Surface-enhanced magnetization for uniaxial ferromagnets

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We study the surface magnetic excitations for a semi-infinite anisotropic Heisenberg ferromagnet. We take a single-ion uniaxial anisotropy at the surface, which is different from that of the bulk. We determine the layer magnetization and the surface magnon modes in the region of temperatures above the bulk critical temperature. Our phase diagram presents the paramagnetic, the bulk-ferromagnetic, and the surface-ferromagnetic phases that join on a multicritical point. This point is determined as a function of the single-ion surface anisotropy parameter.

I. INTRODUCTION

In a recent paper[1] we have determined the layer magnetization and the surface magnons of a ferromagnet with single-ion uniaxial anisotropy in a semi-infinite cubic lattice. We have showed that the onset of the surface ordering occurs when the surface magnon modes start to become more energetic than any bulk mode.

In this paper we give a detailed analysis of the layer magnetization and the surface magnon modes in the region of temperatures above the bulk critical temperature. We determine the phase diagram that presents the paramagnetic (PM), the bulk-ferromagnetic (BFM), and the surface-ferromagnetic (SFM) phases. These three phases join on a multicritical point which is determined as a function of the single-ion surface anisotropy parameter. We also exhibit a diagram showing the behavior of the critical surface anisotropy parameter as a function of the corresponding bulk parameter. In Sec. II we present the model Hamiltonian and the calculations performed within the Green's-function formalism. In Sec. III the results obtained for the layer magnetization and for the phase diagram are discussed.

II. HAMILTONIAN MODEL AND CALCULATIONS

We consider, in what follows, the same model Hamiltonian on a semi-infinite simple-cubic lattice as in Ref. 1, i.e.,

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

where J represents the exchange interactions between spins which are nearest neighbors and $\tilde{D}$ is the single-ion uniaxial anisotropy due to the crystalline field. For the ions on the surface plane ($l=0$) we take $\tilde{D}=D_S$ and for the other ions, $\tilde{D}=D$. We choose the surface 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. First we write the equations of motion for the Fourier transform over time of the Green's function $\langle\langle S_1^+(t); S_m^-(t')\rangle\rangle$. Then, after employing the random-phase approximation, the system of equations can be solved. We have also assumed that the mean value $\langle S_1^z\rangle$ is the same for all ions in the plane l, that is,

$$\langle S_1^z\rangle=\langle S_l^z\rangle , \tag{2}$$

where $l=0$ stands for the surface plane, $l=1$, for the next inner plane, and so on. By considering that just after the second plane we reach the bulk ($l\geq 2$) it is easy to obtain the following expression for the Green's functions:

$$\underline{g}=\frac{1}{2\pi}T^{-1}\underline{\sigma} , \tag{3}$$

where

$$T=\begin{bmatrix} T_{00} & 0 & 0 & 0 & \cdots & \\ \sigma_1 & T_{11} & \sigma_1 & 0 & 0 & \\ 0 & 0 & T_{22} & 0 & 0 & \\ 0 & 0 & 0 & \nu & 0 & \\ 0 & 0 & 0 & 0 & \nu & 0\ldots \\ \vdots & \vdots & \vdots & \vdots & & \end{bmatrix} , \tag{4}$$

and we have the following diagonal elements:

$$T_{00}=\nu-\sigma_0[d_s+z(1-\gamma_{\mathbf{k}_\parallel})]-\sigma_1 , \tag{5}$$

$$T_{11}=\nu-\sigma_0-\sigma_1[d+z(1-\gamma_{\mathbf{k}_\parallel})] , \tag{6}$$

$$T_{22}=\nu-\sigma_1 . \tag{7}$$

We have also defined that

$$\sigma_l=\langle S_l^z\rangle,\quad \underline{g}(\mathbf{k}_\parallel,\nu)=J\underline{G}(\mathbf{k}_\parallel,E) , \tag{8}$$

$$\nu=\frac{E}{2J},\quad d=\frac{D}{J},\quad d_s=\frac{D_s}{J},\quad \tau=\frac{k_BT}{zSJ} , \tag{9}$$

and $\gamma_{\mathbf{k}_\parallel}=\frac{1}{2}[\cos(ak_x)+\cos(ak_z)]$ is the structure factor for a square lattice ($z=4$) of spacing a. In the preceding equations, the matrix $\underline{G}(\mathbf{k}_\parallel,E)$ is the Fourier transform of the Green's functions, and the wave vectors $\mathbf{k}_\parallel$ belong to the two-dimensional Brillouin zone of a square lattice. The simplicity of the matrix T is due to the fact that we have put $\langle S_l^z\rangle=0$ for $l\geq 2$, because we are interested in

magnetic surface excitations for temperatures greater than bulk critical temperature τ_c^b. We are interested in the values of the anisotropy parameter for which we could have σ_0 and σ_1, the magnetization of the first and second layers, respectively, different from zero for $\tau > \tau_c^b$.

