Surface spin waves and surface spin correlations in the presence of magnetic surface reconstruction*

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We examine the nature of surface spin waves in a ferromagnetic crystal for which the surface spin configuration is unstable with respect to ferromagnetic alignment. Magnetic surface reconstruction then occurs, and the spectrum of surface spin waves is found to differ qualitatively from the case where the spins align ferromagnetically. In particular, with the reconstructed phase, there is a surface-spin-wave branch with a dispersion relation $\Omega_s(k_\parallel)$ that approaches zero linearly with $k_\parallel$, as $k_\parallel$ vanishes. In the long-wavelength limit, the spin deviation associated with the mode is localized to the surface. While we consider only a simple model here, we argue that symmetry considerations lead to the existence of such modes whenever magnetic surface reconstruction occurs. We also examine the nature of spin fluctuations in the reconstructed state by studying the behavior of spin correlation functions for a two-dimensional layer of canted spins in a strong exchange field. Large-amplitude spin fluctuations occur in the presence of the low-frequency surface wave; these fluctuations are subdued by the presence of surface anisotropy fields.

I. INTRODUCTION

There is by now a considerable body of theoretical literature on the behavior of spins near the surface of Heisenberg ferromagnets.[1] Most of these analyses presume that the ferromagnetic arrangement of the spin array is present right up to the surface. In the more recent literature,[2–4] attention has focused on circumstances where the spin configuration in and near the surface may be unstable with respect to the ferromagnetic state. This may occur if the surface exchange differs in sign[5] from that in the bulk of the material, or if both ferromagnetic and antiferromagnetic exchange are present simultaneously, with ferromagnetism favored in the bulk. The latter situation occurs in many well-known magnetic crystals, and the former may prove of interest for an overlayer on a magnetic substrate, or if appreciable expansion of the lattice occurs near the surface.[6]

In a recent paper,[4] two of the present authors have explored the stability of the ground state of a semi-infinite fcc lattice of spins, and the dependence of the surface spin configuration on temperature and magnetic field was examined through use of mean-field theory. A similar study has been described recently by Castiel.[3] It was demonstrated for the semi-infinite fcc lattice with a (100) surface that when a surface instability occurs, the surface spins reorder into a new configuration with two sites in each unit cell of the spins in the outermost atomic layer. One has here the phenomenon of magnetic surface reconstruction, a spin analog of the well-known phenomenon of (crystallographic) surface reconstruction.[7]

The purpose of the present paper is to investigate the nature of surface spin waves in the presence of magnetic surface reconstruction. We confine our attention here to the simple model used earlier by Trullinger and Mills[2] in which only spins in the outer most atomic layer are unstable with respect to the ferromagnetic arrangement.

We find that in the presence of surface spin reconstruction, the surface spin wave spectrum differs qualitatively from the case where all spins align ferromagnetically. In particular, there is a surface mode with dispersion relation $\Omega_s(k_\parallel)$ that approaches zero linearly with $k_\parallel$. This is so when an external magnetic field H_0 is applied parallel to the bulk magnetization. In the semi-infinite ferromagnet (i.e., no surface magnetic reconstruction), in the presence of an external field, there is a Zeeman gap $g\mu_B H_0$, and all long-wavelength excitations including the surface spin waves have frequencies equal to or greater than $g\mu_B H_0$.[8]

This new mode, while described here in the context of an analysis of a simple model, is expected to be a general feature present in the surface spin wave spectrum whenever magnetic surface reconstruction occurs. The mode may be called a surface Goldstone mode; in the reconstructed state, its frequency approaches zero in the long-wavelength limit by virtue of a symmetry present in the system. The canted surface spin array may be rotated rigidly about the bulk magnetization, at no cost in energy. This symmetry is always present in both structures examined in Ref. 4, although it is only for the simple model examined here that the spin canting is confined to the outermost atomic layer. Also, since it is a symmetry argument that leads one to expect this mode to be a general feature of the problem, it is also clear that surface anisotropy fields (transverse to the bulk magnetization) present in all real materials will produce a gap in this surface spin wave branch.

If one considers the theory of crystallographic surface reconstruction, then there is no surface phonon analogous to the surface Goldstone mode just described, as long as the reconstructed configuration is commensurate with the underlying crystal structure. Thus, while in the present magnetic problem, we shall be led to conclude that there are large amplitude fluctuations in the reconstructed surface layer (in the absence of surface anisotropy fields of the type discussed below), there are no fluctuations similar to those discussed here, in the theory of crystallographic surface reconstruction.

In addition to presenting a study of the surface spin-wave dispersion relation in the reconstructed state, we also wish to examine the nature of spin fluctuations in the surface to assess the importance of the low-frequency surface waves. This is a difficult task for the semi-infinite solid. However, since we find that in the long-wavelength limit the spin deviation in the surface Goldstone mode is confined only to the outermost layer of spins, we may replace the semi-infinite solid by a simple two-dimensional layer of antiferromagnetically aligned spins, in a strong exchange field from the aligned bulk spins. For this picture we study the spin-correlation functions within the framework of spin-wave theory,[9] to find large amplitude fluctuations in the spin system which in fact diverge in amplitude in the absence of surface anisotropy fields. Even in the presence of such fields, the fluctuations in the surface of a magnet which experiences surface spin reconstruction may be expected, under some circumstances, to be enhanced substantially over the values appropriate to the bulk material. Thus, one conclusion we reach is that the phenomenon of surface spin reconstruction can be accompanied by large surface spin fluctuations, although the analysis here presents a rather crude study of them.

The outline of this paper is as follows. In Sec. II we present a study of surface spin waves in the model of a semi-infinite fcc ferromagnet used in Ref. 2 to obtain the dispersion relation in the presence of surface spin reconstruction. In Sec. III we examine within spin-wave theory spin-correlation functions for a two-dimensional layer of antiferromagnetically coupled spins placed in a strong exchange field. In Sec. IV we make some concluding observations.

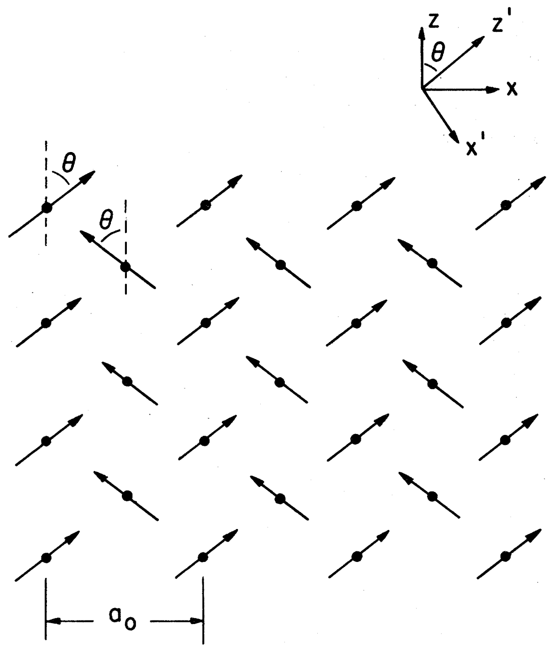

FIG. 1. Configuration of the spins in the outermost layer of the model crystal in the presence of magnetic surface reconstruction.

II. SURFACE SPIN WAVES IN A MODEL CRYSTAL WITH MAGNETIC SURFACE RECONSTRUCTION

As remarked in Sec. I, we consider here the nature of surface spin waves in a model of a semi-infinite magnetic material in which surface spin reconstruction occurs. The model is that examined in Ref. 2: we have a semi-infinite fcc lattice of spins with a (100) surface. The spins in the bulk of the material are coupled by nearest-neighbor Heisenberg-exchange interactions J, while the spins within the outermost layer are coupled by antiferromagnetic exchange J_s. The sign convention is such that $J_s > 0$. The geometry and choice of coordinate axes may be found in Fig. 1.

