^{-1}) . \tag{13}$$

The explicit forms for $\mathcal{F}(k_\perp)$ in the different cases are reported in Appendix A.

For $J_2=0$, having $\mathcal{M}(\mathbf{k}_\parallel)\equiv 1$, we recover the results obtained by Döring:[16] we have only bulk magnons with eigenvectors given by

$$S(l)=\cos[\bar{\alpha}_m(l-\tfrac{1}{2})] \quad \text{with } \bar{\alpha}_m=m\frac{\pi}{N}(m=0,1,\ldots,N-1) . \tag{14}$$

For the energies we have

$$\omega(\mathbf{k}_\parallel,\bar{\alpha}_m)=2J_1(1-\cos\bar{\alpha}_m)+4J_1(1-\gamma_1) . \tag{15}$$

It is worthwhile to note that for any $\mathbf{k}_\parallel$ we have always the uniform solution $\alpha=0$ which corresponds to the acoustic mode: i.e., $\omega\to 0$ for $\mathbf{k}_\parallel\to 0$.

In the general case $J_2\neq 0$ and for any value of $\mathbf{k}_\parallel$, we must have N values of α for which Eq. (11) is satisfied. The results can be briefly summarized.

(a) If $J(\mathbf{k}_\parallel;1)>0$, it is possible to have only monotonic surface magnons in addition to the bulk ones and the localized modes are the lowest energy ones. The separation edge between surface and bulk excitations is

$$\omega_{S-B}(\mathbf{k}_\parallel)=H_i-J(\mathbf{k}_\parallel;0)-2J(\mathbf{k}_\parallel;1) =4J_1(1-\gamma_1)+4J_2(1-\gamma_2)+8J_2(1-\gamma_1) , \tag{16}$$

which represents the energy mode with wave vector $(k_x,0,k_z)$ for a 3D system.

(b) If $J(\mathbf{k}_\parallel;1)<0$ as localized modes we have only oscillating magnons with energy lower than the bulk ones.

(c) Finally, we can have at the most two surface magnons (one symmetric and one antisymmetric).

In Fig. 1 we represent schematically the evolution, within the first Brillouin zone, of the number and type of surface excitations for different values of N and of the ratio $\tau=J_1/4J_2$. In correspondence to the $\mathbf{k}_\parallel$ values for which $J(\mathbf{k}_\parallel;1)=0$ (solid line) $\alpha\to\infty$, i.e., the two surface modes are completely localized at the first and the last plane and the surface magnons change their character from monotonic to oscillating. The volume modes are localized in the other $N-2$ planes; in fact, in this condition the different planes are decoupled and the matrix $\underline{A}$ is diagonal with only two distinct frequencies

$$\omega_S[J(\mathbf{k}_\parallel;1)=0]=A_{11}=A_{NN}=H_s-J(\mathbf{k}_\parallel;0)=J^*+4J_1(1-\gamma_1)+4J_2(1-\gamma_2)\ , \tag{17a}$$

$$\omega_B[J(\mathbf{k}_\parallel;1)=0]=A_{22}=\cdots=A_{N-1\,N-1}=H_i-J(\mathbf{k}_\parallel;0)=2J^*+4J_1(1-\gamma_1)+4J_2(1-\gamma_2)\ . \tag{17b}$$

ω_S is twofold degenerate, while ω_B presents an $(N-2)$ degeneracy of the bulk excitations.

In Fig. 2 we show the effect of NNN exchange on the dispersion curves of a multilayer ($N=5$): the curves are no more parallel as in the Döring[16] case ($J_2=0$). The value of k_x, for which $\alpha\to\infty$, is clear from the figure, and we have only two different eigenvalues.

It is possible to obtain the expression for the mode with lowest energy in the $N\to\infty$ limit (for the details see Appendix B) that with $k_z=0$ is given by

$$\omega_S(k_x,0)=\omega_B(k_x,0)-16\frac{J_2^2}{J^*}\sin^4(k_x/2) \tag{18}$$

with penetration length (for $|\mathbf{k}_\parallel|\to 0$)

$$d=\frac{1}{\alpha}\simeq\frac{J^*}{J_2}\frac{1}{k_\parallel^2}\sim\lambda^2\ , \tag{19}$$

i.e., we recover the results for the semi-infinite system obtained by Mills and Maradudin.[7]

It is also possible to obtain an analytical expression for the energy of the localized excitation and the $N-1$ bulk modes for $k_\parallel\to 0$ (from Fig. 1 we can see that in this limit we always have only one surface magnon). In order to determine α, this limit is equivalent to the $J_2\to 0$ one because both give $\mathcal{M}(\mathbf{k}_\parallel)\to 1$ and the localized character is lost. Consequently, for $\mathbf{k}_\parallel\to 0$ the allowed values of α are the $\bar{\alpha}$ defined in Eq. (14). As shown in Appendix B the frequencies of the bulk modes are

$$\omega_B(\mathbf{k}_\parallel)\underset{\mathbf{k}_\parallel\to 0}{\cong}2J^*[1-\cos\bar{\alpha}_m]+4J_1(1-\gamma_1)+4J_2(1-\gamma_2)+8J_2(1-\gamma_1)\left[\left[1-\frac{1}{N}\right]\cos\bar{\alpha}_m-\frac{1}{N}\right] \tag{20}$$

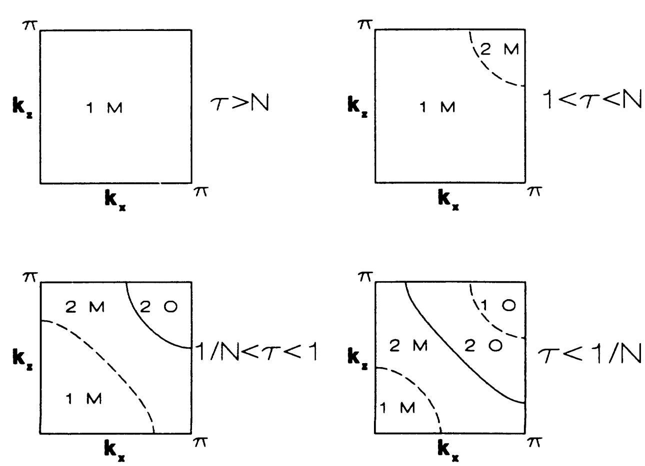

FIG. 1. Schematic plot for the $\mathbf{k}_\parallel$ dependence of the number and type of surface modes (M = monotonic, O = oscillating) for different values of N and $\tau=J_1/4J_2$. Along the solid line, $\alpha\to\infty$, and there are only two distinct frequencies.

