Surface magnons for ferromagnets with single-ion uniaxial anisotropy

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We consider a semi-infinite Heisenberg ferromagnet with nearest-neighbor exchange interactions in a simple-cubic lattice. A single-ion uniaxial anisotropy is taken for the free surface, which is different from that of the bulk. The Green functions at finite temperature are employed to evaluate the magnetization of each layer as well as the surface- and bulk-magnon spectrum up to the bulk critical temperature. We show that the onset of the surface ordering occurs when the energy of the surface magnons begins to be greater than the energy of either bulk mode.

I. INTRODUCTION

The use of Green's functions in the study of surface magnetism is interesting because it can give us information about the spectrum of the surface magnons and simultaneously the layer magnetization of Heisenberg ferromagnets.[1–3] Recent experimental investigations[4,5] on this subject have stimulated the studies on those systems where the lack of full translational symmetry is crucial.

In this paper we consider a semi-infinite Heisenberg ferromagnetic model in a simple-cubic lattice with a (010) free surface. We have also included a single-ion uniaxial anisotropy with the value D_S for the surface and D for the other planes. We have employed Green's function techniques[6] within the random-phase approximation (RPA) to evaluate self-consistently the layer magnetizations of the first three planes from the surface. We have also assumed for simplicity that the bulk magnetization value is reached at the third plane.[1] In this approximation we have determined the surface magnetization for selected values of the parameters D and D_S. Our main goal in this paper is to show that the onset of the surface ordering occurs when the surface magnon modes start to become more energetic than any bulk mode. In Sec. II we present the model Hamiltonian and the calculations for the Green's functions of interest. In Sec. III we discuss the results obtained for the surface-magnon excitations and for the layer magnetization.

II. HAMILTONIAN AND SURFACE GREEN'S FUNCTIONS

We consider the following model Hamiltonian on a semi-infinite simple-cubic lattice

$$H=-\sum_{(\mathrm{i,j})}J_{\mathrm{ij}}\mathbf{S}_i\cdot\mathbf{S}_j-\tilde{D}\sum_{\mathrm{i}}(S_{\mathrm{i}}^z)^2 , \quad (1)$$

where J represents the exchange couplings between nearest neighbors and $\tilde{D}$ is the contribution due to the single-ion uniaxial anisotropy. For the ions on the surface plane ($l=0$) we take $\tilde{D}=D_S$ and for the other ions, $\tilde{D}=D$. The surface is parallel to the (010) plane and we assume that the spins will be oriented preferentially parallel to the surface, so that demagnetizing fields can be neglected.

We write the equations of motion for the Fourier transform of the Green's functions $\langle\langle S_l^+(t);S_{\mathrm{m}}^-(t')\rangle\rangle$,

$$\left[E-2\left[\tilde{D}\langle S_l^z\rangle+\sum_{\mathrm{j}(\neq l)}J_{\mathrm{j}l}\langle S_j^z\rangle\right]\right]G_{l\mathrm{m}}(E)+2\langle S_l^z\rangle\left[\sum_{\mathrm{j}(\neq l)}J_{\mathrm{j}l}G_{\mathrm{jm}}(E)\right]=\frac{1}{\pi}\langle S_l^z\rangle , \quad (2)$$

where $G_{l\mathrm{m}}(E)$ are the Fourier transform of the Green's functions and we have employed the RPA decoupling. We also have assumed that the mean value $\langle S_l^z\rangle$ is the same for all ions in plane l, that is,

$$\langle S_l^z\rangle=\langle S_l^z\rangle , \quad (3)$$

where $l=0$ is the surface plane; $l=1$, the next inner plane and so on. For $l\geq 2$, we have also taken $\langle S_l^z\rangle=\langle S^z\rangle_b$, where $\langle S^z\rangle_b$ is the bulk magnetization per site.