In Ref. 2 it was demonstrated that in the absence of an external magnetic field, if $J_s > \frac{1}{2}J$, then the spins in the outermost atomic layer are unstable with respect to the ferromagnetically aligned state. In the new ground state, the spins in the surface layer break up into two sublattices, each of which is canted at the angle θ relative to the bulk magnetization. The surface spin geometry is illustrated in Fig. 1. The spins in all the interior layers remain aligned, since in the presence of nearest-neighbor exchange only, no torque is exerted on interior spins by the realignment of the surface spins. This simple model is a special limiting case of the more general discussion of Ref. 4.

We wish to study the spin excitations of the above array, in the spin-wave limit. To do this we use the Holstein-Primakoff transformation to cast the Hamiltonian into a quadratic form in Boson annihilation and creation operators. For all interior layers, the standard procedure may be employed. The surface spins must be treated differently.

We divide the surface spins into an A and a B sublattice, and write for the A sites

$$\vec{S}(\vec{l}_A)=\hat{z}\,[\cos\theta\, S_{z'}(\vec{l}_A)-\sin\theta\, S_{x'}(\vec{l}_A)] + \hat{x}\,[\cos\theta\, S_{x'}(\vec{l}_A)+\sin\theta\, S_{z'}(\vec{l}_A)] + \hat{y}S_{y'}(\vec{l}_A)\ , \tag{2.1}$$

where $S_{x'}(\vec{l}_A)$, $S_{y'}(\vec{l}_A)$, and $S_{z'}(\vec{l}_A)$ are the Cartesian components of the spin $\vec{S}(\vec{l}_A)$ in a coordinate system aligned with the magnetization of the A sublattice. For the B spins, we write a form analogous to Eq. (2.1), with θ replaced by $-\theta$. Then the Holstein-Primakoff transformation is applied to the operators in the primed coordinate systems.

For the interior spins, since they remain ferromagnetically aligned, in principle one need not divide them into two sublattices. However, we find it convenient to use the magnetic unit cell appropriate to the outer reconstructed layer for each interior layer of spins. Thus, we divide each interior layer into an A and a B sublattice, even though the two spins in the unit cell are aligned paralled.

When the transformation to boson variables is carried out, if the angle θ is allowed to be general, then terms linear in the boson operators appear in the Hamiltonian. If $a(l_x,0,l_z)$ and $b(l_x,0,l_z)$ denote the boson annihilation operators for A and B spins in the surface layer ($l_y=0$), we find the linear terms have the form

$$H^{(1)}=(1/\sqrt{2})\,S^{1/2}\,[4SJ_s\sin 2\theta-(4JS+g\mu_BH_0)\sin\theta] \times\Big(\sum_{\vec{l}_B}[b(l_x,0,l_z)+b^\dagger(l_x,0,l_z)] - \sum_{\vec{l}_A}[a(l_x,0,l_z)+a^\dagger(l_x,0,l_z)]\Big)\ , \tag{2.2}$$

We have presumed a uniform external magnetic field H_0 is applied parallel to the bulk magnetization.

For the configuration of the surface spins to be a stable equilibrium configuration, one requires the linear times to vanish. Thus, we have

$$\sin\theta(4JS+g\mu_BH_0-8J_sS\cos\theta)=0\ , \tag{2.3}$$

and if $J_s^{(c)}=\frac{1}{2}J+g\mu_BH_0/8S$, the equilibrium configuration of the surface spins has

$$\theta=\begin{cases}0\ , & J_s<J_s^{(c)}\\ \cos^{-1}(J_s^{(c)}/J_s)\ , & J_s>J_s^{(c)}\end{cases}\ . \tag{2.4}$$

The analysis below applies to either the case $J_s \le J_s^{(c)}$ or the case $J_s>J_s^{(c)}$, although it is the second case of primary interest here.

For the quadratic terms, we Fourier transform the two spatial coordinates parallel to the surface by writing

$$a_{\vec{k}_\parallel}(l_y)=\frac{1}{\sqrt{N_s}}\sum_{l_xl_z} e^{+i\vec{k}_\parallel\cdot\vec{l}_\parallel}a(\vec{l}_A)\ , \tag{2.5a}$$

$$a^\dagger_{\vec{k}_\parallel}(l_y)=\frac{1}{\sqrt{N_s}}\ {}_{l_xl_z}\ e^{-i\vec{k}_\parallel\cdot\vec{l}_\parallel}a^\dagger(\vec{l}_A)\ , \tag{2.5b}$$

with a similar transformation for the B operators. Here N_s is the number of magnetic unit cells in a given layer of spins.

The quadratic terms in the Hamiltonian may then be broken down into the following arrangement of terms: (i) terms which couple only spins within the surface layer:

$$H(00)=(g\mu_BH_0\cos\theta-4J_sS\cos 2\theta+4SJ\cos\theta)\sum_{\vec{k}_\parallel}[b^\dagger_{\vec{k}_\parallel}(0)\,b_{\vec{k}_\parallel}(0)+a^\dagger_{\vec{k}_\parallel}(0)a_{\vec{k}_\parallel}(0)] + 4SJ_s\cos^2\theta\sum_{\vec{k}_\parallel}\gamma(\vec{k}_\parallel)\,[a^\dagger_{\vec{k}_\parallel}(0)\,b_{\vec{k}_\parallel}(0)+\text{H.c.}]-4SJ_s\sin^2\theta\sum_{\vec{k}_\parallel}\gamma(\vec{k}_\parallel)[a^\dagger_{\vec{k}_\parallel}(0)b^\dagger_{-\vec{k}_\parallel}(0)+\text{H.c.}]\ . \tag{2.6a}$$

(ii)Terms which couple surface spins ($l_y=0$) to spins in the first interior layer ($l_y=1$):

$$H(01)=-2SJ\cos^2\frac{\theta}{2}\sum_{\vec{k}_\parallel}\gamma_z(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(1)\,a^\dagger_{\vec{k}_\parallel}(0)+b_{\vec{k}_\parallel}(1)\,b^\dagger_{\vec{k}_\parallel}(0)+\text{H.c.}] - 2SJ\cos^2\frac{\theta}{2}\sum_{\vec{k}_\parallel}\gamma_x(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(1)\,b^\dagger_{\vec{k}_\parallel}(0)+b_{\vec{k}_\parallel}(1)\,a^\dagger_{\vec{k}_\parallel}(0)+\text{H.c.}] + 2SJ\sin^2\frac{\theta}{2}\sum_{\vec{k}_\parallel}\gamma_z(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(1)\,a_{-\vec{k}_\parallel}(0)+b_{\vec{k}_\parallel}(1)\,b_{-\vec{k}_\parallel}(0)+\text{H.c.}]+2SJ\sin^2\frac{\theta}{2}\sum_{\vec{k}_\parallel}\gamma_x(\vec{k}_\parallel)[b_{\vec{k}_\parallel}(1)\,a_{-\vec{k}_\parallel}(1)\,b_{-\vec{k}_\parallel}(0)+\text{H.c.}]\ . \tag{2.6b}$$

(iii) Terms which involve operators for spins in layer $l_y=1$:

$$H(1,1)=(g\mu_B H_0+8SJ+4SJ\cos\theta)\sum_{\vec{k}_\parallel}[a^\dagger_{\vec{k}_\parallel}(1)\,a_{\vec{k}_\parallel}(1)+b^\dagger_{\vec{k}_\parallel}(1)\,b_{\vec{k}_\parallel}(1)]-4SJ\sum_{\vec{k}_\parallel}\gamma(\vec{k}_\parallel)[a^\dagger_{\vec{k}_\parallel}(1)\,b_{\vec{k}_\parallel}(1)+\text{H.c.}]\ . \qquad (2.6c)$$