Of course, in the $N\gg 1$ limit Eq. (20) gives the frequencies of the excitations with $\mathbf{k}=(\mathbf{k}_\parallel,\bar{\alpha}_m)$ of the three-dimensional system. For the surface mode we have

$$\omega_S(\mathbf{k}_\parallel)\underset{\mathbf{k}_\parallel\to 0}{\cong}4J_1(1-\gamma_1)+4J_2(1-\gamma_2)+8J_2\left[1-\frac{1}{N}\right](1-\gamma_1)\ . \tag{21}$$

For the eigenvectors we have

$$S(l)\simeq 2-\alpha(N-1)\quad \text{finite } N\ , \tag{22}$$

$$S(l)\simeq 1-\alpha(l-1)\quad N\to\infty,\ \text{and small } l\ . \tag{23}$$

It is interesting to note that the quantity $8(1-1/N)$ in Eqs. (20) and (21), represents the average number $\bar{z}$ of next-nearest neighbors in different planes for a simple cubic lattice. This quantity is obtained as $\mathbf{k}_\parallel\to 0$ limit from a more complicated expression

$$\bar{z}(k_\perp)=\frac{\sum_l z(l)S(l)}{\sum_l S(l)}\ , \tag{24}$$

where the next-nearest neighbors in different planes are dynamically weighted by the eigenvectors. The meaning is particularly clear for the acoustic mode: in this case the magnon is localized on the surface planes and consequently they must have a larger weight. We observe that when expression (24) for $\bar{z}$ is put in (21) instead of $8(1-1/N)$, we obtain an exact expression for $\omega_S(\mathbf{k}_\parallel)$.

IV. EXCHANGE INTERACTIONS ONLY: MAGNETIZATION PROFILE

In the preceding section we have studied the elementary excitations of a system in presence of only exchange interactions, using the method of equation of motion for the spin operators because of its remarkable simplicity.

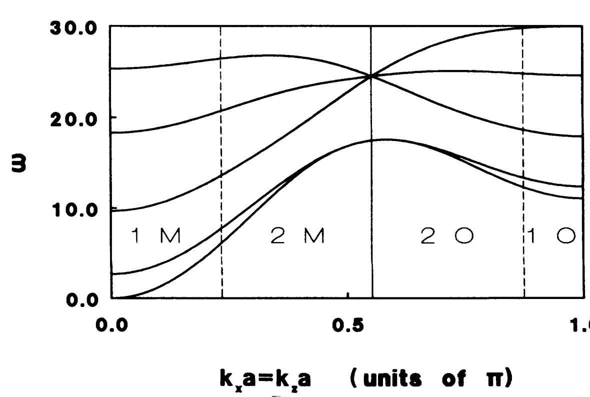

FIG. 2. Dispersion curves for $N=5$, $J_1=1$, $J_2=1.5$.

In order to study the thermodynamical properties, more accessible from the experimental point of view, it is opportune to carry out a boson transformation of the spin operators.

Because of the dimensionality $D=2$, long-range order is forbidden by the theorem of Mermin and Wagner,[17] so we introduce a small magnetic field h that, in the free-spin-wave approximation, works like a uniaxial single-ion anisotropy.

Let us start from the well known Holstein-Primakoff transformation:

$$S^{+}=\sqrt{2S}\left[1-\frac{a^{\dagger}a}{2S}\right]^{1/2}a\ , \tag{25a}$$

$$S^{-}=\sqrt{2S}\,a^{\dagger}\left[1-\frac{a^{\dagger}a}{2S}\right]^{1/2}\ , \tag{25b}$$

$$S^{z}=S-a^{\dagger}a\ . \tag{25c}$$

Owing to the translational invariance in the xz plane and to the absence of this symmetry in the y direction, it is necessary to use a mixed representation for which

$$a_{l}^{\dagger}=N_{\parallel}^{-1/2}\sum_{\mathbf{k}_{\parallel}}a^{\dagger}_{\mathbf{k}_{\parallel},l_y}\exp(i\mathbf{k}_{\parallel}\cdot\boldsymbol{l}_{\parallel})\ , \tag{26a}$$

$$a_{l}=N_{\parallel}^{-1/2}\sum_{\mathbf{k}_{\parallel}}a_{\mathbf{k}_{\parallel},l_y}\exp(-i\mathbf{k}_{\parallel}\cdot\boldsymbol{l}_{\parallel})\ . \tag{26b}$$

The Hamiltonian is diagonal in $\mathbf{k}_{\parallel}$ (from now on we drop the y subscript)

$$\mathcal{H}=\sum_{i,j}\underline{A}_{ij}(\mathbf{k}_{\parallel})a^{\dagger}_{\mathbf{k}_{\parallel},i}a_{\mathbf{k}_{\parallel},j}\ , \tag{27}$$

where

$$\underline{A}_{ij}(\mathbf{k}_{\parallel})=\delta_{ij}H^{\mathrm{eff}}(i)-SJ(\mathbf{k}_{\parallel};i-j) \tag{28}$$

is, of course, the matrix $\underline{A}$ defined in Eq. (4) using the method of the equation of motion for the spin operators.

The matrix $\underline{A}$ is real and symmetric; it is diagonalized by a orthogonal matrix $\underline{U}(\underline{U}^{T}=\underline{U}^{-1})$. This assures the conservation of the boson commutation rules for the new operators $b_{\mathbf{k}_{\parallel},i},b^{\dagger}_{\mathbf{k}_{\parallel},i}$

$$a_{\mathbf{k}_{\parallel},i}=\sum_{l}\underline{U}_{il}b_{\mathbf{k}_{\parallel},l}\ , \tag{29a}$$

$$a^{\dagger}_{\mathbf{k}_{\parallel},i}=\sum_{l}\underline{U}_{il}b^{\dagger}_{\mathbf{k}_{\parallel},l} \tag{29b}$$

so that

$$\mathcal{H}=\sum_{\mathbf{k}_{\parallel}}\sum_{i,j}\underline{A}_{ij}(\mathbf{k}_{\parallel})\sum_{l,m}\underline{U}_{il}\underline{U}_{jm}b^{\dagger}_{\mathbf{k}_{\parallel},l}b_{\mathbf{k}_{\parallel},m} \tag{30}$$

with

$$\sum_{i,j}\underline{A}_{ij}(\mathbf{k}_{\parallel})\underline{U}_{il}\underline{U}_{jm}=[\underline{U}^{T}\underline{A}(\mathbf{k}_{\parallel})\underline{U}]_{lm}$$
$$=\omega_{l}(\mathbf{k}_{\parallel})\delta_{l,m}\ . \tag{31}$$

The diagonalized Hamiltonian is

$$\mathcal{H}=\sum_{l}\sum_{\mathbf{k}_{\parallel}}\omega_{l}(\mathbf{k}_{\parallel})b^{\dagger}_{\mathbf{k}_{\parallel},l}b_{\mathbf{k}_{\parallel},l}\ . \tag{32}$$

For the thermal average of the magnon number operator we have

$$\langle a^{\dagger}_{\mathbf{k}_{\parallel},i}a_{\mathbf{k}_{\parallel},i}\rangle=\sum_{l,m}\underline{U}_{il}\underline{U}_{im}\langle b^{\dagger}_{\mathbf{k}_{\parallel},l}b_{\mathbf{k}_{\parallel},m}\rangle$$
$$=\sum_{l}\underline{U}_{il}^{2}\langle b^{\dagger}_{\mathbf{k}_{\parallel},l}b_{\mathbf{k}_{\parallel},l}\rangle \tag{33}$$

where

$$\langle b^{\dagger}_{\mathbf{k}_{\parallel},l}b_{\mathbf{k}_{\parallel},m}\rangle=\delta_{lm}\left[\exp\left[\frac{\omega_{l}(\mathbf{k})}{T}\right]-1\right]^{-1}.$$

The matrix $\underline{U}$ has elements given by

$$\underline{U}_{il}=S_{l}(r_{y}=i)\ , \tag{34}$$

i.e., $\underline{U}_{il}$ represents the amplitude of the oscillation on the ith plane when the lth mode is excited, provided that the eigenvector is normalized to one.