In order to determine the layer magnetizations σ_0 and σ_1 for $\tau > \tau_c^b$ we need to calculate the matrix elements of T^{-1}. It is easy to show that

$$[T^{-1}(\mathbf{k}_\parallel,\nu)]_{ll} = \frac{N_l(\mathbf{k}_\parallel,\nu)}{D(\mathbf{k}_\parallel,\nu)} , \tag{10}$$

where

$$N_0(\mathbf{k}_\parallel,\nu) = T_{11}; \quad N_1(\mathbf{k}_\parallel,\nu) = T_{00} \tag{11}$$

and

$$D(\mathbf{k}_\parallel,\nu) = T_{11}\cdot T_{00} - \sigma_0\sigma_1 . \tag{12}$$

Finally, the expressions for the layer magnetizations can be calculated through the use of the Green's functions.[2,3] We obtain that

$$\sigma_l = \frac{[S-\phi_l(S)][1+\phi_l(S)]^{2S+1}+[1+S+\phi_l(S)][\phi_l(S)]^{2S+1}}{[1+\phi_l(S)]^{2S+1}-[\phi_l(S)]^{2S+1}} , \tag{13}$$

where

$$\phi_l(S) = \left[\frac{a}{2\pi}\right]^2 \int d\mathbf{k}_\parallel \frac{1}{(\nu_1-\nu_2)} \left[\frac{N_l(\mathbf{k}_\parallel,\nu_1)}{e^{2J\nu_1/k_BT}-1} - \frac{N_l(\mathbf{k}_\parallel,\nu_2)}{e^{2J\nu_2/k_BT}-1}\right] . \tag{14}$$

In Eq. (14), ν_1 and ν_2 are the roots of $D(\mathbf{k}_\parallel,\nu)$, that is, the spectrum of the surface magnons for temperatures greater than the bulk critical temperature. The two self-consistent equations (13) and (14) can now be solved for the two unknowns σ_0 and σ_1. We evaluated the two-dimensional integrals over the Brillouin zone through the special points of Cunningham.[4]

In this paper we have used the random-phase approximation in order to decouple our chain of equations for the Green's function. This approximation is widely employed in the study of the magnetic surface excitations (see Selzer and Majlis[5] and the references therein). Other approximations[3] could be used to break the chain of the Green's function, like the "Callen decoupling," but the problem would become very difficult to handle, and the results are essentially the same as in the RPA case, except at very low temperatures.

We would like to stress that we can get much information about the critical behavior of systems with free surfaces through the real-space renormalization-group method. As we will show in the next section, our results obtained through the Green's-function formalism and the RPA are very similar to the ones obtained by Mariz[6] *et al.* in the study of the critical properties of a Heisenberg model with anisotropic exchange interaction on a semi-infinite lattice. For a detailed discussion of the critical behavior of systems with free surfaces, we refer the formidable revision work by Binder.[7] In the next section we present the main results obtained for the surface magnetization and for the dispersion relations as a function of the temperature and of the single-ion surface anisotropy.

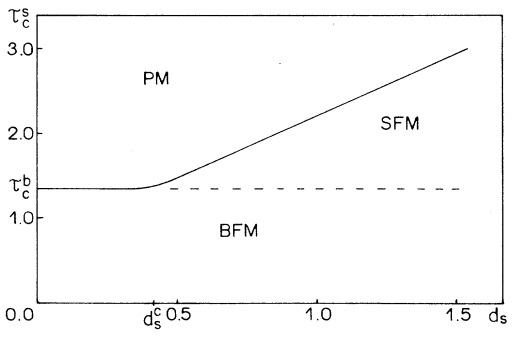

FIG. 1. Surface critical temperature (τ_c^s) as a function of the single-ion surface anisotropy parameter d_s. BFM, SFM, and PM, respectively, represent the bulk-ferromagnetic, surface-ferromagnetic, and paramagnetic phases. We have $S=1$, $d=0.2$, and τ_c^b is the bulk critical temperature.

III. RESULTS AND CONCLUSIONS

We have plotted in Fig. 1 the surface critical temperature ($\tau = k_BT/zSJ$) as a function of the single-ion surface anisotropy parameter ($d_s = DS/J$). We have chosen $S=1$ and $d=0.2$ in our calculations. The phase diagram obtained exhibits three distinct phases, namely: the paramagnetic, the surface ferromagnetic, and the bulk ferromagnetic. They meet at the multicritical point

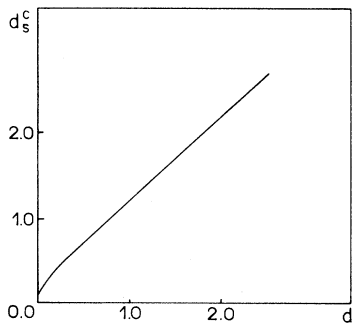

FIG. 2. Critical surface parameter d_s^c as a function of the bulk anisotropy parameter d for $S=1$.

