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Proximity effects in magnetic interfaces

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The Green's-function method in the random-phase approximation is applied to calculate the magnetization of the (111) surface planes on both sides of an interface between two semi-infinite Heisenberg ferromagnets with a face-centered-cubic structure. Both bulk systems are chosen with anisotropic exchange interactions. When there is an appreciable difference in the transition temperatures of both sides, one finds that the stronger ferromagnet induces a permanent magnetization in the weaker one, which can be sustained at temperatures higher than the transition temperature of the latter. Several branches of surface magnons are also found.

I. INTRODUCTION

The current interest in interfaces, both from the basic and from the technological points of view, has stimulated the study of the properties of magnetic interfaces. Yaniv[1] has considered an interface between two simple-cubic Heisenberg ferromagnets. He obtained the excitation spectrum of the system at low temperatures and applied the results to obtain the transmission coefficient for propagating magnons.[2]

We study in this paper an interface between two semi-infinite fcc ferromagnets. We apply for this problem the Green's-function formalism in the random-phase approximation (RPA) to obtain the manetization profile and the dispersion relation for the magnons localized at the interface as a function of temperature.

Section II of the present paper contains the description of the formalism applied. In Sec. III we describe the results obtained. One interesting point is that, in general, *isotropic* bulk exchange interactions lead to surface instabilities, i.e., one acoustic surface-magnon branch turns negative at small $|\mathbf{k}_{\parallel}|$. The effect of such instability upon the ground state is obviously a problem in itself, but it is outside the scope of the present paper, so we have adopted a Hamiltonian with an exchange interaction exhibiting a uniaxial anisotropy for the bulk and on the surface planes which constitute the interface.

II. DESCRIPTION OF THE MODEL AND METHOD OF CALCULATION

It is customary to assume that the presence of the surface—or interface—does not perturb the translation invariance of the spin arrangement in the ground state along the surface plane or indeed along the whole family of planes parallel to the surface or interface.

This assumption might be cast in doubt if the surface instabilities mentioned in the Introduction were in fact present. Under such conditions, the magnetization of a certain number of planes near the surface may show a periodic oscillation along those planes.

Under the assumption that no instabilities arise, as would be the case if the anisotropy gap in the bulk spectrum were sufficiently wide, we can Fourier transform away the coordinates of the spin sites parallel to the interface in the equations for the Green matrix, thereby obtaining a RPA Hamiltonian which maps the original three-dimensional problem onto a one-dimensional model where the nondiagonal (on-site) interactions depend on $\mathbf{k}_{\parallel}$, the wave vector for propagation along the (111) planes.[3,4]

The Green's function in this mixed representation depends on $\mathbf{k}_{\parallel}$ and on the indices of the planes to which the corresponding spins belong, and it satisfies the equation:[3]

$$\underline{\Omega}\,\underline{G}=\underline{\sigma}\ , \tag{1}$$

where

$$\Omega_{im}(\omega,\mathbf{k}_{\parallel})=\left[\omega-2\sum_{l}\langle S_l^z\rangle\eta_{il}I_{il}(\mathbf{k}_{\parallel}=0)\right]\delta_{im}+2\langle S_i^z\rangle\sum_{l}I_{lm}(\mathbf{k}_{\parallel})\delta_{il} \tag{2}$$

and

$$\eta_{il}=\begin{cases}\eta_0 & \text{at the surface on the left}\\ \eta_{\bar{0}} & \text{at the surface on the right}\\ -\eta_1 & \text{in the bulk on the left}\\ \eta_2 & \text{in the bulk on the right .}\end{cases} \tag{3}$$

