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Influence of surface anisotropy on the magnetization of the Heisenberg ferromagnet

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We examine theoretically the influence of surface anisotropy on the magnetization of the Heisenberg ferromagnet in its outermost layers. Emphasis is on the case where the surface spins sense an easy axis normal to the surface and at temperatures where spin-wave theory may be applied. For parameters in the range of those that emerge from recent analyses of Fe surfaces and interfaces, we find the influence of surface anisotropy to be very modest, except at rather low temperatures (10-K range). A key element in the analysis is a cancellation between the surface spin-wave contribution to the magnetization and that from a "hole" produced in the density of the bulk waves, when the surface wave is removed from the bulk spin-wave bands. Our theoretical analysis is based on a Green's-function method.

I. INTRODUCTION

The nature of magnetism at crystal surfaces, and at the interface between magnetic solids and other materials, has been an active topic of discussion in the recent literature. Advances in both sample preparation and experimental technique now allow one to explore these issues in a remarkably quantitative manner.

It is clear from recent experiments that the spins that reside in the outermost layer of a ferromagnetic crystal or very thin film can experience anisotropy fields very much larger than realized in the bulk of crystals. For materials such as Fe, where one has cubic site symmetry in the bulk, such a result is expected when the influence of spin-orbit coupling on the magnetic energy is considered, in combination with the low site symmetry in the surface.[1] It is found quite frequently[2,3] that there is an easy axis normal to the surface, for spins in the surface of single crystal Fe, or ultrathin Fe films. The effective surface anisotropy field can be inferred to be in the range of 50–100 kG in such samples. The purpose of this paper is to explore the influence of such a surface anisotropy field on the temperature variation of the magnetization near the surface of semi-infinite Heisenberg ferromagnet. We begin with comments on the motivation for our study.

The temperature variation of the magnetization near the surface of the Heisenberg ferromagnet, with surface anisotropy absent, has been explored in the theoretical literature. Suppose we let $\langle S_z(l)\rangle$ be the magnetization within the layer l atomic planes from the surface, and write

$$\langle S_z(l)\rangle = S - \Delta(l)\ .$$

Deep in the bulk, and at temperatures low enough for spin-wave theory to be valid, we have the well-known Bloch law $\Delta(\infty)=C_\infty T^{3/2}$, with T the temperature. One inquires about the behavior of $\Delta(l)$, as l approaches the surface.

This question was addressed first by Rado,[4] in a very brief abstract. An expression was given for $\Delta(l)$ in the spin-wave regime, for a simple cubic Heisenberg ferromagnet with nearest-neighbor exchange, and (100) surface. With $l=0$ the surface layer, Rado's result gave $\Delta(0)=2C_\infty T^{3/2}$. One realizes the $T^{3/2}$ law in the surface also, with coefficient larger than the bulk by a factor of 2.

The model explored by Rado is a very special, indeed almost singular, example. Quite generally, surfaces of Heisenberg ferromagnet support surface spin waves as elementary excitations, as noted in an example some years ago.[5] If the exchange interactions are short ranged (not necessarily confined to nearest neighbors), subsequent discussion showed that one realizes surface spin waves below the bulk spin wave bands quite similar to those explored in Ref. 5 for a broad class of models. Such waves are found any time exchange bonds nonnormal to the surface are broken when the surface is formed by cutting all exchange couplings which cross a mathematical plane located between two adjacent atomic planes.[6] This statement assumes all exchange couplings near the surface are identical to the corresponding couplings in the bulk; the surface spin waves remain even if surface exchange constants differ considerably from the bulk.

Rado's model admits no such surface spin waves, and in fact the bulk waves are simple standing waves with wave vector perpendicular to the surface $k_\perp^{(n)}\equiv n\pi/L$, with L the film thickness.[7] If we write $\Delta(0)=C_s T^{3/2}$, the result $C_s=2C_\infty$ follows at once by noting each spin wave has a simple antinode right at the surface.