(iv) Terms which involve operators in layers $l_y\geq 2$:

$$\begin{aligned}H_B=&(g\mu_B H_0+12SJ)\sum_{l=2}^{\infty}\sum_{\vec{k}_\parallel}[a^\dagger_{\vec{k}_\parallel}(l)\,a_{\vec{k}_\parallel}(l)+b^\dagger_{\vec{k}_\parallel}(l)\,b_{\vec{k}_\parallel}(l)]-4SJ\sum_{l=2}^{\infty}\sum_{\vec{k}_\parallel}\gamma(\vec{k}_\parallel)[a^\dagger_{\vec{k}_\parallel}(l)\,b_{\vec{k}_\parallel}(l)+\text{H.c.}]\\&-2SJ\sum_{l=2}^{\infty}\sum_{\vec{k}_\parallel}\gamma_z(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(l)\,a^\dagger_{\vec{k}_\parallel}(l-1)+b_{\vec{k}_\parallel}(l)\,b^\dagger_{\vec{k}_\parallel}(l-1)+\text{H.c.}]\\&-2SJ\sum_{l=2}^{\infty}\sum_{\vec{k}_\parallel}\gamma_x(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(l)\,b^\dagger_{\vec{k}_\parallel}(l-1)+b_{\vec{k}_\parallel}(l)\,a^\dagger_{\vec{k}_\parallel}(l-1)+\text{H.c.}]\ .\end{aligned} \qquad (2.6d)$$

In these expressions,

$$\gamma_x(\vec{k}_\parallel)=\cos(\tfrac{1}{2}a_0k_x)\ , \qquad (2.7a)$$

$$\gamma_z(\vec{k}_\parallel)=\cos(\tfrac{1}{2}a_0k_z)\ , \qquad (2.7b)$$

$$\gamma(\vec{k}_\parallel)=\gamma_x(\vec{k}_\parallel)\gamma_z(\vec{k}_\parallel)\ . \qquad (2.7c)$$

From the boson Hamiltonian displayed above, we form the equations of motion for the various operators. Again, this is a standard procedure. To find the spin-wave frequencies of the system, one seeks solutions with the time dependence

$$a_{\vec{k}_\parallel}(l,t)=a_{\vec{k}_\parallel}(l)e^{-i\Omega t}\ , \qquad (2.8a)$$

$$a^\dagger_{\vec{k}_\parallel}(l,t)=a^\dagger_{-\vec{k}_\parallel}(l)e^{-i\Omega t}\ , \qquad (2.8b)$$

and similarly for $b_{\vec{k}_\parallel}(l,t)$ and $b^\dagger_{-\vec{k}_\parallel}(l,t)$.

For the operator $a_{\vec{k}_\parallel}(l)$, when $l\geq 2$ we find

$$\begin{aligned}\Omega a_{\vec{k}_\parallel}(l)=&(g\mu_B H_0+12SJ)a_{\vec{k}_\parallel}(l)-4SJ\gamma(\vec{k}_\parallel)\,b_{\vec{k}_\parallel}(l)\\&-2SJ\gamma_z(\vec{k}_\parallel)[a_{\vec{k}_\parallel}(l+1)+a_{\vec{k}_\parallel}(l-1)]\\&-2SJ\gamma_x(\vec{k}_\parallel)[b_{\vec{k}_\parallel}(l+1)+b_{\vec{k}_\parallel}(l-1)]\ .\end{aligned} \qquad (2.9)$$

For $l\geq 2$, the equation of motion for $b_{\vec{k}_\parallel}(l)$ is the same as Eq. (2.9), except $b_{\vec{k}_\parallel}(l)$ and $a_{\vec{k}_\parallel}(l)$ are everywhere interchanged. The equations of motion for $a^\dagger_{-\vec{k}_\parallel}(l)$ and $b^\dagger_{-\vec{k}_\parallel}(l)$ may be found by making the replacements

$$a_{\vec{k}_\parallel}(l)\rightarrow a^\dagger_{-\vec{k}_\parallel}(l)\ , \qquad (2.10a)$$

$$b_{\vec{k}_\parallel}(l)\rightarrow b_{-\vec{k}_\parallel}(l)\ , \qquad (2.10b)$$

$$\Omega\rightarrow-\Omega \qquad (2.10c)$$

everywhere in the equations of motion for $a_{\vec{k}_\parallel}(l)$ and $b_{\vec{k}_\parallel}(l)$.

Note that for $l\geq 2$, there are no terms which couple the annihilation operators to the creation operators. This will not be true for $l=0$ and $l=1$. The equations of motion for the $l=0$ and $l=1$ operators will be written down shortly. To search for surface spin waves, we shall seek solutions of the system of equations in the form

$$a_{\vec{k}_\parallel}(l)=\begin{cases}a_{\vec{k}_\parallel}(0)\,, & l=0\\ a_{\vec{k}_\parallel}(1)\,e^{-Q(l-1)}\,, & l\geq 1\end{cases} \qquad (2.11a)$$

$$a^\dagger_{-\vec{k}_\parallel}(l)=\begin{cases}a^\dagger_{-\vec{k}_\parallel}(0), & l=0\\ a^\dagger_{-\vec{k}_\parallel}(1)\,e^{-\tilde{Q}(l-1)}, & l\geq 1\,.\end{cases} \qquad (2.11b)$$

Expressions for Q and $\tilde{Q}$ may be found by inserting Eqs. (2.11a) and (2.11b) into the equations of motion for the operators for layers with $l\geq 2$. When this is done, for a given frequency and given value of $\vec{k}_\parallel$, one finds two allowed values of Q, and two allowed values of $\tilde{Q}$. We call these $Q_\pm$ and $\tilde{Q}_\pm$, where

$$\cosh Q_\pm=(h+3\mathcal{J}\pm\gamma\mathcal{J}-\Omega)/\mathcal{J}(\gamma_z\mp\gamma_x) \qquad (2.12a)$$

and

$$\cosh\tilde{Q}_\pm=(h+3\mathcal{J}\pm\gamma\mathcal{J}+\Omega)/\mathcal{J}(\gamma_z\mp\gamma_x)\ . \qquad (2.12b)$$

We have introduced the abbreviations $\mathcal{J}=4JS$, $H=g\mu_B H_0$, and explicit reference to $\vec{k}_\parallel$ is dropped from $\gamma(\vec{k}_\parallel)$, $\gamma_x(\vec{k}_\parallel)$, and $\gamma_z(\vec{k}_\parallel)$.

To satisfy the equations of motion for $l=0$ and $l=1$, solutions with each allowed value of Q and each allowed value of $\tilde{Q}$ must be superimposed for $l\geq 1$. The bulk equations ($l\geq 2$) require the solutions to have the form

$$a_{\vec{k}_\parallel}(l)=a_{\vec{k}_\parallel}(1+)e^{-Q_+(l-1)}+a_{\vec{k}_\parallel}(1-)e^{-Q_-(l-1)}\ , \qquad (2.13a)$$

$$b_{\vec{k}_\parallel}(l)=-a_{\vec{k}_\parallel}(1+)e^{-Q_+(l-1)}+a_{\vec{k}_\parallel}(1-)e^{-Q_-(l-1)}\ , \qquad (2.13b)$$

$$a^\dagger_{-\vec{k}_\parallel}(l)=a^\dagger_{-\vec{k}_\parallel}(1+)e^{-\tilde{Q}_+(l-1)}+a^\dagger_{-\vec{k}_\parallel}(1-)e^{-\tilde{Q}_-(l-1)}\ , \qquad (2.13c)$$

$$b^\dagger_{-\vec{k}_\parallel}(l)=-a^\dagger_{-\vec{k}_\parallel}(1+)e^{-\tilde{Q}_+(l-1)}+a^\dagger_{-\vec{k}_\parallel}(1-)e^{-\tilde{Q}_-(l-1)}\ . \qquad (2.13d)$$

That is to say, the bulk equations lead to the requirements

$$b_{\vec{k}_\parallel}(1\pm) = \mp a_{\vec{k}_\parallel}(1\pm) \ , \quad (2.14a)$$

$$b^\dagger_{-\vec{k}_\parallel}(1\pm) = \mp a^\dagger_{-\vec{k}_\parallel}(1\pm) \ . \quad (2.14b)$$