η_{il} is the exchange anisotropy parameter. When $\eta_{il}=1$, that pair has an isotropic exchange interaction. All pairs (i,l) are nearest-neighbor spins. For neighbors in the bulk, the exchange integrals I_{ij} have, respectively, values I_1 and I_2. We denote with index 0, quantities on the left surface, and with $\bar{0}$, those on the right surface. The quantities $I_{lm}(\mathbf{k}_{\parallel})$,

$$I_{i,i\pm1}(\mathbf{k}_{\parallel})=\begin{cases}3I_1\phi(\mathbf{k}_{\parallel}) & \text{on the left,}\ \ (i,i-1)\neq0\\ 3I_2\phi(\mathbf{k}_{\parallel}) & \text{on the right,}\ \ (i,i\pm1)\neq\bar{0}\ ,\end{cases} \tag{4}$$

where

$$\phi(\mathbf{k}_{\parallel})=\tfrac{1}{3}\{3+2[\cos2\pi(k_1-k_2)+\cos2\pi k_1+\cos2\pi k_2]\}^{1/2}\ . \tag{5}$$

$\mathbf{k}_{\parallel}$ is a wave vector contained in the first Brillouin zone (BZ) of the two-dimensional hexagonal surface k space:[1]

$$I_{00}(\mathbf{k}_{\parallel})=3I_1(3\phi^2-1)\ , \tag{6}$$

$$I_{\bar{0}\bar{0}}(\mathbf{k}_{\parallel})=3I_2(3\phi^2-1)\ . \tag{7}$$

The matrix $\underline{\sigma}$ is diagonal:

$$\sigma_{nn}=\begin{cases} \dfrac{\langle S_0^z\rangle}{\pi}, \quad n=0; \quad \langle S_{\bar{0}}^z\rangle, \quad n=\bar{0} \\ \dfrac{\langle S_n^z\rangle}{\pi}, \quad n>0; \quad \dfrac{\langle S_{\bar{n}}^z\rangle}{\pi}, \quad \bar{n}>\bar{0}\ . \end{cases} \tag{8}$$

$\langle \cdots \rangle$ denotes the thermodynamic average. We shall assume that for $n>0$,

$$\sigma_{nn}=\sigma_1\ , \qquad \sigma_{\bar{n}\bar{n}}=\sigma_2\ , \tag{9}$$

while σ_{00} and $\sigma_{\bar{0}\bar{0}}$ are to be determined self-consistently.

We assume for simplicity that

$$\begin{aligned} &\langle S_n^z\rangle \equiv S_1 \ \text{ bulk average on the left, for } n>0 \\ &\langle S_{\bar{n}}^z\rangle \equiv S_2 \ \text{ bulk average on the right, for } \bar{n}>\bar{0}\ , \end{aligned} \tag{10}$$

so that we calculate self-consistently only the magnetization on both surfaces 0 and $\bar{0}$, while that of all other planes to the right and left of the surface on both sides will be taken equal to the bulk equilibrium magnetization at the same temperature, which was previously evaluated also in the RPA for the bulk.[5]

We can separate the Hamiltonian into two parts:

$$\underline{H}=\underline{H}^0+\underline{V}\ , \tag{11}$$

where $\underline{H}^0$ contains only interactions between pairs of spins both on the right or on the left, and V only has elements in the subspace of two dimensions spanned by the planes 0 and $\bar{0}$, and in this subspace it can be written

$$\underline{V}=6I_{12}\begin{array}{cc} 0 & \bar{0} & \\ \left[\begin{array}{cc} \langle S_{\bar{0}}^z\rangle & -\phi\langle S_0^z\rangle \\ -\phi\langle S_{\bar{0}}^z\rangle & \langle S_0^z\rangle \end{array}\right. & \left|\begin{array}{c} 0 \\ \bar{0} \end{array}\right. \end{array}\ . \tag{12}$$

Let us introduce a matrix $\underline{U}$ such that

$$G_{jm}=\sum_s U_{js}\langle S_s^z\rangle\delta_{sm}\ . \tag{13}$$

Then,

$$\underline{\Omega}\,\underline{U}=\underline{1}/\pi\ . \tag{14}$$

Upon defining

$$\underline{\Omega}_0=\omega\underline{1}-\underline{H}^0\ , \tag{15}$$

we have

$$\underline{U}=\frac{1}{\pi}(1-\underline{\Omega}_0^{-1}\underline{V})^{-1}\underline{\Omega}_0^{-1}\ . \tag{16}$$