We have noted, however, that low-frequency long-wavelength surface spin waves occur in the model quite generally.[8] These are present as thermal excitations, and will lead to a contribution $\Delta_s(l)$ to the magnetization near the surface not contained in Rado's special case. Maradudin and Mills[9] carried out a detailed analysis of $\Delta(l)$ for a model that contains surface spin waves. They demonstrated that one must consider, in addition to $\Delta_s(l)$, the influence of the surface on the frequency distribution and amplitude of bulk spin waves, to obtain the total magnetization deficit $\Delta(l)$. These authors showed the total bulk spin-wave contribution is given by

$$\Delta_B(l)=2C_\infty T^{3/2}-\Delta_s(l) ,$$

so the total is once again $2C_\infty T^{3/2}$. From a subsequent discussion,[6] one sees this cancellation occurs not only for the particular model structure explored by Maradudin and Mills,[9] but for a wide class of surface geometries.

What has happened is the following. The long-wavelength surface spin waves are rather weakly bound on the surface of the Heisenberg ferromagnet, in a sense discussed earlier[5,6,9] and mentioned again in the following. The perturbation provided by the surface pulls them out of and below the bulk spin-wave bands in frequency; when this is done, a "hole" is left behind in the density of bulk spin-wave states, near the bottom of the band. This hole adds the piece $-\Delta_s(l)$ to the bulk spin-wave contribution $\Delta_B(l)$ to the mean spin deviation near the surface. When the surface and the bulk contributions are added together, the piece from the hole cancels the surface wave contribution. We refer to this result as the cancellation theorem. The analysis of Maradudin and Mills derived this result, again for a particular model, within the framework of a Green's function analysis. The present author showed[6] how it emerges from an analysis of standing spin waves in a film of thickness L, in the limit $L\rightarrow\infty$. This was done within a calculation that can be applied to a variety of low index surfaces for a range of crystal structures, with the exchange in the surface layer possibly different from the bulk. This shows the result $\Delta(0)=2C_\infty T^{3/2}$ to be rather general in the limit of low temperatures.

Quite recently Rado[10] has presented a calculation which explores the role of surface anisotropy on the temperature dependence of $\Delta(0)$. He argues that thermally excited surface spin waves, which owe their presence to easy-axis surface anisotropy, can produce a term in $\Delta(l)$ "quasilinear" in the absolute temperature T. In his analysis, Rado does not explore the influence of bulk spin waves on the behavior of $\Delta(l)$ near the surface. Mössbauer studies of the magnetization of an Fe film overlaid by MnF_2 suggests $\Delta(0)$ exhibits a linear variation in temperature over a wide range.[11]

While the connection between Rado's model and the sample used in the experiment is not entirely clear, his remarks suggest one should explore theoretically the influence of the surface anisotropy field on the temperature variation of the surface magnetization. The purpose of this paper is to address this question in the spin-wave regime. A central issue is the cancellation theorem, and the question of whether the presence of surface anisotropy changes its character. The analysis presented here shows that corrections to the result $\Delta(0)=2C_\infty T^{3/2}$ are quite small except at rather low temperatures ($T\lesssim 10$ K), if we have parameters appropriate to Fe surfaces and interfaces in mind. The basic reason is that the cancellation theorem holds to good approximation, even when the thermally excited surface spin waves and their bulk counterparts are perturbed by the presence of surface anisotropy. We obtain a "quasi linear" term equivalent to that displayed in Rado's paper with origin in surface spin waves, but as we shall see this is canceled, leaving a small residue.

Our conclusions depend on certain assumptions about the relative order of magnitude of characteristic energies in the problem. These are outlined in Sec. II, and will be invoked as the discussion proceeds. Our conclusions do not apply, for example, if the strength of the surface anisotropy field approaches the strength of the exchange field felt by a spin in the lattice. This circumstance might be realized if the exchange itself is highly anisotropic within the surface layer; from a physical point of view, there is little difference in the influence of single-site anisotropy and exchange anisotropy at low temperatures, where the wavelength of thermally excited spin waves exceeds the (assumed microscopic) range of the exchange interactions. So one can conceive of surfaces and interfaces described by parameters whose relative orders of magnitude differ substantially from the assumptions used here.

We proceed by means of a Green's-function approach that generates an exact and complete solution to the model Hamiltonian, in the spin-wave regime. Because of this, strictly speaking, we need not invoke the assumptions just mentioned. The general expressions for $\Delta(l)$ are quite cumbersome and suitable only for numerical computation. Our aim in this paper is to provide insight into the various contributions and to obtain analytic results that are simple. As we shall see, this can be accomplished for models whose parameters approximate an important class of systems studied experimentally.