For the thermal deviation $\Delta_i(T)$ on the ith plane we have

$$\Delta_{i}(T)\equiv S-\langle S^{z}(r_{y}=i)\rangle=\sum_{l}(2\pi)^{-2}\int d\mathbf{k}_{\parallel}S_{l}^{2}(\mathbf{k}_{\parallel};r_{y}=i)\left\{\exp\left[\frac{\omega_{l}(\mathbf{k}_{\parallel})}{T}\right]-1\right\}^{-1}\ . \tag{35}$$

From Eq. (35) it is apparent that the magnetization profile is also determined by the eigenvectors. For real systems such a property can be measured by means of conversion electron Mössbauer spectroscopy.[3] In order to have the deviation per spin of the multilayer

$$\bar{\Delta}(T)=N^{-1}\sum_{i}\Delta_{i}(T) \tag{36}$$

being $\sum_i \underline{U}_{il}^{2}=1$, we have

$$\bar{\Delta}(T)=N^{-1}\sum_{l}(2\pi)^{-2}\int d\mathbf{k}_{\parallel}\left\{\exp\left[\frac{\omega_{l}(\mathbf{k}_{\parallel})}{T}\right]-1\right\}^{-1}. \tag{37}$$

In the presence of a NN interaction only $S_{l}^{2}(i)=N^{-1}$ for the acoustic mode and $S_{l}^{2}(i)=2N^{-1}\cos^{2}[\bar{\alpha}_{l}(i-1/2)]$ for the optical ones. It is apparent that the acoustic mode gives a uniform spin deviation. Furthermore, it is easy to note that, while all modes contribute to the surface $(i=1)$ spin deviation, the spin deviation of the central layer $(i=N/2)$ is given only by the symmetric modes. Quantitatively, for ultrathin films and very low temperatures with respect to J we have that the spin deviation is determined only by the acoustic mode,

$$\Delta(T)=\frac{1}{N}\frac{1}{4\pi}\frac{T}{J}\ln[1-e^{-h/T}]^{-1}\underset{T\gg h}{\sim}\frac{1}{N}\frac{1}{4\pi}\frac{T}{J}\ln\left[\frac{T}{h}\right] \tag{38}$$

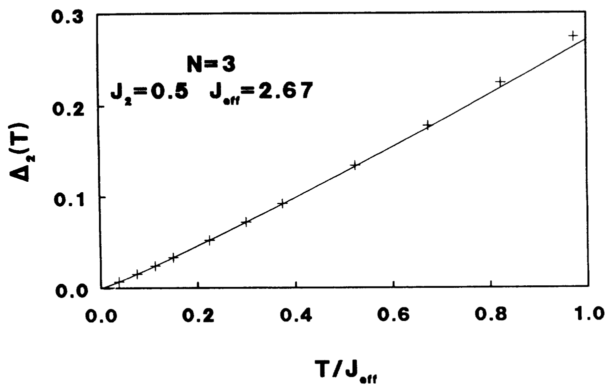

FIG. 3. Temperature dependence of the thermal deviation on the central plane of an $N=3$ film. Crosses: numerical values; solid line: Eq. (38). $J_{\rm eff}=J_1+4J_2(1-1/2N)$, as follows from (47).

similarly to the monolayer system. The result (38) has been experimentally observed by Paul, Taborelli, and Landolt for Fe/Au(100).[18] In Fig. 3 this quasilinear T dependence is shown for a film with $N=3$ layers. J_2 is different from zero but for such a small value of N the localized character of the surface is not important ($\alpha \ll 1$). This quantity, as the other thermodynamical properties shown in this section, has been calculated introducing a very small magnetic field, $h=10^{-4}$, in order to avoid the usual 2D infrared divergence. In the $N \gg 1$ limit with $S_l^2(1)\simeq(2/N)[1-(l\pi/N)^2/2]$ and at low temperatures (so that we can put $\epsilon_{\mathbf{k}_\parallel}\simeq Jk_\parallel^2$) we have

$$\Delta_1(T)=2\Delta_B(T)+O(T/J)^{5/2} \tag{39}$$

[where $\Delta_B(T)$ is the spin deviation for a 3D system]. For $\Delta_{N/2}(T)$ the summation in Eq. (35) is restricted to N an even integer, and consequently

$$\Delta_{N/2}(T)=\Delta_1(T)/2=\Delta_B(T)\ . \tag{40}$$

The expressions (39) and (40) are the well-known results obtained by Rado[19] and Mills and Maradudin[7] for the semi-infinite system.

In Fig. 4 the crossover between the quasilinear T dependence (dashed line) and the $T^{3/2}$ law (solid line) with increasing T is shown for the surface and central planes in an $N=21$ film. At very low temperatures only the acoustic mode statistically weights and $\Delta_i(T)$ follows a $T\ln T$ law; instead at higher temperatures we have to invoke a $T^{3/2}$ law. The comparison of $\Delta_1(T)$ and $\Delta_{N/2}(T)$ shows that all the modes are important for the former but only the even ones for the latter. So, we have to take into account a much larger number of modes to reproduce $\Delta_1(T)$ than those necessary for the central plane. However, while analytically a $T^{3/2}$ law results from an infinite number of modes, Fig. 4 shows that a rather small number of modes (~ 5) is sufficient.

The results obtained for the spin deviation in the presence of the NNN interaction J_2 are shown in Figs. 5 and 6. In the former it is reported the normalized quantity $[\Delta_i-\Delta_{N/2}]/\Delta_{N/2}$ vs the plane index i at fixed T and $N=43$. For comparison, also the result obtained in the

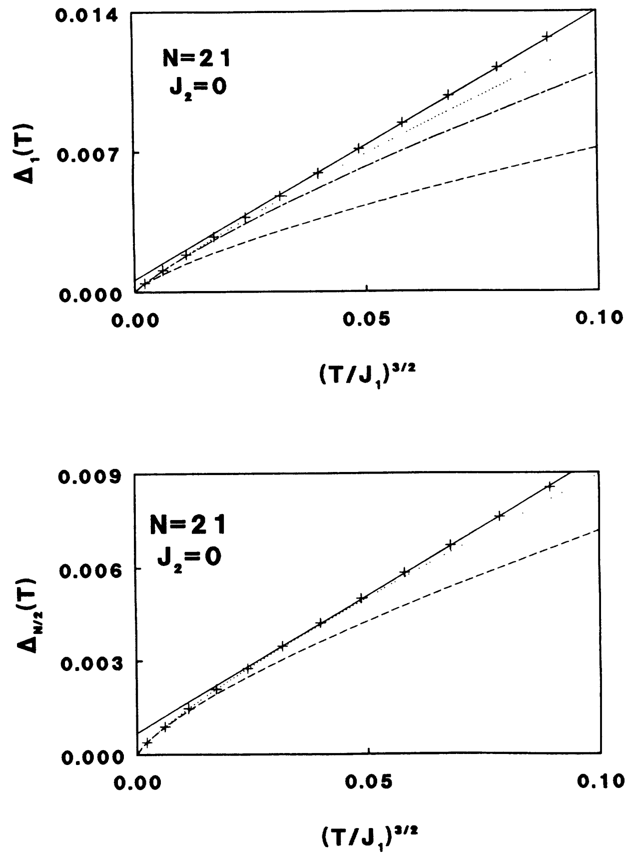

FIG. 4. Thermal deviations on the first and central plane of a film ($N=21$). Crosses: numerical values; solid line: $T^{3/2}$ law; dashed line: contribution of the acoustic mode ($\propto(1/N)T\ln T$); short-and-long-dashed line: acoustic mode plus first optical mode; dotted line: acoustic, first and second optical modes.

absence of NNN interaction is shown. In order to put into clear evidence the effect of the surface modes, we have chosen an effective stiffness in the second case.