The matrix $\underline{U}^0$, being the inverse of $\omega\underline{1}-\underline{H}^0$ is deblocked in two parts, each one being the Greenian of the effective Hamiltonian $\underline{H}^0$ evaluated on the left or right spaces, respectively. The matrix $\underline{V}$ connects both blocks. Correspondingly, we can express the left and right blocks of $\underline{U}^0$ in terms of the well-known Green matrices for semi-infinite systems.[3]

It must be noticed that, according to Eq. (2), the matrix elements of $\underline{U}^0$ depend on the averages $\sigma_{00},\sigma_{\bar{0}\bar{0}}$ and these are evaluated self-consistently with both sides coupled so that the effective Hamiltonian can only be known after the whole problem has been solved.

We now define the dimensionless quantities

$$g^0=\frac{(U^0)_{00}}{2I_1S_1}\ , \tag{17}$$

$$d^0=\frac{(U^0)_{\bar{0}\bar{0}}}{2I_2S_2}\ . \tag{18}$$

We shall take for simplicity $I_1=I_2$. Then, we define $\epsilon_{12}=I_{12}/I$ and call

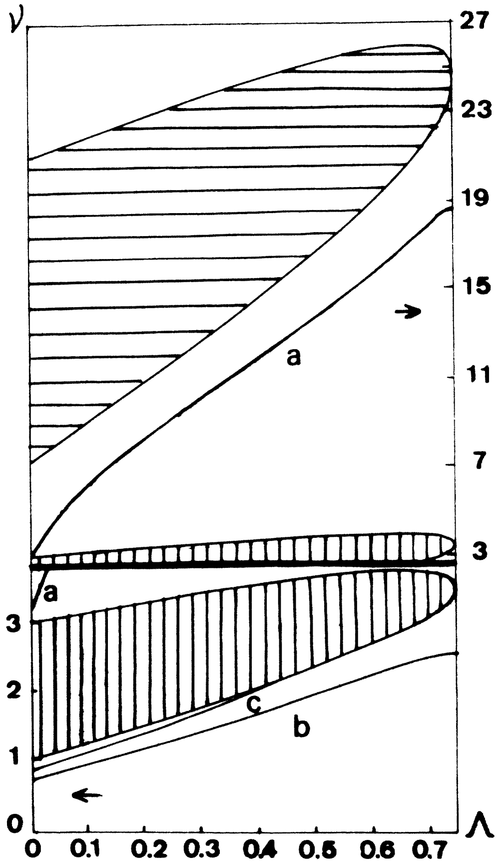

FIG. 1. Dispersion relations for the interface localized magnons. a, b, and c are interface modes. In the lower part of the figure below the thick horizontal line, frequencies ν (in units of $12\ I_1S_1$) are read on the left vertical scale, while in the upper part, the scale is on the right, as indicated by the arrows. The vertically hatched region is the lower continuum. The upper continuum is hatched horizontally. $\Lambda(\mathbf{k}_{\parallel})=\frac{3}{4}(1-\phi^2)$. $S_1=\frac{1}{2}$, $S_2=\frac{7}{2}$.

$$u_0=6\epsilon_{12}\sigma_{\bar{0}}\ ,\qquad v_0=6\epsilon_{12}\sigma_0 \tag{19}$$

and

$$u=\phi u_0\ ,\qquad v=\phi v_0\ . \tag{20}$$

In terms of these quantities, we write the diagonal elements of U as

$$U_{00}=g^0(1-g^0v_0)/D\ , \tag{21}$$

$$U_{\bar{0}\bar{0}}=d^0(1-d^0u_0)/D\ , \tag{22}$$

$$D=1-g^0u_0-d^0v_0+g^0d^0u_0v_0(1-\phi^2)\ , \tag{23}$$

so that the zeros of D are the poles of $\underline{U}$ and determine the frequencies of the localized modes. In order to obtain the magnetization of the two interface planes and the spectrum of the coupled system, we must solve self-consistently a system of two equations:[1,3]