The outline of this paper is as follows. Section II is devoted to setting up the Green's-function formalism, and here we obtain an exact expression for it, in the presence of uniaxial surface anisotropy. In Sec. III, we study the effect of surface anisotropy on surface spin waves and obtain explicit expressions for the various contributions to the mean spin deviation. The latter discussion is necessarily rather technical, unfortunately. In Sec. IV, we collect together various results and discuss their implication.

II. GENERAL REMARKS AND FORMAL RESULTS

While we have Fe surfaces and interfaces in mind, we use a Heisenberg model rather than the proper itinerant electron description appropriate to such a material. It remains a challenge to carry through a complete description of surface spin dynamics in an itinerant model, even in the spin-wave regime.[12]

We have a semi-infinite Heisenberg ferromagnet placed in a magnetic field H_0 parallel to the surface. We suppose the spins in the outermost layer experience an effective anisotropy field H_s normal to the surface, and thus normal to H_0. Our primary emphasis will be on the case where the direction normal to the surface is an easy axis. A spin also sits in an exchange field H_x from its neighbors; we assume exchange couplings within the surface layer may differ from those in the bulk, but that the exchange field felt by a surface spin does not differ in order of magnitude by that experienced by bulk spin. We are interested in the case where H_x is substantially larger than H_0 and H_s. Thus, we assume $H_0, H_s \ll H_x$. The temperature T is such that $k_B T \ll H_x$, but except at the lowest temperatures (~ 10 K) we also have $H_0, H_s < k_B T \ll H_x$. We can obtain rather simple results in the end if we invoke these assumptions.

As the spins precess when a surface or bulk spin wave is excited, dipolar fields are generated. Their strength is measured by $4\pi M$, with M the magnetization. One has $4\pi M \sim H_0, H_s$, but in the interest of simplicity we ignore the influence of dipolar fields here. Earlier studies of surface spin waves show that for these modes, and bulk waves as well, one must superimpose three waves, each with its own propagation constant normal to the surface to satisfy the boundary conditions there.[13,14] The past analyses which include dipolar coupling also confine their attention to an approximate description of exchange by introducing a term proportional to ∇^2 in the equations of motion of the spin system. Such a procedure fails to generate the exchange dominated surface spin waves studied in Ref. 5 and which, in our view, play the primary role in the thermodynamics of the surface region, in the range of temperatures of interest here. Because the introduction of dipolar effects in the lattice description of the problem used here produces substantial technical complications, we ignore them in this study. It would be of interest to explore their role in subsequent work.

We shall orient a Cartesian coordinated system with z axis parallel to the surface and to an applied external magnetic field H_0. The y axis is normal to the surface. The position of a given spin is given by $\boldsymbol{l} = \boldsymbol{l}_\parallel + \hat{\mathbf{y}} l_y$, and $l_y = 0$ refers to the surface plane. Our Hamiltonian is written, with $\mathbf{S}(\boldsymbol{l}_\parallel l_y)$ the spin at site $\boldsymbol{l}$,

$$\begin{aligned} H = & -\tfrac{1}{2} \sum_{\boldsymbol{l}_\parallel} \sum_{\boldsymbol{\delta}_\parallel} J_s(\boldsymbol{\delta}_\parallel) \mathbf{S}(\boldsymbol{l}_\parallel 0) \cdot \mathbf{S}(\boldsymbol{l}_\parallel + \boldsymbol{\delta}_\parallel, 0) \\ & -\tfrac{1}{2} \sum_{\boldsymbol{l}_\parallel} \sum_{\boldsymbol{\delta}_\parallel} \sum_{l_y=1}^{\infty} J(\boldsymbol{\delta}_\parallel) \mathbf{S}(\boldsymbol{l}_\parallel l_y) \cdot \mathbf{S}(\boldsymbol{l}_\parallel + \boldsymbol{\delta}_\parallel, l_y) \\ & - \sum_{l_y=0}^{\infty} \sum_{\boldsymbol{l}_\parallel} \sum_{\boldsymbol{\Delta}_\parallel} J(\boldsymbol{\Delta}_\parallel) \mathbf{S}(\boldsymbol{l}_\parallel l_y) \cdot \mathbf{S}(\boldsymbol{l}_\parallel + \boldsymbol{\Delta}_\parallel, l_y + 1) \\ & - K_s \sum_{\boldsymbol{l}_\parallel} S_y^2(l_y, 0) - H_0 \sum_{\boldsymbol{l}_\parallel} \sum_{l_y=0}^{\infty} S_z(\boldsymbol{l}_\parallel l_y) . \end{aligned} \tag{2.1}$$