Generally, we have a fast decrease of spin deviation toward the central plane value, but in the presence of a NNN interaction we have a stronger effect on the surface plane. In Fig. 6 we report the ratio between the surface

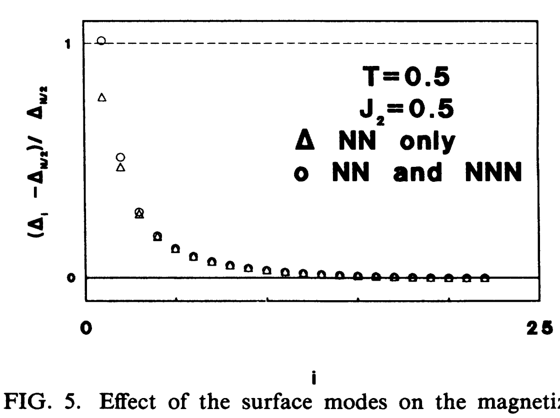

FIG. 5. Effect of the surface modes on the magnetization profile of an $N=43$ multilayer. Triangles are calculated for $J_1=J_{\rm eff}$.

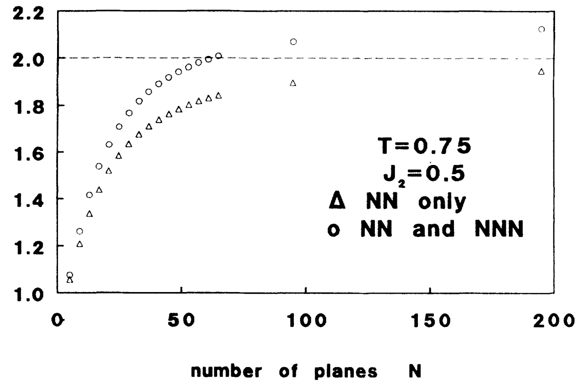

FIG. 6. Effect of NNN exchange on the ratio between thermal deviations on first and central planes. Again, triangles are calculated for $J_1 = J_{\rm eff}$.

plane spin deviation and the central plane spin deviation vs the plane number of the multilayer. It is well known that for $N \to \infty$, in the temperature region in which the Bloch law holds this ratio must tend to 2 for any value of J_2.[7] For the multilayers, it is apparent that with $J_2 \neq 0$ we have a much quicker rise. The values greater than 2 reported for $N > 65$ seem to suggest that for $J_2 \neq 0$ this ratio shows a maximum, indicating that for an intermediate region of N there is a very important contribution of the surface mode.

In conclusion, it is important to understand what is the temperature region in which it is simple to observe the contribution of the localized modes to the magnetization profile. At very low temperature only the acoustic mode is excited but for $\mathbf{k}_\parallel \to 0$ the factor α in the eigenfunction $S(l) = \exp[-\alpha(l-1)]$ is very small and consequently this mode is not much localized. It is necessary to increase the temperature, so that greater $\mathbf{k}_\parallel$ are important, but without a sensible increase of the optical modes contribution which have bulk character.

V. DIPOLAR INTERACTION AND SURFACE ANISOTROPY

In this section we report the results obtained for the spectrum and the magnetization profile for the complete Hamiltonian (1): i.e., $\lambda, w \neq 0$.

A. The spectrum

We assume that the dipolar interaction prevails over the uniaxial surface anisotropy and consequently a collinear ground state with the spins in the surface plane xz results:

$$W = \frac{3}{4} w \frac{\mathcal{D}(N)}{N} > A = S\lambda(N)/N \ , \tag{41}$$

where the dipolar summation $\mathcal{D}(N)$ is defined in Appendix C. The assumptions of a collinear structure and the spins in the film plane are in agreement with many experimental studies.

Using the transformation (25) we obtain the following boson Hamiltonian:

$$\mathcal{H} = \sum_{i,j} \sum_{\mathbf{k}_\parallel} \left\{ \underline{A}_{ij}(\mathbf{k}_\parallel) a^\dagger_{\mathbf{k}_\parallel, i} a_{\mathbf{k}_\parallel, j} + \frac{\underline{B}_{ij}(\mathbf{k}_\parallel)}{2} [a^\dagger_{\mathbf{k}_\parallel, i} a^\dagger_{-\mathbf{k}_\parallel, j} + a_{\mathbf{k}_\parallel, i} a_{-\mathbf{k}_\parallel, j}] \right\} , \tag{42}$$

where only quadratic terms have been retained and i,j denote the plane indices. The matrices $\underline{A}$ and $\underline{B}$ and their properties are defined in Appendix C. Now we develop a Green's function formalism in order to find both the spin-wave frequencies and the magnetization profile. We define the Fourier transformed retarded Green's functions

$$\underline{G}_{lm}(\mathbf{k}_\parallel, E) = \langle\langle a_{\mathbf{k}_\parallel, l}; a^\dagger_{\mathbf{k}_\parallel, m} \rangle\rangle_E \ , \tag{43a}$$

$$\underline{G}'_{lm}(\mathbf{k}_\parallel, E) = \langle\langle a^\dagger_{-\mathbf{k}_\parallel, l}; a^\dagger_{\mathbf{k}_\parallel, m} \rangle\rangle_E \ . \tag{43b}$$

Their equation of motion in terms of $(N \times N)$ matrices are

$$[\underline{A}(\mathbf{k}_\parallel) - E\underline{I}]\underline{G}(\mathbf{k}_\parallel) + \underline{B}(\mathbf{k}_\parallel)\underline{G}'(\mathbf{k}_\parallel) = -\frac{1}{2\pi}\underline{I} \ , \tag{44a}$$

$$-\underline{B}(-\mathbf{k}_\parallel)\underline{G}(\mathbf{k}_\parallel) + [-\underline{A}(\mathbf{k}_\parallel) - E\underline{I}]\underline{G}'(\mathbf{k}_\parallel) = \underline{O} \ , \tag{44b}$$

where $\underline{I}$ and $\underline{O}$ denote the unitary and zero matrix, respectively. The spin-wave frequencies are obtained from the poles of $\underline{G}(\mathbf{k}_\parallel)$ as the eigenvalues of the nonsymmetric $(2N) \times (2N)$ real matrix $\underline{T}$:

$$\underline{T}(\mathbf{k}_\parallel) = \begin{bmatrix} \underline{A}(\mathbf{k}_\parallel) & \underline{B}(\mathbf{k}_\parallel) \\ -\underline{B}(-\mathbf{k}_\parallel) & -\underline{A}(\mathbf{k}_\parallel) \end{bmatrix} . \tag{45}$$

It is easy to demonstrate[12] that $\underline{T}(\mathbf{k}_\parallel)$, $-\underline{T}(\mathbf{k}_\parallel)$, and $\underline{T}(-\mathbf{k}_\parallel)$ have the same eigenvalues; consequently half of the $2N$ eigenvalues are positive and half negative, with the same absolute value:

$$\omega_{l+N}(\mathbf{k}_\parallel) = -\omega_l(\mathbf{k}_\parallel) \quad (l = 1, 2, \ldots, N) \ . \tag{46}$$

For the monolayer case $(N=1)$ $\underline{A}$ and $\underline{B}$ are scalar quantities, and in the continuum limit, $\mathbf{k}_\parallel \to 0$, one recovers the result first found by Maleev[10] for $h=0$, $\lambda=0$. Also in the case of a bilayer $(N=2)$, it is possible to obtain the explicit expressions for the acoustic and optical modes in the limit $w/J \ll 1$ and $k_\parallel a \ll 1$. Both these results are reported in Appendix C.