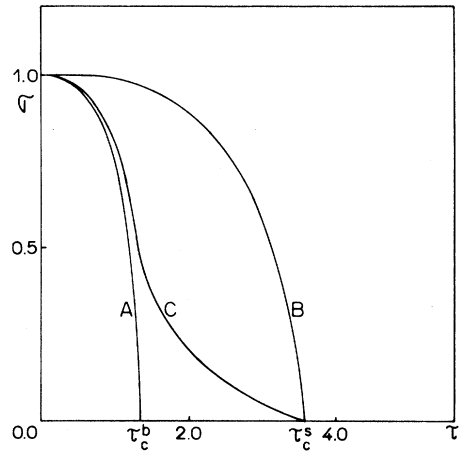

FIG. 3. Magnetization per spin (σ) as a function of the temperature. A, B, and C, respectively, represent the bulk, first layer, and second layer magnetizations. We have $S=1$, $d=0.2$, and $d_s=2.0$.

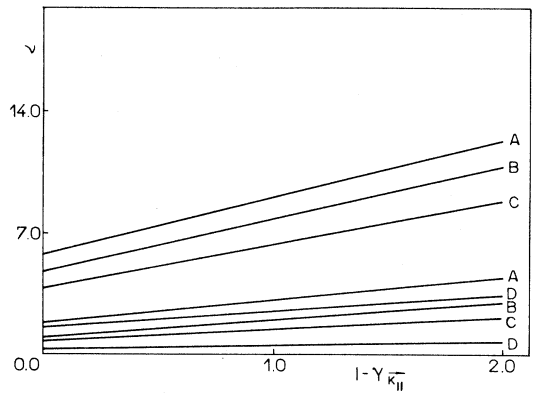

FIG. 4. Dispersion relation for surface magnons for different values of the temperature. The abscissa measures $1-\gamma_{k_\parallel}$. The different curves correspond to $A(\tau=1.38)$, $B(\tau=1.60)$, $C(\tau=1.80)$, and $D(\tau=2.10)$. We have $S=1$, $d=0.2$, $d_s=1.0$, $\tau_c^b=1.36$, and $\tau_c^s=2.18$.

$(d_s^c,\tau_c^b)\equiv(0.408,1.36)$. The value of d_s^c is defined as the particular value of d_s above which we can have surface ordering even for a paramagnetic bulk. For the values of d_s less than d_s^c, the bulk and surface critical temperatures, τ_c^b and τ_c^s, respectively, are identical. For this range of values of d_s we have employed the formalism given in Ref. 1.

In Fig. 2 we exhibit the behavior of the critical surface parameter d_s^c as a function of the corresponding bulk parameter d. It is interesting to observe the appearance of surface ordering even for an isotropic Heisenberg bulk ($d=0$). It is necessary to have a finite anisotropy parameter on the surface. This is to be expected because a completely isotropic Heisenberg model on the surface layer cannot sustain a spontaneous magnetization at a finite temperature.[8]

In Fig. 3 we show the behavior of the magnetization of the two first layers and of the bulk as a function of the temperature. For the chosen values, $d=0.2$ and $d_s=2.0$, the surface critical temperature is larger than twice the corresponding bulk temperature. The calculations for $\tau<\tau_c^b$ were performed using the formalism given in Ref. 1. Finally, in Fig. 4, we show the dispersion relations for the surface magnons for temperatures above the critical bulk temperature. We have found two branches for each value of the temperature and we note that they tend to disappear as we approach the surface critical temperature. Our results for ferromagnets with a finite uniaxial single-ion anisotropy at the surface are similar to those obtained for surface exchange anisotropy Heisenberg ferromagnets employing the Green's function with the RPA.[2] A detailed real-space renormalization-group calculation has been considered by Mariz[6] *et al.* to study the critical properties of a Heisenberg model with anisotropic exchange interactions on a semi-infinite lattice. Although our main objective in this work is not an accurate determination of the critical points, we would like to stress that our phase diagram, shown in Fig. 1, exhibits the same essential features presented in their phase diagram. For the parameters of Fig. 3, we have considered the calculations for three layers, that is, the bulk is attained in the fourth plane. The increase in the surface magnetization $\langle S_0^z\rangle$ when we pass from two to three independent planes is of 1%. This small increase on $\langle S_0^z\rangle$ is to be expected because with three independent planes the effective field on the first plane is slightly greater than using two independent planes. We believe that the main conclusions of this paper are not affected by these small differences.

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