The first two terms describe intraplanar exchange couplings, and the third describes interplanar couplings. Exchange within the surface layer may differ from that in the bulk. The parameter K_s is the strength of the surface anisotropy. We have an easy axis normal to the surface with the choice $K_s > 0$.

We proceed in the spin-wave regime by resorting to the Holstein-Primakoff transformation.[15] If $a(\boldsymbol{l}_\parallel l_y)$ and $a^\dagger(\boldsymbol{l}_\parallel l_y)$ are the boson annihilation and creation operation in the site representation, we let

$$a(\boldsymbol{l}_\parallel l_y) = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}_\parallel} a(\mathbf{k}_\parallel l_y) \exp(i \mathbf{k}_\parallel \cdot \boldsymbol{l}_\parallel) , \tag{2.2}$$

with a similar transformation applied to $a^\dagger(\mathbf{k}_\parallel l_y)$. Here N_s is the number of sites in a basic quantization area, and $\mathbf{k}_\parallel$ lies within the surface Brillouin zone. When constant terms in H are discarded, we have the spin-wave Hamiltonian

$$\begin{aligned} H_{\text{sw}} = & \sum_{\mathbf{k}_\parallel} \{ H_0 - \tfrac{1}{2} H_s + [I_s(0) - I_s(\mathbf{k}_\parallel)] + I_\perp(0) \} a^\dagger(\mathbf{k}_\parallel 0) a(\mathbf{k}_\parallel 0) \\ & + \sum_{\mathbf{k}_\parallel} \sum_{l_y=1}^{\infty} \{ H_0 + [I(0) - I(\mathbf{k}_\parallel)] + 2 I_\perp(0) \} a^\dagger(\mathbf{k}_\parallel l_y) a(\mathbf{k}_\parallel l_y) \\ & - \sum_{\mathbf{k}_\parallel} \sum_{l_y=0}^{\infty} I_\perp(\mathbf{k}_\parallel) [a^\dagger(\mathbf{k}_\parallel l_y) a(\mathbf{k}_\parallel l_y + 1) + a^\dagger(\mathbf{k}_\parallel l_y + 1) a(\mathbf{k}_\parallel l_y)] + \tfrac{1}{4} H_s \sum_{\mathbf{k}_\parallel} [a^\dagger(\mathbf{k}_\parallel 0) a^\dagger(-\mathbf{k}_\parallel 0) + a(\mathbf{k}_\parallel 0) a(-\mathbf{k}_\parallel 0)] . \end{aligned} \tag{2.3a}$$

We have introduced $H_s = 2 K_s S$, which may be viewed as an effective magnetic field acting on the surface spins, with origin in the anisotropy. In Eq. (2.3) we have defined

$$I_s(\mathbf{k}_\parallel) = S \sum_{\boldsymbol{\delta}_\parallel} J_s(\boldsymbol{\delta}_\parallel) \exp(i \mathbf{k}_\parallel \cdot \boldsymbol{\delta}_\parallel) , \tag{2.3b}$$

$$I(\mathbf{k}_\parallel) = S \sum_{\boldsymbol{\delta}_\parallel} J(\boldsymbol{\delta}_\parallel) \exp(i \mathbf{k}_\parallel \cdot \boldsymbol{\delta}_\parallel) , \tag{2.3c}$$

and

$$I_\perp(\mathbf{k}_\parallel) = S \sum_{\boldsymbol{\Delta}_\parallel} J(\boldsymbol{\Delta}_\parallel) \exp(i \mathbf{k}_\parallel \cdot \boldsymbol{\Delta}_\parallel) . \tag{2.3d}$$