For the multilayer case with generic N, one must resort to numerical methods. However, it is possible to generalize the results obtained for $N=1$ and 2 in order to obtain an expression for the acoustic mode ($k \equiv |\mathbf{k}_\parallel|$ and φ_k is the angle between $\mathbf{k}_\parallel$ and the z direction) in the limits $w, \lambda \ll J$ and for small wave vectors $(ka) \ll 1$,

$$\omega_A^2(\mathbf{k}_\parallel)=(A_{\mathbf{k}_\parallel}-B_{\mathbf{k}_\parallel})(A_{\mathbf{k}_\parallel}+B_{\mathbf{k}_\parallel})$$
$$=\left\{\Delta_N-2\pi Q(N)w(ka)+\frac{\pi^2}{y_0}w(ka)^2+SJ_{\text{eff}}(ka)^2\right\}$$
$$\times\left\{h+2\pi w\sin^2\varphi_k Q(N)ka-\frac{\pi^2}{8y_0}(1+6\sin^2\varphi_k)w(ka)^2+SJ_{\text{eff}}(ka)^2\right\}, \tag{47}$$

where

$$J_{\text{eff}}\equiv[J_1+4J_2(1-1/2N)]$$

and

$$Q(N)=[1-\exp(-Nka)]/[1-\exp(-ka)] .$$

The quantity $(h\Delta_N)^{1/2}$, with

$$\Delta_N=h-2S\frac{2\lambda}{N}f_s+\frac{3}{2}w\bar{y} ,$$

represents the gap of a multilayer of N planes. $f_s=(1-1/2S)$ is the kinematic factor necessary for a correct quantum treatment of the single-ion anisotropy.[20] y_0 and $\bar{y}$ are some of the numerous dipolar sums shown in Appendix C. For $Nka \ll 1$, $Q(N)\rightarrow N$ and the terms in $w(ka)^2$ can be neglected, so that the dipolar interaction contributes to the squared frequency of the acoustic mode with a term linear in k and in the number of planes. This is exactly what was suggested by Yafet, Kwo, and Gyorgy.[11] It is clear that with increasing N, the region of validity of such behavior becomes more and more limited: this is consistent with the fact that in three dimensions the dipolar interaction does not give a term linear in k, even for very low wave vectors.[21]

In Fig. 7 we report $\omega_A(\mathbf{k}_\parallel)$ vs $(k_x a)$ for low k, for different values of the number of planes N and $h=\lambda=0$. For comparison we report, in the case $N=15$, the prediction by Yafet, Kwo, and Gyorgy[11] in which the k expansion for the dipolar sums is limited to linear terms. We see that no gap is present and for $Nka \ll 1$ the dipolar interaction gives rise to a $(Nka)^{1/2}$ behavior. Increasing k and N, expression (47) results in closer agreement with the numerical results than the prediction of Yafet, Kwo, and Gyorgy.

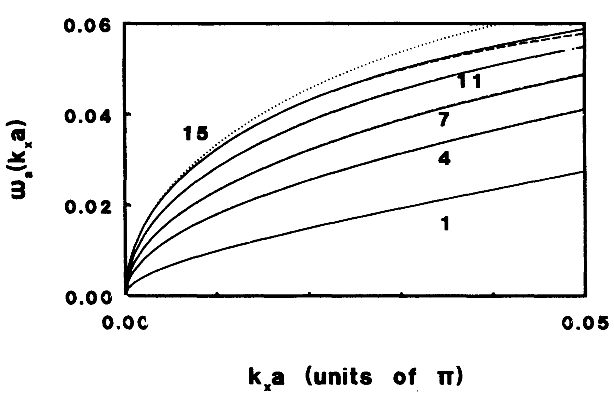

FIG. 7. Dispersion curve of the acoustic mode of a multilayer ($N=1,4,7,11,15$) in presence of exchange ($J_{\text{eff}}=1$) and dipolar interaction ($w=0.01$). Solid line: analytical expression (47); dashed line: numerical results; dotted line: prediction of Yafet, Kwo, and Gyorgy (Ref. 11).

It is worthwhile to note from Eq. (47) that we recover, in the limit $N\rightarrow\infty$ and $a\rightarrow 0$ and for very low wave vectors, the result of the magnetostatic mode theory[4] for the frequency $\omega_S(\mathbf{k}_\parallel)$ of the surface mode of a ferromagnetic slab of finite thickness $L=Na$. With $\mathbf{k}_\parallel$ along the x direction perpendicular to the magnetization $\omega_S(\mathbf{k}_\parallel)$ is given by

$$\omega_S(\mathbf{k}_\parallel)=\left[\left[\omega_0+\frac{\omega_m}{2}\right]^2-\frac{\omega_m^2}{4}\exp(-2kL)\right]^{1/2} \tag{48}$$

with $\omega_0\equiv h$ and $\omega_m\equiv 4\pi g\mu_B M_S=4\pi w$. ω_S is found to lie above the k independent frequency of the bulk mode $\omega_0=[\omega_0(\omega_0+\omega_m)]^{1/2}$.

B. Magnetization profile

Using the spectral theorem the magnetization profile can be obtained from the diagonal elements of the matrix $\underline{G}$

$$\langle a^\dagger_{\mathbf{k}_\parallel,l}a_{\mathbf{k}_\parallel,l}\rangle=-2\int_{-\infty}^{+\infty}dE\frac{\text{Im}\langle\langle a_{\mathbf{k}_\parallel,l};a^\dagger_{\mathbf{k}_\parallel,l}\rangle\rangle_{E+i0^+}}{\exp(\beta E)-1} \tag{49}$$

so that $\Delta_l(T)=N_\parallel^{-1}\sum_{\mathbf{k}_\parallel}\langle a^\dagger_{\mathbf{k}_\parallel,l}a_{\mathbf{k}_\parallel,l}\rangle$. In order to calculate $\underline{G}_{l,l}(\mathbf{k}_\parallel,E)$ let us first observe that the system (44a) and (44b) can be rewritten as

$$[\underline{T}(\mathbf{k}_\parallel)-E\underline{I}]\underline{F}(\mathbf{k}_\parallel)=-\frac{1}{2\pi}\underline{L} \tag{50}$$

in terms of the matrix $\underline{T}$ and of the $(2N\times 2N)$ auxiliary matrices $\underline{F},\underline{L}$ defined as

$$\underline{F}(\mathbf{k}_\parallel)=\begin{bmatrix}\underline{G}(\mathbf{k}_\parallel) & \underline{O}\\ \underline{G}'(\mathbf{k}_\parallel) & \underline{O}\end{bmatrix}\quad \underline{L}=\begin{bmatrix}\underline{I} & \underline{O}\\ \underline{O} & \underline{O}\end{bmatrix} . \tag{51}$$