In the interest of brevity, we present only a summary of the lengthy manipulations of the equations of motion for layers $l=1$ and $l=0$. For example, when the equation for $a_{\vec{k}_\parallel}(1)$ is written down, after some manipulation with the formulas in Eq. (2.13a), the result may be written

$$(2\sin^2\tfrac{1}{2}\theta - \gamma_- e^{+Q_+})a_{\vec{k}_\parallel}(1+) + (2\sin^2\tfrac{1}{2}\theta - \gamma_+ e^{+Q_-})a_{\vec{k}_\parallel}(1-) + \tfrac{1}{2}\gamma_z\cos^2\tfrac{1}{2}\theta\, a_{\vec{k}_\parallel}(0) + \tfrac{1}{2}\gamma_x\cos^2\tfrac{1}{2}\theta\, b_{\vec{k}_\parallel}(0) - \tfrac{1}{2}\gamma_z\sin^2\tfrac{1}{2}\theta\, a^\dagger_{-\vec{k}_\parallel}(0) - \tfrac{1}{2}\gamma_x\sin^2\tfrac{1}{2}\theta\, b^\dagger_{-\vec{k}_\parallel}(0) = 0 \ , \quad (2.15)$$

with three similar equations formed from the equation of motion for $b_{\vec{k}_\parallel}(1)$, and $b^\dagger_{-\vec{k}_\parallel}(1)$. We have introduced

$$\gamma_\pm = \tfrac{1}{2}(\gamma_z \pm \gamma_x) \ . \quad (2.16)$$

From the four equations for the layer $l=1$, expressions may be obtained for the four amplitudes $a_{\vec{k}_\parallel}(1+)$, $a_{\vec{k}_\parallel}(1-)$, $a^\dagger_{-\vec{k}_\parallel}(1+)$, and $a^\dagger_{-\vec{k}_\parallel}(1-)$ in terms of the four variables $a_{\vec{k}_\parallel}(0)$, etc., that describe the spin motion in the outermost layer $l=0$. Finally, in the equations of motion for the operators with $l=0$, all operators that refer to layers other than $l=0$ may be now eliminated, to find four equations which involve only $a_{\vec{k}_\parallel}(0)$, $b_{\vec{k}_\parallel}(0)$, $a^\dagger_{-\vec{k}_\parallel}(0)$, and $b^\dagger_{-\vec{k}_\parallel}(0)$. The last step is to break these four surface equations into two sets of equations decoupled from each other through use of the transformation

$$A^{(+)}_{\vec{k}_\parallel} = a_{\vec{k}_\parallel}(0) + b_{\vec{k}_\parallel}(0) \ , \quad (2.17a)$$

$$A^{(-)}_{\vec{k}_\parallel} = a_{\vec{k}_\parallel}(0) - b_{\vec{k}_\parallel}(0) \ , \quad (2.17b)$$

$$\tilde{A}^{(+)}_{\vec{k}_\parallel} = a^\dagger_{-\vec{k}_\parallel}(0) + b^\dagger_{-\vec{k}_\parallel}(0) \ , \quad (2.17c)$$

$$\tilde{A}^{(-)}_{\vec{k}_\parallel} = a^\dagger_{-\vec{k}_\parallel}(0) - b^\dagger_{-\vec{k}_\parallel}(0) \ . \quad (2.17d)$$

The final set of equations has the form

$$(\Omega - \alpha^{(+)} - \cos^4\tfrac{1}{2}\theta\, g_1^{(+)} - \sin^4\tfrac{1}{2}\theta\, g_2^{(+)})A^{(+)}_{\vec{k}_\parallel} + [\beta + \sin^2\tfrac{1}{2}\theta\cos^2\tfrac{1}{2}\theta(g_1^{(+)} + g_2^{(+)})]\tilde{A}^{(+)}_{\vec{k}_\parallel} = 0, \quad (2.18a)$$

$$-[\beta + \sin^2\tfrac{1}{2}\theta\cos^2\tfrac{1}{2}\theta(g_1^{(+)} + g_2^{(+)})]A^{(+)}_{\vec{k}_\parallel} + (\Omega + \alpha^{(+)} + \sin^4\tfrac{1}{2}\theta\, g_1^{(+)} + \cos^4\tfrac{1}{2}\theta\, g_2^{(+)})\tilde{A}^{(+)}_{\vec{k}_\parallel} = 0, \quad (2.18b)$$

$$(\Omega - \alpha^{(-)} - \cos^4\tfrac{1}{2}\theta\, g_1^{(-)} - \sin^4\tfrac{1}{2}\theta\, g_2^{(-)})A^{(-)}_{\vec{k}_\parallel} - [\beta - \sin^2\tfrac{1}{2}\theta\cos^2\tfrac{1}{2}\theta(g_1^{(-)} + g_2^{(-)})]\tilde{A}^{(-)}_{\vec{k}_\parallel} = 0, \quad (2.19a)$$

$$[\beta - \sin^2\tfrac{1}{2}\theta\cos^2\tfrac{1}{2}\theta(g_1^{(-)} + g_2^{(-)})]A^{(-)}_{\vec{k}_\parallel} + (\Omega + \alpha^{(-)} + \sin^4\tfrac{1}{2}\theta\, g_1^{(-)} + \cos^4\tfrac{1}{2}\theta\, g_2^{(-)})\tilde{A}^{(-)}_{\vec{k}_\parallel} = 0. \quad (2.19b)$$

In these expressions, we have introduced

$$\alpha^{(\pm)} = (h + \mathcal{J})\cos\theta - \mathcal{J}_s\cos 2\theta \pm \gamma\mathcal{J}_s\cos^2\theta \ , \quad (2.20)$$

$$\beta = \gamma\mathcal{J}_s\sin^2\theta \ , \quad (2.21)$$

$$g_1^{(\pm)} = \mathcal{J}\gamma_\pm^2/(2\sin^2\tfrac{1}{2}\theta - \gamma_\pm e^{Q_\mp}) \ , \quad (2.22)$$

$$g_2^{(\pm)} = \mathcal{J}\gamma_\pm^2/(2\sin^2\tfrac{1}{2}\theta - \gamma_\pm e^{\tilde{Q}_\mp}) \ , \quad (2.23)$$

where $\mathcal{J}_s = 4J_sS$.

The remainder of this section will be devoted to exploration of the solutions of Eqs. (2.18) and (2.19). To find the surface spin-wave frequencies, one picks a value of $\vec{k}_\parallel$ in the Brillouin zone of the *reconstructed* surface spin layer, and searches for frequencies where either of the 2×2 determinants vanishes. Before we proceed with a description of these solutions for the general case, we look at two special examples.

A. Case $\theta = 0$ (no surface spin reconstruction)

If the antiferromagnetic surface exchange J_s is less than the critical value $J_s^{(c)}$ required for magnetic surface reconstruction to occur, then from Eq. (2.4) we have $\theta=0$; the spins in the surface aligned ferromagnetically, with moment parallel to the bulk spins. Then Eqs. (2.18) and (2.19) may be solved trivially. For each $\vec{k}_\parallel$, there are two positive frequency solutions we denote by $\Omega_+(\vec{k}_\parallel)$ and $\Omega_-(\vec{k}_\parallel)$. These are

$$\Omega_\mp(\vec{k}_\parallel) = h + \mathcal{J} - \mathcal{J}_s[1 \pm \gamma(\vec{k}_\parallel)] - \frac{\mathcal{J}\gamma_\pm^2(\vec{k}_\parallel)}{1 + (1 + \mathcal{J}_s/\mathcal{J})[1 \pm \gamma(\vec{k}_\parallel)]} \ . \quad (2.24)$$

The mode Ω_+ emerges from Eqs. (2.18), while that labeled Ω_- emerges from Eqs. (2.19).