We wish to calculate the spin deviation $\Delta(l_y)$, defined as

$$\Delta(l_y) = S - \langle S_z(\boldsymbol{l}_\parallel l_y) \rangle = \frac{1}{N_s} \sum_{\mathbf{k}_\parallel} \langle a^\dagger(\mathbf{k}_\parallel l_y) a(\mathbf{k}_\parallel l_y) \rangle_T . \tag{2.4}$$

As remarked earlier, we do this by means of a Green's-function method. We introduce

$$G(\mathbf{k}_\parallel t; l_y l_y') = i \theta(t) \langle a(\mathbf{k}_\parallel l_y; t), a^\dagger(\mathbf{k}_\parallel l_y'; 0)] \rangle , \tag{2.5}$$

where $a(\mathbf{k}_\parallel l_y; t)$ is the operator $a(\mathbf{k}_\parallel l_y)$ in the Heisenberg representation. One introduces the Fourier transform with respect to time by writing

$$G(\mathbf{k}_\parallel t; l_y l_y') = \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} e^{-i\Omega t} G(\mathbf{k}_\parallel \Omega; l_y l_y') . \tag{2.6}$$

It is straightforward to show that

$$\Delta(l_y)=\frac{1}{i\pi}\sum_{\mathbf{k}_\parallel}\int_{-\infty}^{+\infty}d\Omega\, n(\Omega)\mathrm{Im}[G(\mathbf{k}_\parallel\Omega+i\eta;l_y l_y)] . \tag{2.7}$$

where $n(\Omega)=(e^{\beta\Omega}-1)^{-1}$ and $\beta=1/k_B T$. The reader should note we use units within which $\hbar=1$. For what follows, it is important to keep in mind that the integral on frequency in Eq. (2.7) ranges over negative as well as positive frequencies.

The equation of motion of the Green's function is

$$i\frac{\partial}{\partial t}G(\mathbf{k}_\parallel t;l_y l_y')=-\delta(t)\delta_{l_y l_y'}+i\Theta(t)\langle[a(\mathbf{k}_\parallel l_y;t),H_{\mathrm{sw}}],a^\dagger(\mathbf{k}_\parallel l_y;0)\rangle . \tag{2.8}$$

One finds

$$\Omega G(\mathbf{k}_\parallel\Omega;l_y l_y')=-\delta_{l_y l_y'}+\delta_{l_y 0}d_\parallel^{(s)}(\mathbf{k}_\parallel)G(\mathbf{k}_\parallel\Omega;0l_y')+(1-\delta_{l_y 0})d_\parallel(\mathbf{k}_\parallel)G(\mathbf{k}_\parallel\Omega;l_y l_y')$$
$$-d_\perp(\mathbf{k}_\parallel)G(\mathbf{k}_\parallel\Omega;l_y+1,l_y')-(1-\delta_{l_y o})G(\mathbf{k}_\parallel\Omega;l_y-1,l_y')-\tfrac{1}{2}H_s\delta_{l_y 0}[G(\mathbf{k}_\parallel\Omega;0l_y')-D(\mathbf{k}_\parallel\Omega;0l_y')] . \tag{2.9}$$

In this equation, we encounter a new Green's function, $D(\mathbf{k}_\parallel\Omega;l_y l_y')$, which is the Fourier transform with respect to time of

$$D(\mathbf{k}_\parallel t;l_y l_y')=i\Theta(t)\langle[a^\dagger(-\mathbf{k}_\parallel l_y;t),a^\dagger(\mathbf{k}_\parallel l_y'0)]\rangle . \tag{2.10}$$