We now introduce the Fourier transform of the Green's functions, $G(\mathbf{K}_\parallel,E)$, where the wave vectors $\mathbf{K}_\parallel$ belong to the two-dimensional Brillouin zone of a square lattice. It is easy to show that the Green's function can be determined by the following reduced matrix equation:

$$\underline{g}=\frac{1}{2\pi}T^{-1}\underline{\sigma} , \quad (4)$$

where T is given by

$$T=\begin{vmatrix} T_{00} & \sigma_0 & 0 & 0 & \cdots & & & \\ \sigma_1 & T_{11} & \sigma_1 & 0 & \cdots & & & \\ 0 & 1 & T_{22} & 1 & 0 & \cdots & & \\ 0 & 0 & 1 & 2t & 1 & 0 & \cdots & \\ 0 & 0 & 0 & 1 & 2t & 1 & 0 & \\ \vdots & \vdots & & & & & & \cdots \end{vmatrix} \quad (5)$$

with the following diagonal elements. If $i\geq 3$,

$$T_{ii}=2t=w-d-2-z(1-\gamma_{\mathbf{K}_\parallel}) , \quad (6)$$

otherwise

$$T_{22}=T_{33}+(1-\sigma_1) , \quad (7)$$

$$T_{11}=T_{33}+1+(1-\sigma_1)[d+z(1-\gamma_{\mathbf{K}_\parallel})] , \quad (8)$$

$$T_{00}=T_{33}+2+z[1-\sigma_0-\gamma_{\mathbf{K}_\parallel}(1-\sigma_0)]+(d-\sigma_0 d_s)-\sigma_1 . \quad (9)$$

We have also defined that

$$\sigma_l=\frac{\langle S_l^z\rangle}{\langle S^z\rangle_b} , \quad \underline{g}(\mathbf{K}_\parallel,w)=J\underline{G}(\mathbf{K}_\parallel,E) , \quad (10)$$

$$w=\frac{E}{2J\langle S^z\rangle_b} , \quad d=\frac{D}{J} , \quad d_S=\frac{D_S}{J} , \quad \tau=\frac{k_BT}{zSJ} , \quad (11)$$

and $\gamma_{\mathbf{k}_\parallel}=\frac{1}{2}[\cos(k_xa)+\cos(k_za)]$ is the structure factor for a square lattice ($z=4$) of spacing a.

Following the procedure outlined by Selzer and Majlis[1] to calculate the elements of T^{-1}, it is straightforward to show that

$$(T^{-1})_{00}=\cfrac{1}{T_{00}-\cfrac{\sigma_0\sigma_1}{T_{11}-\cfrac{\sigma_1}{T_{22}-\xi}}} , \quad (12)$$

$$(T^{-1})_{11}=\frac{1}{T_{11}-\dfrac{\sigma_0\sigma_1}{T_{00}}-\dfrac{\sigma_1}{T_{22}-\xi}} , \quad (13)$$

where

$$\xi+\xi^{-1}=2t . \quad (14)$$

From Eq. (4) we see that the poles of the Green's functions coincide with the roots of the det(T). The diagonal elements of $\underline{g}$ can be expressed as the ratio between two polynomials,

$$g_{ll}(\mathbf{K}_\parallel,\xi)=\frac{A_l(\mathbf{K}_\parallel,\xi)}{B(\mathbf{K}_\parallel,\xi)} , \quad (15)$$

where $B(\mathbf{K}_\parallel,\xi)$ is a fifth-degree polynomial which does not depend on l. The roots of Eq. (14), $\xi(t)$, are complex for $|t|<1$. In this case we can write that $t=-\cos(k_ya)$ and if we put this in Eq. (6), we obtain the bulk dispersion relation for the magnons. On the other hand, if $|t|>1$, the roots $\xi(t)$ will be real and only those for which $|\xi|<1$ will have a physical meaning. The spectrum of the surface magnons can be obtained from the real roots of $B(\mathbf{K}_\parallel,\xi_S)=0$, with $|\xi_S|<1$. The Eqs. (6) and (14) then give

$$w_S(\mathbf{K}_\parallel)=\xi_S+\xi_S^{-1}+d+2+z(1-\gamma_{\mathbf{K}_\parallel}) . \quad (16)$$