This dispersion relation in Eq. (2.24) is identical to that which forms the basis of the earlier discussion by Trullinger and Mills.[2] To see the equivalence of the two forms, one must first note that in the present work, the orientation of the two coordinate axes parallel to the surface (the y and the z axes) differs by 45° from the axes used in Ref. 2. Also, we use here the Brillouin zone appropriate to the reconstructed surface spin configuration, while Ref. 2 uses that for the unreconstructed one. This is why we obtain two distinct branches, while only a single branch is described in Ref. 2;

our Ω_- branch is a portion of the dispersion relation of the single branch folded back into a smaller Brillouin zone. The two Brillouin zones are illustrated in Fig. 2. Because the dispersion relation is examined in Ref. 2, we do not comment in detail here.

B. Two-dimensional surface spin layer

The terms in Eqs. (2.18) and (2.19) which involve g_1 and g_2 have their physical origin in the motion of the interior spins (layers with $l \geq 1$), which feeds back to affect the motion of the spins in the surface layer. If we set $g_1 = g_2 = 0$, then the dispersion relation becomes that of a two-dimensional layer of spins (the surface spins) which are excited, and the only role of the interior spins is to provide a fixed exchange field within which the surface spins precess. The presence of the exchange field from the surface spins enters through the factor of $\mathcal{J}$ which enters the definition of α.

If we set $g_1 = g_2 = 0$ to obtain the approximate description of the surface spin dynamics just described then we find the two-branch dispersion relation (assume $\theta \neq 0$)

$$\Omega_\pm(\vec{k}_\parallel) = \mathcal{J}_s[1 \pm \gamma(\vec{k}_\parallel)]^{1/2}[1 \pm \gamma(\vec{k}_\parallel)\cos 2\theta]^{1/2}. \tag{2.25}$$

Once again, the mode labeled "+" emerges from Eqs. (2.18) while the labeled "−" emerges from Eqs. (2.19). In this expression, we have eliminated h and $\mathcal{J}$ in favor of $\mathcal{J}_s$ through use of Eq. (2.3).

In the limit $\vec{k}_\parallel \to 0$, we have

$$\gamma(\vec{k}_\parallel) \cong 1 - \tfrac{1}{8}a_0^2 k_\parallel^2 + \cdots, \tag{2.26}$$

so we have in the long-wavelength limit

$$\Omega_-(k_\parallel) = \tfrac{1}{2}\mathcal{J}_s a_0 k_\parallel[\sin^2\theta + \tfrac{1}{16}\cos 2\theta(a_0 k_\parallel)^2]^{1/2} \tag{2.27a}$$

and

$$\Omega_+(k_\parallel) = 2\mathcal{J}_s \cos\theta[1 + O((k_\parallel a_0)^2)]. \tag{2.27b}$$

Note that as $k_\parallel \to 0$, the frequency of the lower branch vanishes linearly with $k_\parallel$. This is the case even when the Zeeman field H_0 is present. From a physical point of view, this mode has vanishing frequency as $k_\parallel \to 0$ because the two canted sublattices may be rigidly rotated about the bulk magnetization (always keeping the two sublattices in the same plane) with no cost in energy. There is a symmetry operation present for the reconstructed surface spin configuration that is absent when no surface spin reconstruction occurs. The $\Omega_-(\vec{k}_\parallel)$ mode displayed in Eq. (2.25) is the "surface Goldstone mode" described in Sec. I.

Of course, the discussion above is based on the presumption that we may set g_1 and g_2 equal to zero, to obtain a surface spin wave confined entirely to the reconstructed surface layer. We shall shall see shortly that this procedure is justifiable, in the long-wave length limit.

We next turn to a study of the full equations (2.18) and (2.19).

In Fig. 3(a), we show the $\Omega_+(\vec{k}_\parallel)$ and $\Omega_-(\vec{k}_\parallel)$ curves for $h = 0.3\mathcal{J}$ and $\mathcal{J}_s = 0.6\mathcal{J}$, in the direction $k_z = 0$. For these parameters, $\mathcal{J}_s$ is small enough that $\theta = 0$, and no surface spin reconstruction occurs. Note that both $\Omega_+(\vec{k}_\parallel)$ and $\Omega_-(\vec{k}_\parallel)$ are finite and nonzero for $\vec{k}_\parallel = 0$. In Fig. 3(b), we show the dispersion curves when $\mathcal{J}_s = 0.65\mathcal{J}$, and again $h = 0.3\mathcal{J}$. For this value of h, the value of $\mathcal{J}_s$ is the critical

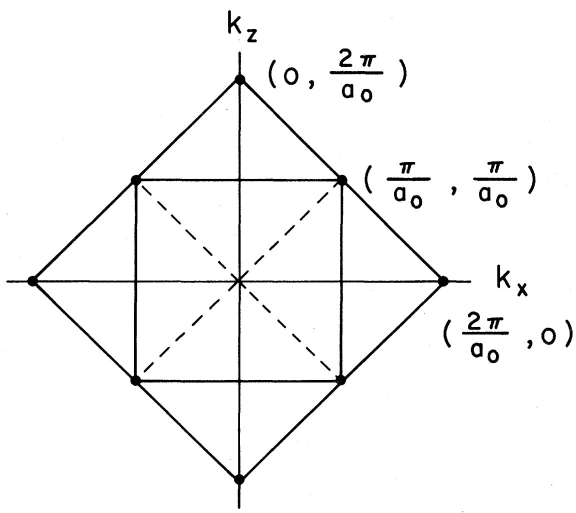

FIG. 2. Brillouin zone for the unreconstructed surface spin configuration (large diamond) and reconstructed spin configuration (small square).

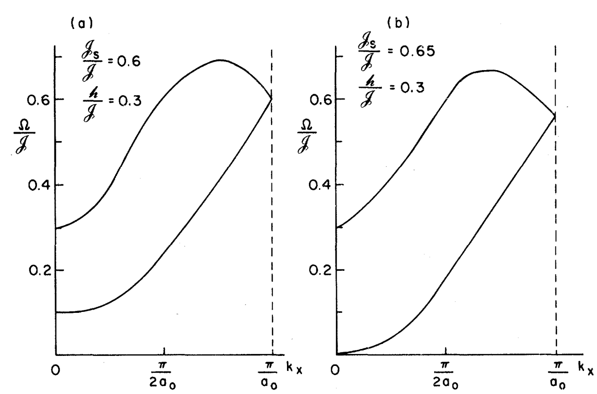

FIG. 3. Surface spin-wave dispersion relations for values of $\mathcal{J}_s$ given by (a) $\mathcal{J}_s = 0.6\mathcal{J}$, a value too small to provide surface reconstruction, and (b) $\mathcal{J}_s = 0.65\mathcal{J}$, the critical value of $\mathcal{J}_s$ where reconstruction just sets in. We have taken $h = 0.3\mathcal{J}$ for these calculations.

value $\mathcal{J}_s^{(c)}$ at which surface spin reconstruction occurs. At this point, $\Omega_-(k_\parallel)$ drops to zero at $k_\parallel = 0$, and the lower branch varies quadratically with wave vector, for $k_\parallel a_0 \ll 1$. The curves in Fig. 3 may be calculated from the analytic formula in Eq. (2.24).

In Fig. 4 we show surface spin-wave dispersion curves for values of $\mathcal{J}_s$ large enough to drive the surface spins into a reconstructed configuration. To obtain these curves, we have solved numerically for the roots of the 2×2 determinants formed from Eqs. (2.18) and (2.19). The main point to note is that the frequency of the lower branch vanishes linearly with $\vec{k}_\parallel$, as $\vec{k}_\parallel \to 0$. We explored other directions of the two dimensional Brillouin zone and found similar behavior.