Denoting by $\underline{P}(\mathbf{k}_\parallel)$ the real nonunitary matrix, which diagonalizes $\underline{T}(\mathbf{k}_\parallel)$,

$$\underline{T}'(\mathbf{k}_\parallel)=\underline{P}^{-1}(\mathbf{k}_\parallel)\underline{T}(\mathbf{k}_\parallel)\underline{P}(\mathbf{k}_\parallel) , \tag{52}$$

we obtain, multiplying Eq. (50) by $\underline{P}^{-1}(\mathbf{k}_\parallel)$ on the left and $\underline{P}(\mathbf{k}_\parallel)$ on the right:

$$[\underline{T}'(\mathbf{k}_\parallel)-E\underline{I}]\underline{F}'(\mathbf{k}_\parallel)=-\frac{1}{2\pi}\underline{L}' ,$$

where

$$\underline{F}'(\mathbf{k}_\parallel)=\underline{P}^{-1}(\mathbf{k}_\parallel)\underline{F}(\mathbf{k}_\parallel)\underline{P}(\mathbf{k}_\parallel)$$

and

$$\underline{L}'(\mathbf{k}_\parallel)=\underline{P}^{-1}(\mathbf{k}_\parallel)\underline{L}(\mathbf{k}_\parallel)\underline{P}(\mathbf{k}_\parallel) .$$

The matrix $[\underline{T}'(\mathbf{k}_\parallel)-E\underline{I}]$ is diagonal, so that

$$[\underline{T}'(\mathbf{k}_\parallel)-E\underline{I}]_{ij}^{-1}=\frac{\delta_{ij}}{\omega_i(\mathbf{k}_\parallel)-E} , \tag{53}$$

giving

$$\begin{aligned}\underline{F}'_{ij}(\mathbf{k}_\parallel)&=-\frac{1}{2\pi}\sum_l [\underline{T}'(\mathbf{k}_\parallel)-E\underline{I}]_{il}^{-1}\underline{L}'_{lj}\\ &=-\frac{1}{2\pi}\frac{\underline{L}'_{ij}}{\omega_i(\mathbf{k}_\parallel)-E}\end{aligned} \tag{54}$$

and thus

$$\begin{aligned}\underline{F}_{ij}(\mathbf{k}_\parallel)&=-\frac{1}{2\pi}\sum_{l,m}\underline{P}_{il}(\mathbf{k}_\parallel)\frac{\underline{L}'_{lm}}{\omega_l-E}\underline{P}_{mj}^{-1}(\mathbf{k}_\parallel)\\ &=-\frac{1}{2\pi}\sum_l\frac{\underline{P}_{il}(\mathbf{k}_\parallel)\underline{P}_{l,j}^{-1}(\mathbf{k}_\parallel)\underline{L}_{jj}}{\omega_l-E} .\end{aligned} \tag{55}$$

In conclusion, the imaginary part of the Green's function $\langle\langle a_{\mathbf{k}_\parallel,i};a^\dagger_{\mathbf{k}_\parallel,j}\rangle\rangle_{E+i0^+}$ can be expressed as

$$\mathrm{Im}\underline{F}_{ii}(E+i0^+)=-\tfrac{1}{2}\sum_{l=1}^{2N}\underline{P}_{il}(\mathbf{k}_\parallel)\underline{P}_{li}^{-1}(\mathbf{k}_\parallel)\delta(E-\omega_l) \tag{56}$$

where $i=1,\dots,N$.

The spin-wave magnetization profile is then obtained integrating

$$\langle a^\dagger_{\mathbf{k}_\parallel,n}a_{\mathbf{k}_\parallel,n}\rangle=\sum_{j=1}^{2N}\underline{P}_{nj}\underline{P}_{jn}^{-1}\frac{1}{e^{\beta\omega_j}-1}, \quad n=1,\dots,N \tag{57}$$

over the two-dimensional Brillouin zone.

Taking into account the property (46) of the eigenvalues, it is possible to separate the temperature dependent contribution from the zero-point spin reduction

$$\Delta_l(T)=\frac{1}{N_\parallel}\sum_{\mathbf{k}_\parallel}\sum_{j=1}^{N}\left[\frac{\underline{P}_{lj}\underline{P}_{jl}^{-1}-\underline{P}_{lj'}\underline{P}_{j'l}^{-1}}{\exp(\beta\omega_j)-1}-\underline{P}_{lj'}\underline{P}_{j'l}^{-1}\right] \quad (j'=j+N) . \tag{58}$$

In the presence of only exchange interactions $\underline{P}(\mathbf{k}_\parallel)$ is an orthogonal $(N\times N)$ matrix with $\underline{P}_{lj}\underline{P}_{jl}^{-1}=\underline{P}_{lj}^2=S_j^2(l)$; in this case, from Eq. (57) we reobtain Eq. (35).

For $N=1$ we recover the monolayer result.[10,11] Equation (58) becomes

$$\langle a^\dagger_{\mathbf{k}_\parallel}a_{\mathbf{k}_\parallel}\rangle=\frac{\underline{P}_{11}\underline{P}_{11}^{-1}-\underline{P}_{12}\underline{P}_{21}^{-1}}{\exp(\beta\omega-1)}-\underline{P}_{12}\underline{P}_{21}^{-1} \tag{59}$$

and $\underline{T}$ is a (2×2) matrix with eigenvalues

$$E^\pm_{\mathbf{k}_\parallel}\pm[A^2_{\mathbf{k}_\parallel}-B^2_{\mathbf{k}_\parallel}]^{1/2}=\pm E_{\mathbf{k}_\parallel} . \tag{60}$$

The final result is

$$\langle a^\dagger_{\mathbf{k}_\parallel}a_{\mathbf{k}_\parallel}\rangle=\left[\frac{A_{\mathbf{k}_\parallel}}{E_{\mathbf{k}_\parallel}}\right]\frac{1}{\exp(\beta E_{\mathbf{k}_\parallel})-1}+\left[\frac{A_{\mathbf{k}_\parallel}-E_{\mathbf{k}_\parallel}}{2E_{\mathbf{k}_\parallel}}\right] . \tag{61}$$

For the spin deviation the temperature dependence is $\Delta(T)\propto(T/J)^{3/2}$ if $T\ll w(w/J)^{1/2}$ and $\Delta(T)\propto(T/J)\ln[(T/w)(J/w)^{1/2}]$ for $T\gg w(w/J)^{1/2}$.[10]

For $N>1$, if only the acoustic mode is statistically important, we can generalize Eq. (61) in a simple way: the quantities $A_{\mathbf{k}_\parallel},E_{\mathbf{k}_\parallel}$ are modified according to (47) and a factor $1/N$, as in (38) is present. Otherwise, if the values of N and T are not small and more than one mode has to be taken into account, a numerical diagonalization of the matrix $\underline{T}$ is necessary.