Meanwhile, in order to calculate the roots of $B(\mathbf{K}_\parallel,\xi)$, it is necessary to evaluate the layer magnetizations σ_0, σ_1 and the bulk magnetization $\langle S^z\rangle_b$. From the properties of the Green's functions[7] we can show that

$$\sigma_l=\frac{1}{\langle S^z\rangle_b}\frac{[S-\phi_l(S)][1+\phi_l(S)]^{2S+1}+[S+1+\phi_l(S)][\phi_l(S)]^{2S+1}}{[1+\phi_l(S)]^{2S+1}-[\phi_l(S)]^{2S+1}} , \quad (17)$$

where

$$\phi_l(S)=-\lim_{\varepsilon\to 0+}\left[\frac{a^2}{2\pi^3}\right]\int d\mathbf{K}_\parallel\left[\int_{-1}^{+1}dt\frac{\mathrm{Im}[T^{-1}(\mathbf{K}_\parallel,t+i\varepsilon)]_{ll}}{(e^{\beta E}-1)}+\frac{\pi}{2}\sum_\alpha\frac{A_l(\mathbf{K}_\parallel,\xi_\alpha)}{B'(\xi_\alpha)}\frac{(1-\xi_\alpha^2)}{\xi_\alpha^2(e^{\beta E}-1)}\right] , \quad (18)$$

ξ_α being the real roots of the polynomial $B(\xi)$ and $B'(\xi_\alpha)$ its derivative calculated at the point $\xi=\xi_\alpha$. We also remember that

$$E=2J\langle S^z\rangle_b w=2J\langle S^z\rangle_b[2t+d+2+z(1-\gamma_{\mathbf{K}_\parallel})] . \quad (19)$$

The bulk magnetization $\langle S^z\rangle_b$ is calculated for each value of the temperature from the equations:

$$\langle S^z\rangle_b=\frac{[S-\chi(S)][1+\chi(S)]^{2S+1}+[1+S+\chi(S)][\chi(S)]^{2S+1}}{[1+\chi(S)]^{2S+1}-[\chi(S)]^{2S+1}} , \quad (20)$$

where

$$\chi(S)=\frac{1}{N}\sum_{\mathbf{q}}(e^{\beta\varepsilon_{\mathbf{q}}}-1)^{-1} \quad (21)$$

and

$$\varepsilon_{\mathbf{q}}=2J\langle S^z\rangle_b[d+z(1-G_{\mathbf{q}})] \quad (22)$$

is the spectrum of the bulk magnons. Here the $\mathbf{q}$ values run over the first Brillouin zone of a simple cubic lattice ($z=6$) with structure factor $G_{\mathbf{q}}$. The sum in Eq. (21) was performed considering a set of 816 special points in the zone that can be obtained from the work of Chadi and Cohen.[8] Equations (17)–(19) can now be solved self-consistently for σ_0 and σ_1. The two-dimensional integrals over the Brillouin zone were evaluated through the special points of Cunningham.[9] In this way we are able to determine, for each value of the temperature, the bulk magnetization and the first- and second-layer magnetizations, as well as the spectrum of the bulk and surface magnons for a semi-infinite anisotropic Heisenberg ferromagnet.

III. RESULTS AND CONCLUSIONS

We present in Fig. 1 the spectrum of the surface and bulk magnons for several values of the temperature. [The reduced temperature τ defined by Eq. (11), appears through Bose factors in Eqs. (18) and (21).] For the values of the anisotropy parameters considered ($d=0.2$ and $d_S=0.2$) we show that the energies of the surface

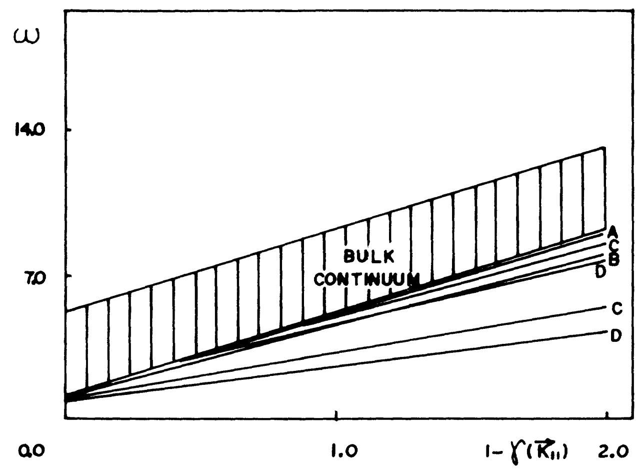

FIG. 1. Dispersion relations for surface and bulk magnons. The dashed region is the bulk continuum. The abcissa measures $1-\gamma_{\mathbf{k}_{\parallel}}$. The different curves correspond to $\tau_c^b=1.36$, A ($\tau=0.69$), B ($\tau=0.97$), C ($\tau=1.26$), D ($\tau=1.34$), all with $S=1$, $d=0.2$, $d_S=0.2$.

magnons are always smaller than the corresponding bulk ones for all temperatures τ below the bulk transition temperature (τ_c^b). We also note the unfolding of the spectrum of the surface magnons as we approach τ_c^b. Besides, one surface-magnon branch moves away from the continuum at large values of the wave vector.