From the structure of Eqs. (2.19), one may show that as $\vec{k}_\parallel \to 0$, the reconstructed surface spins behave as a two-dimensional layer of spins decoupled in a dynamical sense from the bulk spins. The only role of the bulk spins is to provide a strong exchange field [the term $\mathcal{J}$ in Eq. (2.20)]. We believe this to be an important observation, since the existence of the low-frequency surface mode necessarily leads to the presence of large amplitude spin fluctuations in the surface, as we shall see in Sec. III. To describe these large fluctuations which originate from the surface Goldstone mode, one may replace the problem of the semi-infinite magnet with a reconstructed surface by the problem of a two-dimensional layer of spins in a strong exchange field. The model explored here is a special one, in that only the spins in the surface layer reconstruct. Since the surface Goldstone mode has its origin in an underlying symmetry in the reconstructed ground state, it should exist quite generally, with properties similar in a qualitative sense to the mode described here.

To see the correctness of the assertion just made, first note that as $\vec{k}_\parallel \to 0$, the attenuation constants Q_+ and $\tilde{Q}_+$ defined in Eqs. (2.12) both approach infinity. We have $e^{\tilde{Q}_+}$ and e^{Q_+} both proportional to $k_\parallel^{-2}$, as $k_\parallel \to 0$. With this information in hand, we see that the quantities $\gamma_- e^{Q_+}$ and $\gamma_- e^{\tilde{Q}_+}$ both approach a constant as $k_\parallel \to 0$:

$$\lim_{k_\parallel \to 0} \gamma_- e^{\tilde{Q}_+} = \frac{h + 4\mathcal{J} + \Omega}{\mathcal{J}} \tag{2.28a}$$

and

$$\lim_{k_\parallel \to 0} \gamma_- e^{Q_+} = \frac{h + 4\mathcal{J} - \Omega}{\mathcal{J}} . \tag{2.28b}$$

This implies that $g_1^{(-)}$ and $g_2^{(-)}$ both vanish as the *fourth* power of $k_\parallel$ as $k_\parallel \to 0$.

This result means that if in the expressions for $\alpha^{(-)}$ and β, we replace γ by the long-wavelength form $\gamma \cong 1 - \frac{1}{8}(a_0 k_\parallel)^2$, the contributions from $g_1^{(-)}$ and $g_2^{(-)}$ are the next highest order in the expansion in powers of $(a_0 k_\parallel)^2$. Thus, in the long-wavelength limit, both $g_1^{(-)}$ and $g_2^{(-)}$ fail to contribute to the two leading terms of the dispersion relation and $\Omega_-(k_\parallel)$ is given by the two-dimensional layer result displayed in Eq. (2.27a), with the neglected terms being of order $(a_0 k_\parallel)^4$ inside the square root. We see that the two-dimensional layer model produces not only the linear term in $k_\parallel$ correctly in the dispersion relation, but the first correction as well. In Sec. III we study the behavior of spin fluctuations in the reconstructed surface layer by exploiting the analogy with the two-dimensional canted spin array in a strong exchange field.

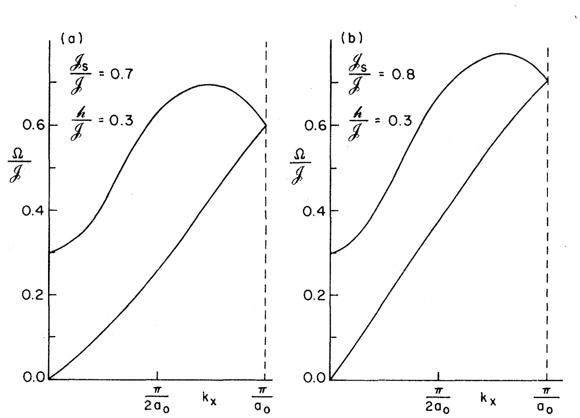

FIG. 4. Surface spin-wave dispersion relation for values of $\mathcal{J}_s$ large enough to produce surface reconstruction. We have, again for $h = 0.3\mathcal{J}$, calculations for (a) $\mathcal{J}_s = 0.7\mathcal{J}$ and (b) $\mathcal{J}_s = 0.8$.

III. COMMENTS ON THE NATURE OF SPIN FLUCTUATIONS IN THE RECONSTRUCTED SURFACE

In this section we comment on the nature of spin fluctuations in canted layers of spins of the sort described in Sec. II. One knows well that that in systems in less than three dimensions, long-wavelength fluctuations (spin waves in the present case) can break up long-range order. In Sec. II we saw that to excellent approximation, the long-wavelength low-frequency spin waves may be regarded as quite localized to the surface layer. Thus, the role of these long-wavelength modes may be assessed by confining one's attention to a two-dimensional layer of canted spins in a strong external field. The field represents the sum of the applied Zeeman field and the exchange field from the ferromagnetically aligned bulk spins. We investigate the nature of the spin-correlation functions for such a layer of spins.

The two-dimensional layer we consider is illustrated in Fig. 1. We presume that the spins lie in the plane of the layer in the equilibrium configuration. The Hamiltonian has the form

$$H=H_z+H_x+H_A, \tag{3.1}$$

where

$$H_z=-g\mu_B H_E\left(\sum_{l_A} S_z(l_A)+\sum_{l_B} S_z(l_B)\right) \tag{3.2}$$

is the Zeeman interaction of the surface spins with the effective field (the sum of the externally applied field plus the exchange field from the bulk spins), and

$$H_x=+J_s\sum_{l_A}\sum_{\vec\delta}\vec S(\vec l_A)\cdot\vec S(\vec l_A+\vec\delta) \tag{3.3}$$

is the exchange coupling between the spins. In Eq. (3.3), $\vec\delta$ is a vector from a site on the A sublattice to a nearest site on the B sublattice. Finally in H_A, we introduce an anisotropy field which acts on the spins. Because the surface sites have lower symmetry than bulk sites, additional anisotropy fields will always be present in the surface. We shall see that such anisotropy fields play a crucial role in damping the large amplitude spin fluctuations which we find below with no anisotropy present. For H_A, we take the form

$$\begin{aligned}H_A=&-K_z\left(\sum_{l_A} S_z^2(l_A)+\sum_{l_B} S_z^2(l_B)\right)\\&-K_x\left(\sum_{l_A} S_x^2(l_A)+\sum_{l_B} S_x^2(l_B)\right)\\&-K_y\left(\sum_{l_A} S_y^2(l_A)+\sum_{l_B} S_y^2(l_B)\right).\end{aligned} \tag{3.4}$$

If constant terms are discarded, Eq. (3.4) may be rewritten

$$\begin{aligned}H_A=&-\overline{K}\left(\sum_{l_A}[S_x^2(l_A)+S_y^2(l_A)]+\sum_{l_B}[S_x^2(l_B)+S_y^2(l_B)]\right)\\&-\frac{\Delta K}{2}\left(\sum_{l_A}[S_x^2(l_A)-S_y^2(l_A)]\right.\\&\left.+\sum_{l_B}[S_x^2(l_B)-S_y^2(l_B)]\right).\end{aligned} \tag{3.5}$$

where $\Delta K=K_x-K_y$; $\overline{K}=K_x+K_y-2K_z$.

If the lattice in Fig. 1 is a square lattice, we should take $K_z=K_x$. If we were to rotate the spins through 90° so that the net moment of the spin array is directed normal to the plane, then we should choose $K_x=K_y$. It is then easy to see for this latter choice that $\Delta K=0$. The parameter ΔK will play a crucial role in the discussion below; for the case where the net moment is normal to the plane, effects similar to those encountered below from ΔK will be encountered if contributions to the anisotropy which are quartic in the spin operators are introduced.

The next step is to find the spectrum of spin waves provided by the Hamiltonian displayed above, and study the behavior of the spin-correlation functions in the spin-wave regime. The problem of finding the form of the spin-wave spectrum is a standard one, so we only sketch the details.