An expression analogous to (58) is obtained also for $w=0$ but in presence of a single-ion easy-plane anisotropy. In this case the nonsymmetric matrix $\underline{T}$ takes a simple form, since the matrix $\underline{B}$ is multiple of the unitary matrix. This allows us to obtain analytically the eigenvalues and eigenvectors of the matrix $\underline{T}$ with no more effort than in the case of a model with NN and NNN interactions. The explicit results will be shown in a future publication, where the total magnetization of the superlattice $(Fe_3/Ag_x)_8$ with different number x of Ag planes will be investigated.[22]

VI. CONCLUSIONS

We have studied the linear excitations and magnetization profile for ultrathin films with a few layers thickness, and different peculiar behaviors due to the absence of translational invariance are found. Using a microscopic approach we have shown that in the presence of NNN J_2, a situation meaningful physically, different numbers and types of localized modes as a function of the ratio J_2/J_1, the number of layers N and the 2D wave vectors $\mathbf{k}_\parallel$, are present. In particular, in addition to the usual monotonic surface modes, for sufficiently high wave vectors surface modes, called oscillating modes are predicted. These modes always have the lowest energies and for the acoustic one we have been able to give an analytical expression. Their effects on the magnetization profile are very strong, giving for external planes a spin deviation much larger than the inner ones: in ultrathin films these effects are much more relevant than in the semi-infinite case. This behavior has been experimentally observed in iron ultrathin films using conversion electron Mössbauer spectroscopy.[3,23] For fixed N, with increasing temperature it is possible to observe a transition between a 2D regime ($T\ln T$) and a 3D one ($T^{3/2}$).

Also the effects due to the dipolar interaction and a single-ion surface anisotropy have been considered. Using a Green's-function formalism, the energies of excitations as functions of a number N of planes and of the wave vectors $\mathbf{k}_\parallel$ are studied. In particular, for the acoustic mode an analytical expression is obtained improving the suggestion by Yafet, Kwo, and Gyorgy[11] about the N dependence of the $\mathbf{k}_\parallel$ linear term given by the dipolar interaction. These predictions can be experimentally verified by means of Brillouin light scattering. For the magnetization profile we derive an expression valid for any model depicted by a nondiagonal quadratic boson Hamiltonian (consequently a nonsymmetric matrix $\underline{T}$).

APPENDIX A

Using Eqs. (9) and (10) the function $\mathcal{F}(k_\perp)$ is

$$\mathcal{F}^+(k_\perp)=\frac{\cos[k_\perp(N+1)/2]}{\cos[k_\perp(N-1)/2]} \quad \text{(symmetric)} \tag{A1a}$$

$$\mathcal{F}^-(k_\perp)=\frac{\sin[k_\perp(N+1)/2]}{\sin[k_\perp(N-1)/2]} \quad \text{(antisymmetric)} . \tag{A1b}$$

For $k_\perp=\alpha$ (bulk magnons) we define $\mathcal{F}^\pm(\alpha)=\mathcal{F}^\pm(k_\perp=\alpha)$. For $k_\perp=-i\alpha$ (monotonic surface magnons) we define $\mathcal{R}^\pm(\alpha)=\mathcal{F}^\pm(k_\perp=-i\alpha)$ where the functions $\mathcal{R}^\pm(\alpha)$ are obtained from the $\mathcal{F}^\pm(\alpha)$, replacing (sin, cos) with (sinh, cosh). For the oscillating surface magnons $(k_\perp=-i\alpha+\pi)$, in the symmetric case we find

$$\mathcal{F}^+(-i\alpha+\pi)=\begin{cases}-R^-(\alpha), & N=2n\\ -R^+(\alpha), & N=2n+1 ,\end{cases} \tag{A2}$$

while in the antisymmetric one

$$\mathcal{F}^-(-i\alpha+\pi)=\begin{cases}-R^+(\alpha), & N=2n\\ -R^-(\alpha), & N=2n+1 .\end{cases} \tag{A3}$$

APPENDIX B

The frequency of the acoustic (surface) mode is given by

$$\omega_S(\mathbf{k}_\parallel)=H_i-J(\mathbf{k}_\parallel;0)-2J(\mathbf{k}_\parallel;1)\cosh\alpha \tag{B1}$$

with α determined by Eq. (11). When $N\to\infty$ we have

$$\cosh[\alpha(n+1)/2]/\cosh[\alpha(N-1)/2\simeq\exp(\alpha) .$$

Introducing the quantity $\omega_{S-B}(\mathbf{k}_\parallel)$, as defined by Eq. (16), $\omega_S(\mathbf{k}_\parallel)$ becomes

$$\omega_S(\mathbf{k}_\parallel)=\omega_{S-B}(\mathbf{k}_\parallel)-2J(\mathbf{k}_\parallel;1)[\cosh\alpha-1] . \tag{B2}$$

Taking into account that

$$2\cosh\alpha=[J^*/(J_1+4J_2\gamma_1)]+[(J_1+4J_2\gamma_1)/J^*]$$

and putting $k_z=0$, we obtain the result (18) found by Mills and Maradudin.[7]

For a finite number N planes we know that for $|\mathbf{k}_\parallel|\ll 1$ there is a symmetric localized energy, which has the lowest energy and $N-1$ bulk modes. To a certain extent the $\mathbf{k}_\parallel\to 0$ limit is analogous to the $J_2\to 0$ case because in both limits we have $\mathcal{M}(\mathbf{k}_\parallel)\to 1$. Therefore for $\mathbf{k}_\parallel\to 0$ we have that the solutions are very near to the Döring ones.[16] For $\alpha\to 0$ (surface mode),

$$\cosh[\alpha(N+1)/2]/\cosh[\alpha(N-1)/2]\simeq 1+\frac{\alpha^2}{2}N .$$

Consequently $\cosh\alpha\simeq[N-1+\mathcal{M}(\mathbf{k}_\parallel)]/N$; in this way we obtain Eq. (21).

For the symmetric bulk modes, putting $\alpha=\bar{\alpha}_m+\epsilon$, we can obtain ϵ by means of a development at the lowest order in this quantity

$$\mathcal{M}(\mathbf{k}_\parallel)=\frac{\cos[(\alpha/2)(N+1)]}{\cos[(\alpha/2)(N-1)]}\simeq 1-\epsilon N\tan\left[\frac{\bar{\alpha}_m}{2}\right] . \tag{B3}$$

Substituting in Eq. (9) pertinent to the bulk modes we obtain Eq. (20). The result is valid also for the antisymmetric modes.

APPENDIX C

In order to determine the ground state we parametrize the spins as $\mathbf{S}=(S\sin\theta\sin\phi,\ S\cos\theta,\ S\sin\theta\cos\phi)$. The exchange, Zeeman, and anisotropy terms assume usual expressions while the dipolar interaction contribution to the ground state is given by

$$\mathcal{H}^0_{\rm dip}(\theta)=\text{cost}-\frac{3SwN_\parallel}{4}\sin^2\theta\sum_{l_y,m_y}D_{yy}(l_y-m_y) \tag{C1}$$

with

$$D_{ii}(l_y-m_y)=\sum_{l_x,l_z}\frac{1}{|\mathbf{l}-\mathbf{m}|^3}\left[1-3\frac{(l_i-m_i)^2}{|\mathbf{l}-\mathbf{m}|^2}\right] ,$$

$$i=x,y,z . \tag{C2}$$

Expression (C1) is obtained taking into account various properties of the dipolar summation. Let us write

$$\sum_{l_y,m_y}D_{yy}(l_y-m_y)=ND_{yy}(0)+\sum_{\Delta l_y=1}^{N-1}2(N-\Delta l_y)D_{yy}(\Delta l_y)\equiv\mathcal{D}(N) \tag{C3}$$

where $D_{yy}(0)$ is predominant: $D_{yy}(1)\simeq -D_{yy}(0)/30$.