$$\sigma_n=\frac{[s-\psi_n(s)][1+\psi_n(s)]^{2s+1}+[s+1+\psi_n(s)][\psi_n(s)]^{2s+1}}{[1+\psi_n(s)]^{2s+1}-[\psi_n(s)]^{2s+1}}\ , \tag{24}$$

where $\psi_n(s)$ is

$$\psi_n(s)=2\int_{-\infty}^{\infty}d\omega\frac{a^2}{4\pi^2}\int_{\mathrm{BZ}}d^2\mathbf{k}_{\parallel}\frac{\mathrm{Im}\,U_{nn}(\omega+i\epsilon,\mathbf{k}_{\parallel})}{\exp(\omega/kT)-1}\ , \tag{25}$$

with $n=0,\bar{0}$.

III. RESULTS AND DISCUSSIONS

In our example, we chose the strong (right) magnetic side with spin $\frac{7}{2}$ and the weak (left) one with spin $\frac{1}{2}$. The exchange integrals in the bulk on both sides were taken as equal: $I_1=I_2=I$. The ratio of the critical temperature of the right-hand side T_{c2} to that of the left-hand side T_{c1} is $T_{c2}/T_{c1}=21$. The coupling between both surfaces was taken as $I_{12}=\frac{1}{2}I$.

We chose the anisotropy constants n_{ij} equal in both bulk materials, with a value $\eta_b=1.5$ and its value on both surfaces as $\eta_s=1.2$, while the coupling between both sides was taken as isotropic, with $\eta_{0\bar{0}}=1$. There is a gap in the continuum of each side with a value

$$\Delta_\alpha=24I(\eta_b-1)S_\alpha,\quad \alpha=1,2\ .$$

In Fig. 1, we plot the limits of the continuum spectrum of each semi-infinite side and the surface magnon branches for $T=0.155$ in units where $T_{c1}=0.38$ and $T_{c2}=7.98$. Abscissas represent $\Lambda(\mathbf{k}_{\parallel})=\frac{3}{4}(1-\phi^2)$.

We find both acoustic and optic interface magnon branches. Abscissas represent $\Lambda(\mathbf{k}_{\parallel})$. $\Lambda=0$ is at the center of the two-dimensional Brillouin zone. $\Lambda=\frac{3}{4}$ is the zone edge. The thick horizontal line in the figure separates different ranges of frequencies. In the lower part, curve a, the optic magnon branch, starts at $\mathbf{k}_{\parallel}=0$, very near the upper bound of the lower continuum (hatched vertically in the figure) and it grows linearly. Curves b and c are acoustic-magnon branches. Above the horizontal line we plot the uppermost part of the lower continuum, the region of the upper continuum (horizontally hatched), and the whole of the optic magnon branch (curve a).

It is worth while to remark that the interface local modes differ from the simple-cubic (sc) case, wherein no acoustic branches are found. Yaniv[1] has already stressed that the absence of local magnon branches below the lower subband in the case he considered (sc structure) was specific to that case, and that such modes should be expected in a situation where bonds across the interface are nonperpendicular to it, as in the (111) interface in a fcc structure. Our results are in fact a confirmation of those remarks. An acoustic interface magnon branch had already been obtained[6] in a theoretical treatment of an interface produced by a stacking fault in a Heisenberg fcc ferromagnet.

As to the local magnetization, the range of temperatures considered, $0<T<T_{c1}$, does not allow for any noticeable change of the right-hand-side surface plane. On the other hand, in spite of the decrease of the bulk magnetization of the weaker ferromagnet, which tends to zero at $T\rightarrow T_{c1}$, we did not find any change of the left-hand surface either, so that $\langle S_0^z\rangle=\frac{1}{2}\hbar$ up to T_{c1}.

The main conclusion of our calculations is, therefore, that one should expect effects of induced magnetization at an interface, just as those that were found for a system of an anisotropic layer deposited on a semi-infinite isotropic Heisenberg ferromagnet.[4] We expect that similar processes could be found in superlattices consisting of different magnetic materials, and even that bulk magnetism could be induced in a superlattice where one of the materials is paramagnetic.

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