To proceed, we transform the spin operators for the A and B sublattices to a canted coordinate system, as described in Eq. (2.1) and the remarks that follow. Then the Holstein-Primakoff transformation is applied,[10] and the angle θ is found by the requirement that terms linear in the annihilation and creation operators vanish. In the present case, with $\mathcal{J}_s=4SJ_s$, $h_e=g\mu_B H_E$, $\overline{k}=S\overline{K}$, and $\Delta\overline{k}$ $S\Delta K$, we have

$$\sin\theta[(2\mathcal{J}_s+2\overline{k}+\Delta\overline{k})\cos\theta-h_e]=0, \tag{3.6}$$

with sublattice canting ($\theta\neq 0$) when $2\mathcal{J}_s+2\overline{k}+\Delta\overline{k}>h_e$. We assume here that $\Delta\overline{k}>0$, so the transverse moment of the spin array aligns parallel to the x direction. If $\Delta\overline{k}<0$, then the spin array will rotate through 90°, with the transverse moment aligned along y.

To proceed further, we introduce the wave vector $\vec k_\parallel$ parallel to the layer as in Eq. (2.5), and then transform to the variables

$$c_{\vec k_\parallel}=(1/\sqrt2)(a_{\vec k_\parallel}+b_{\vec k_\parallel}) \tag{3.7a}$$

and

$$d_{\vec k_\parallel}=(1/\sqrt2)(a_{\vec k_\parallel}-b_{\vec k_\parallel}). \tag{3.7b}$$

The Hamiltonian then becomes

$$H=H_1+H_2, \tag{3.8}$$

where

$$H_1=\sum_{\vec k_\parallel}A_+(\vec k_\parallel)c^\dagger_{\vec k_\parallel}c_{\vec k_\parallel}-\frac12\sum_{\vec k_\parallel}B_+(\vec k_\parallel)(c^\dagger_{\vec k_\parallel}c^\dagger_{-\vec k_\parallel}+\text{H.c.}) \tag{3.9a}$$

and

$$H_2=\sum_{\vec k_\parallel}A_-(\vec k_\parallel)d^\dagger_{\vec k_\parallel}d_{\vec k_\parallel}-\frac12\sum_{\vec k_\parallel}B_-(\vec k_\parallel)(d^\dagger_{\vec k_\parallel}d^\dagger_{-\vec k_\parallel}+\text{H.c.}), \tag{3.9b}$$

with

$$A_\pm(\vec k_\parallel)=\mathcal{J}_s(1\pm\gamma\cos^2\theta)+\overline{k}\sin^2\theta+\tfrac12\Delta\overline{k}(2+\sin^2\theta) \tag{3.10a}$$

and

$$B_\pm(\vec k_\parallel)=\mathcal{J}_s\gamma\sin^2\theta-\overline{k}\sin^2\theta+\tfrac12\Delta\overline{k}(2-\sin^2\theta). \tag{3.10b}$$

Each of the Hamiltonians in Eq. (3.8) is diagonalized readily by means of a Bogoliubov transformation:

$$c^\dagger_{\vec{k}_\parallel} = \cosh\theta_{\vec{k}_\parallel}(+)\,\alpha^\dagger_{\vec{k}_\parallel}(+) + \sinh\theta_{\vec{k}_\parallel}(+)\,\alpha_{-\vec{k}_\parallel}(+)\,, \quad (3.11)$$

with the "+" replaced by "−" for the operator $d^\dagger_{\vec{k}_\parallel}$. If we choose

$$\tanh 2\theta_{\vec{k}_\parallel}(\pm) = B_\pm(\vec{k}_\parallel)/A_\pm(\vec{k}_\parallel)\,, \quad (3.12)$$

then the Hamiltonian H becomes

$$H_{1,2} = -\frac{1}{2}\sum_{\vec{k}_\parallel} A_\pm(\vec{k}_\parallel) + \sum_{\vec{k}_\parallel} \Omega_\pm(\vec{k}_\parallel)[\alpha^\dagger_{\vec{k}_\parallel}(\pm)\alpha_{\vec{k}_\parallel}(\pm) + \tfrac{1}{2}]\,, \quad (3.13)$$

where the spin-wave frequencies are given by

$$\Omega_\pm(\vec{k}_\parallel) = [\mathscr{G}_s(1\pm\gamma) + 2\Delta\bar{k}]^{1/2} \times [\mathscr{G}_s(1\pm\gamma\cos 2\theta) + (2\bar{k}+\Delta\bar{k})\sin^2\theta]^{1/2}\,. \quad (3.14)$$

If we set $\Delta\bar{k}=0$, then the frequency of the mode $\Omega_-(\vec{k}_\parallel)$ vanishes in the limit $\vec{k}_\parallel \to 0$. This is the "surface Goldstone mode" discussed earlier in the paper. Our primary interest in this section is the role of this low-frequency mode in producing spin fluctuations within the layer.

Note that when $\Delta\bar{k}\neq 0$, then $\Omega_-(0)$ is finite. The anisotropy terms which contribute to $\Delta\bar{k}$ inhibit rotation of the spins in the plane perpendicular to the magnetization of the layer, with the result that a finite restoring force is obtained even for $\vec{k}_\parallel = 0$. The gap in the surface wave branch can be considerable even though $\Delta\bar{k}$ is small. To see this, for exchange-coupled S-state ions (say Eu^{2+}), one may expect to find both $\bar{k}$ and $\Delta\bar{k}$ small compared to $\mathscr{G}_s$. In this circumstance, $\Omega_-(0) = 2(\sin\theta)(\mathscr{G}_s\Delta\bar{k})^{1/2}$. Thus, $\Omega_-(0)$ is proportional to the geometrical mean of the (large) exchange field $\mathscr{G}_s$, and the (small) anisotropy term $\Delta\bar{k}$. A small amount of anisotropy can thus produce a substantial gap in the low-frequency surface spin-wave spectrum. It is well known that this is a general feature of spin configurations with antiferromagnetic character.

For our purposes, only the long-wavelength modes on the lower branch will prove of interest. Indeed, for the short-wavelength excitations, the use of the single layer is a poor approximation to the semi-infinite geometry. For $k_\parallel a_0 \ll 1$, we have to good approximation

$$\Omega_-(k_\parallel) \cong \tfrac{1}{2}\mathscr{G}_s a_0(\sin\theta)(\lambda^2 + k_\parallel^2)^{1/2}\,, \quad (3.15)$$

where $\lambda^2 = 16\Delta\bar{k}/\mathscr{G}_s a_0^2$.

We next turn to a study of the nature of the spin-correlation functions. Of particular concern is the behavior of the spins in the limit that the surface anisotropy $\Delta\bar{k}$ becomes very small. The spin-correlation functions are readily calculated through use of the Holstein-Primakoff transformation outlined above. As a consequence, we only quote the results.