The ground state is obtained minimizing the energy per spin

$$\frac{\mathcal{H}^0}{SNN_\parallel}=\left[\frac{S\lambda(N)}{N}-\frac{3}{4}w\frac{\mathcal{D}(N)}{N}\right]\sin^2\theta-h\sin\theta\cos\phi$$

$$\equiv(A-W)\sin^2\theta-h\sin\theta\cos\phi . \tag{C4}$$

The quantities $\underline{A}_{lm}$ and $\underline{B}_{lm}(\mathbf{k}_\parallel)$ in Eq. (42), are given by

$$\underline{A}_{lm}(\mathbf{k}_\parallel)=\delta_{l,m}h^{\rm eff}(l)-SJ(\mathbf{k}_\parallel;l-m)+\frac{w}{2}[D_{xx}(\mathbf{k}_\parallel;l-m)+D_{yy}(\mathbf{k}_\parallel;l-m)] , \tag{C5a}$$

$$\underline{B}_{lm}(\mathbf{k}_\parallel)=\delta_{l,m}h^{\rm eff}_\lambda(l)+\frac{w}{2}[D_{xx}(\mathbf{k}_\parallel;l-m)-D_{yy}(\mathbf{k}_\parallel;l-m)+2iD_{xy}(\mathbf{k}_\parallel;l-m)] , \tag{C5b}$$

where

$$\begin{aligned}
h^{\rm eff}(l)&=h+h^{\rm eff}_J(l)+h^{\rm eff}_w(l)+h^{\rm eff}_\lambda(l) ,\\
h^{\rm eff}_J(l)&=S\sum_{\mathbf{m}}J(l-\mathbf{m}) ,\\
h^{\rm eff}_w(l)&=-w\sum_{\mathbf{m}}D_{zz}(l-\mathbf{m}) ,\\
h^{\rm eff}_\lambda(l)&=-\lambda(l)Sf_s .
\end{aligned} \tag{C6}$$

We have introduced the Fourier transform

$$J(\mathbf{k}_\parallel;l-m)=\sum_{\mathbf{m}_\parallel} J(\mathbf{l}-\mathbf{m})\exp[i\mathbf{k}_\parallel\cdot(\mathbf{l}_\parallel-\mathbf{m}_\parallel)]\ , \tag{C7a}$$

$$D_{\alpha\beta}(\mathbf{k}_\parallel;l-m)=\sum_{\mathbf{m}_\parallel} D_{\alpha\beta}(\mathbf{l}-\mathbf{m})\exp[i\mathbf{k}_\parallel\cdot(\mathbf{l}_\parallel-\mathbf{m}_\parallel)]\ . \tag{C7b}$$

For exchange interactions only $J(\mathbf{k}_\parallel;0)$ and $J(\mathbf{k}_\parallel;1)$ are different from zero. The dipolar sums, which is convenient to redefine as

$$D_{\alpha\beta}(\mathbf{k}_\parallel;\Delta l)\equiv D_{\alpha\beta}(\mathbf{k}_\parallel=0;\Delta l)+D_{\alpha\beta}^{\mathbf{k}_\parallel}(\Delta l)$$

can be numerically evaluated in a very efficient way,[6] while the analytical expression for $|\mathbf{k}_\parallel|\ll 1$ are reported in Ref. 12. We have that $D_{\alpha\alpha}(\mathbf{k}_\parallel;\Delta l)$ are real, even function of $\mathbf{k}_\parallel$ and Δl, different from zero for $\mathbf{k}_\parallel=0$; $D_{\alpha\beta}(\mathbf{k}_\parallel;\Delta l)$ is a purely imaginary, odd function of $\mathbf{k}_\parallel$ and Δl. Consequently, $\underline{A}$ and $\underline{B}$ are real and their matrix elements satisfy the relations:

$$\underline{A}_{lm}(-\mathbf{k}_\parallel)=\underline{A}_{lm}(\mathbf{k}_\parallel)=\underline{A}_{ml}(\mathbf{k}_\parallel)\ , \tag{C8a}$$

$$\underline{B}_{lm}(-\mathbf{k}_\parallel)=\underline{B}_{ml}(\mathbf{k}_\parallel)\ , \tag{C8b}$$

which assure the hermiticity of the Hamiltonian (42).

For the monolayer we have for the frequency the well known result:

$$\omega^2(\mathbf{k}_\parallel)=\{\Delta_1+wD_{yy}^{\mathbf{k}_\parallel}(0)+S[J(\mathbf{k}_\parallel=0;0)-J(\mathbf{k}_\parallel;0)]\}\times\{h+wD_{xx}^{\mathbf{k}_\parallel}(0)+S[J(\mathbf{k}_\parallel=0;0)-J(\mathbf{k}_\parallel;0)]\}\ , \tag{C9}$$

while for $N=2$, the frequency of the acoustic mode is

$$[\omega_A(\mathbf{k}_\parallel)]^2=\left\{\Delta_2+w\sum_{l=0,1}D_{yy}^{\mathbf{k}_\parallel}(l)+S\sum_{l=0,1}[J(\mathbf{k}_\parallel=0;l)-J(\mathbf{k}_\parallel;l)]\right\}\times\left\{h+w\sum_{l=0,1}D_{xx}^{\mathbf{k}_\parallel}(0)+S\sum_{l=0,1}[J(\mathbf{k}_\parallel=0;l)-J(\mathbf{k}_\parallel;l)]\right\} \tag{C10}$$

and for the optical one:

$$[\omega_+(\mathbf{k}_\parallel)]^2=\left\{\Delta_2-2wy_1+2S(J_1+4J_2)+w\sum_{l=0,1}(-)^lD_{yy}^{\mathbf{k}_\parallel}(l)+S\sum_{l=0,1}(-)^l[J(\mathbf{k}_\parallel=0;l)-J(\mathbf{k}_\parallel;l)]\right\}\times\left\{h+wy_1+2s(J_1+4J_2)+w\sum_{l=0,1}(-)^lD_{xx}^{\mathbf{k}_\parallel}(l)+S\sum_{l=0,1}(-)^l[J(\mathbf{k}_\parallel=0;l)-J(\mathbf{k}_\parallel;l)]\right\}+2[wD_{xy}(\mathbf{k}_\parallel;1)]^2\ , \tag{C11}$$

where $y_{\Delta l}\equiv D_{yy}(\mathbf{k}_\parallel=0;\Delta l)$. For $N>2$ we must define $\bar{y}$ given by $\bar{y}\equiv y_0+(1-1/N)2y_1$.

[1]See, for instance, Appl. Phys. A **49** (1989) (special issue on *Magnetism in Ultrathin Films,* edited by D. Pescia), and references therein.

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[23]A quantitative comparison with such experimental data is deferred to future work.