In Fig. 2 we show the behavior of the spectrum of the surface and bulk magnons as a function of the surface anisotropy parameter d_S. The behavior presented is the same for whatever temperature below the bulk critical temperature. For small values of the parameter d_S the energy of the surface magnons is always smaller than the energy of the corresponding bulk magnons. In this case the bulk and the surface critical temperatures are the same. On the other hand, for d_S larger than a critical value (in our figure this value is around 0.50) the surface magnons have energies greater than those on the bulk continuum. For those values of the parameter d_S the surface is ordered even when the bulk is paramagnetic. For completeness we exhibit in Fig. 3 the reduced magnetization of the surface as a function of the temperature. The curve C, that corresponds to $d_S=1.0$, indicates that at τ_c^b, the surface magnetization is about 80% of this value at $T=0$. That is, the surface is still ferromagnetic while the bulk is in a paramagnetic state. Although we have not presented here the detailed calculations, the contribution of the next-nearest-neighbor exchange interactions does not change the main conclusions of this work. In a following paper[10] we shall give a detailed analysis of the surface magnons and the surface magnetization in the interesting region of temperatures above the bulk critical temperature for various values of the parameters D and D_S.

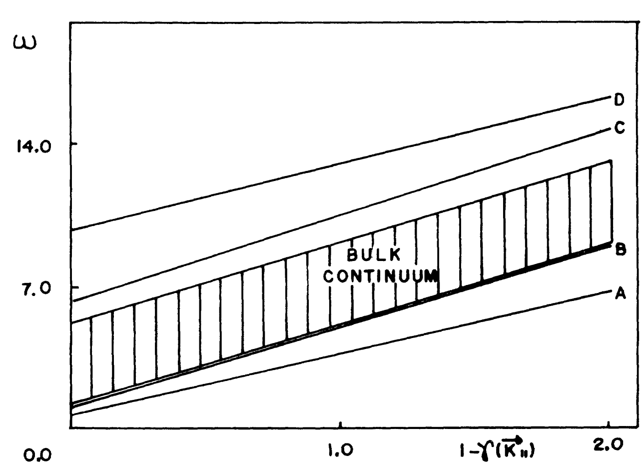

FIG. 2. Dispersion relations for surface and bulk magnons for different values of d_S. The dashed region represents the bulk continuum, the abcissa measures $1-\gamma_{\mathbf{k}_{\parallel}}$. The different curves correspond to A ($d_S=0.02$), B ($d_S=0.2$), C ($d_S=0.75$), and D ($d_S=1.0$), all with $S=1$, $d=0.2$, and $\tau=0.69$ ($\tau_c^b=1.36$).

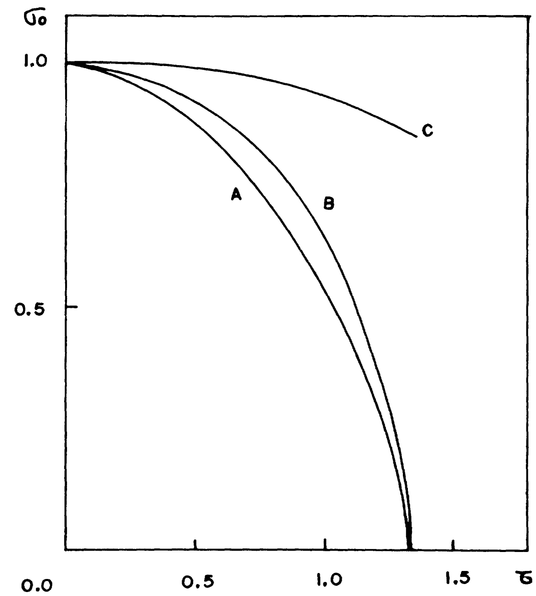

FIG. 3. Reduced magnetization of the surface plane as a function of the temperature. The different curves correspond to A ($d_S=0.02$), B ($d_S=0.2$), C ($d_S=1.0$), all with $S=1$, $d=0.2$, $\tau_c^b=1.36$.

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