To examine the fluctuations in the transverse moment, consider the form of $\langle S_x(\vec{l}_A)S_x(0)\rangle$ and $\langle S_y(\vec{l}_A)S_y(0)\rangle$, where both spin operators refer to the A sublattice. We find after some straightforward calculation that

$$\langle S_y(\vec{l}_A)S_y(0)\rangle = \frac{S}{4N_s} \times \sum_{\vec{k}_\parallel\sigma}[1+2n_\sigma(\vec{k}_\parallel)][A_\sigma(\vec{k}_\parallel) - B_\sigma(\vec{k}_\parallel)] \times [\Omega_\sigma(\vec{k}_\parallel)]^{-1}\cos(\vec{k}_\parallel\cdot\vec{l}_A) \quad (3.16)$$

and

$$\langle S_x(\vec{l}_A)S_x(0)\rangle = S(S+1)\sin^2\theta - \frac{S\sin^2\theta}{2N_s} \times \sum_{\vec{k}_\parallel\sigma}\frac{A_\sigma(\vec{k}_\parallel)}{\Omega_\sigma(\vec{k}_\parallel)}[1+2n_\sigma(\vec{k}_\parallel)] + \frac{S\cos^2\theta}{4N_s} \times \sum_{\vec{k}_\parallel\sigma}\cos(\vec{k}_\parallel\cdot\vec{l}_A)\frac{A_\sigma(\vec{k}_\parallel)+B_\sigma(\vec{k}_\parallel)}{\Omega_\sigma(\vec{k}_\parallel)} \times [1+2n_\sigma(\vec{k}_\parallel)]\,, \quad (3.17)$$

In these expressions, $\sigma =$ "+" or "−" is a branch index and

$$n_\sigma(\vec{k}_\parallel) = [e^{\Omega_\sigma(\vec{k}_\parallel)/k_BT} - 1]^{-1}$$

is the Bose-Einstein factor. It is useful to note that as $k_\parallel \to 0$, one has the limiting forms

$$A_-(\vec{k}_\parallel) + B_-(\vec{k}_\parallel) = \tfrac{1}{8}\mathscr{G}_s a_0^2(\lambda^2 + k_\parallel^2) \quad (3.18a)$$

and

$$A_-(\vec{k}_\parallel) - B_-(\vec{k}_\parallel) = 2\mathscr{G}_s\sin^2\theta\,. \quad (3.18b)$$

Inspection of Eqs. (3.16) and (3.17) show that at $T=0$, the zero-point fluctuations of the spin array do not break up the long-range order in the transverse moment, in the limit $\Delta\bar{k}=0$. That is to say, both $\langle S_y^2(0)\rangle$ and $\langle S_x^2(0)\rangle$ remain finite and well behaved at $T=0$, when $\Delta\bar{k}=0$. However, when the temperature is finite, both of these quantities diverge for $\Delta\bar{k}=0$, since for $k_BT \gg \hbar\Omega_-(k_\parallel)$, one has $n_-(k_\parallel)$ approximately equal to $k_BT/\hbar\Omega_-(k_\parallel)$. Thus, for long-range order in the transverse moment to exist in the layer at nonzero temperature, it is necessary for surface anisotropy to inhibit the transverse fluctuations in the spin system.

If we take only the contribution from the long-wavelength modes associated with the lower branch, and use Eq. (3.15), we find

$$\langle S_y^2(0)\rangle_T - \langle S_y^2(0)\rangle_0 = -\lambda S a_0(\sin\theta) \times[\tau\ln(e^{1/\tau}-1)-1], \qquad (3.19)$$

where λ is defined after Eq. (3.15), and we have

$$\tau = k_B T/\hbar\Omega_-(0). \qquad (3.20)$$

Thus, as $\Delta\bar{k}\to 0$, $\langle S_y^2(0)\rangle_T - \langle S_y^2(0)\rangle_0$ diverges as $\ln[k_B T/\hbar\Omega_-(0)]$, a very weak divergence. This is in accord with the earlier notion that modest amounts of surface anisotropy are most effective in damping the large amplitude spin fluctuations. Note also that $\Omega_-(0)$ is proportional to $\sin\theta$. Application of an external magnetic field parallel to the bulk magnetization will *decrease* the value of θ [see Eq. (3.6) and the results of Ref 4]. Thus, as θ decreases and $\Omega_-(0)$ decreases, the amplitude of the transverse spin fluctuations *increases* in the present model.

All of the conclusions above apply to fluctuations in a two-dimensional array of spins inhibited by planar anisotropy fields. However, since the divergences have their origin in the low-frequency long-wavelength modes (the surface Goldstone modes of Sec. II) for which in the semi-infinite model of Sec. II the surface spins decouple from the bulk to good approximation, we argue that the conclusions apply to reconstructed layers on substrates.

Note that while for small $\Delta\bar{k}$ we find $\langle S_x^2(0)\rangle_T$ and $\langle S_y^2(0)\rangle_T$ to be large, the correlation functions of the form

$$\langle [S_x(\vec{l}_A) - S_x(0)][S_x(\vec{l}_A) - S_x(0)]\rangle$$

are well behaved, with no divergences from the low-frequency long-wavelength modes. Thus, the motion of the spins is highly correlated, although both $\langle S_x^2(0)\rangle_T$ and $\langle S_y^2(0)\rangle_T$ may be large (for small $\Delta\bar{k}$). There is an analogy here between the spin array presently under consideration and the two-dimensional lattice, where the mean-square displacement diverges for each atom, but there remain correlations between the relative positions of the atoms.

One may believe that (for $\Delta\bar{k}=0$), since at $\vec{k}_\parallel = 0$ the zero-frequency mode is a rigid precession of the two sublattices with the z component of the spin fixed, long-range order in S_z will persist even though we have just seen that the fluctuations in $\langle S_x^2\rangle_T$ and $\langle S_y^2\rangle_T$ diverge when $\Delta\bar{k}\to 0$. If this were so, one could think of the layer of fluctuating spins as a system with $d=2$ and $n=2$, as suggested by Blandin and Castiel.[3] From our spin-wave analysis, we find large fluctuations in S_z which diverge as $\Delta\bar{k}\to 0$, just as the fluctuations in the transverse moment diverge. The point is that at finite temperature, the spin sublattices wobble as they precess, to produce fluctuations in S_z comparable to those in S_x and S_y. Thus, the analysis here raises a question about whether the analogy $d=2$, $n=2$ is appropriate when $\Delta\bar{k}=0$.

For $\langle S_z(l_A)S_z(0)\rangle$ we find the result

$$\langle S_z(l_A)S_z(0)\rangle = S(S+1)\cos^2\theta - \frac{S\cos^2\theta}{2N_s} \times\sum_{\vec{k}_\parallel\sigma}\frac{A_\sigma(\vec{k}_\parallel)}{\Omega_\sigma(\vec{k}_\parallel)}[1+2n_\sigma(\vec{k}_\parallel)] + \frac{S\sin^2\theta}{4N_s} \times\sum_{\vec{k}_\parallel\sigma}\cos(\vec{k}_\parallel\cdot\vec{l}_A)\frac{A_\sigma(\vec{k}_\parallel)+B_\sigma(\vec{k}_\parallel)}{\Omega_\sigma(\vec{k}_\parallel)} \times[1+2n_\sigma(\vec{k}_\parallel)]. \qquad (3.21)$$

Examination of this form shows divergences identical to those which occur in $\langle S^2{}_x(0)\rangle_T$ and $\langle S_y^2(0)\rangle_T$, as $\Delta\bar{k}\to 0$.

IV. CONCLUSION

The purpose of this paper has been to outline the qualitative features of the spin behavior in the surface of a semi-infinite magnet which undergoes surface spin reconstruction. Before one can proceed further, it is necessary to have a firmer grasp on the physics of the surface region. For example, whether surface reconstruction can occur at all depends on the nature of the exchange interactions in and near the surface. We know of no simple argument that can lead one to reliable conclusions on the magnitude and sign of surface exchange constants relative to the bulk.

We also see here that the behavior of the surface spins is quite sensitive to the nature of anisotropy fields at the surface. This is another area where little is known. From one recent experimental study that has probed this question in detail one sees that the surface pinning fields may be complex in nature.[11] In the limit $\Delta\bar{k}\to 0$, one encounters an interesting problem in statistical mechanics posed by the existence of the large fluctuations. Our own view is that surface anisotropy fields present in real materials should be sufficiently large that the spin fluctuations in the surface remain well behaved. But this conjecture must await further experimental data for confirmation.

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[8]If the surface spins are stable with respect to the ferromagnetic state, but the exchange constants are such that the surface spins are close to being unstable, then there may be short-wavelength modes of low frequency. See Fig. 3 in Ref. 4.

[9]In systems with no long-range order, but long correlation lengths, Y. Imry, P. Pincus, and D. Scalapino [Phys. Rev. B 12, 1978 (1975)] have argued that spin-wave theory produces the proper form of the spin-correlation functions, so long as one is concerned with spins of spatial separation small compared to the coherence length.

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