We have also defined

$$d_\parallel^{(s)}(\mathbf{k}_\parallel)=H_0+[I_s(0)-I_s(\mathbf{k}_\parallel)]+I_\perp(0) , \tag{2.11a}$$

$$d_\parallel(\mathbf{k}_\parallel)=H_0+[I(0)-I(\mathbf{k}_\parallel)]+2I_\perp(0) , \tag{2.11b}$$

and

$$d_\perp(\mathbf{k}_\parallel)=I_\perp(\mathbf{k}_\parallel) . \tag{2.11c}$$

The theory is closed when we find the equation of motion for $D(\mathbf{k}_\parallel t;l_y l_y')$. For its Fourier transform one has

$$\Omega D(\mathbf{k}_\parallel\Omega;l_y l_y')=-\delta_{l_y 0}d_\parallel^{(s)}(\mathbf{k}_\parallel)D(\mathbf{k}_\parallel\Omega;l_y l_y')-(1-\delta_{l_y 0})d_\parallel(\mathbf{k}_\parallel)D(\mathbf{k}_\parallel\Omega;l_y l_y')+(1-\delta_{l_y 0})d_\perp(\mathbf{k}_\parallel)D(\mathbf{k}_\parallel\Omega;l_y-1,l_y')$$
$$+d_\perp(\mathbf{k}_\parallel)D(\mathbf{k}_\parallel\Omega;l_y+1,l_y')+\tfrac{1}{2}H_s[D(\mathbf{k}_\parallel\Omega;0l_y')-G(\mathbf{k}_\parallel\Omega;0_y')] . \tag{2.12}$$

These equations may be solved in closed form. In what follows, for the sake of brevity, we suppress reference to the dependence of various quantities in the above equations on $\mathbf{k}_\parallel$. It will be useful to replace the frequency Ω by the complex frequency z which in the end will be allowed to approach the real axis from above.

We proceed by introducing the operator

$$M(l_y l_y')=\delta_{l_y l_y'}[\delta_{l_y 0}d_\parallel^{(s)}+(1-\delta_{l_y 0})d_\parallel]$$
$$-\delta_{l_y',l_y+1}d_\perp-\delta_{l_y',l_y-1}(1-\delta_{l_y 0})d_\perp , \tag{2.13}$$

so the two equations of motion become

$$\sum_{l_y''}[z\delta_{l_y l_y''}-M(l_y l_y'')]G(z;l_y''l_y')$$
$$=-\delta_{l_y l_y'}-\tfrac{1}{2}H_s\delta_s\delta_{l_y,0}[G(z;0l_y')-D(z;0l_y')] \tag{2.14a}$$

and

$$\sum_{l_y''}[z\delta_{l_y l_y''}+M(l_y l_y'')]D(z;l_y''l_y')$$
$$=\tfrac{1}{2}H_s\delta_{l_y,0}[D(z;0l_y')-G(z;0l_y')] . \tag{2.14b}$$

If we introduce the Green's function $G_s(z;l_y l_y')$ of the semi-infinite Heisenberg ferromagnet with surface anisotropy H_s set to zero, Eq. (2.14) may be written

$$G(z;l_y l_y')=G_s(z;l_y l_y')+\tfrac{1}{2}H_s G_s(z;l_y 0)$$
$$\times[G(z;0l_y')-D(z;0l_y')] \tag{2.15a}$$

and

$$D(z;l_y l_y')=-\tfrac{1}{2}H_s G_s(-z;l_y 0)[G(z;0l_y')-D(z;0l_y')] . \tag{2.15b}$$

To obtain these results, one uses

$$G_s(z;l_y l_y')=[z\delta_{l_y l_y'}-M(l_y l_y')]^{-1} .$$

It is a simple matter to solve Eqs. (2.15):

$$G(z;l_yl_y')=G_s(z;l_yl_y')+\tfrac{1}{2}H_s\frac{G_s(z;l_y0)G_s(z;0l_y')}{\{1-(H_s/2)[G_s(z;00)+G_s(-z;00)]\}} . \tag{2.16}$$

Our final task is to obtain $G_s(z;l_yl_y')$. This has been done elsewhere, but for completeness we sketch the derivation. The equation obeyed by this function is

$$zG_s(z;l_yl_y')=-\delta_{l_yl_y'}+\delta_{l_y,0}d_{\parallel}^{(s)}G_s(z;0l_y')+(1-\delta_{l_y,0}]d_{\parallel}G_s(z;l_yl_y')-d_{\perp}G_s(z;l_y+1,l_y')-(1-\delta_{l_y,0})d_{\perp}G_s(z;l_y-1,l_y') . \tag{2.17}$$

One considers l_y' fixed, and considers G_s to be a function of l_y. For $l_y>0$, we have the simple structure

$$zG_s(z;l_yl_y')-d_{\parallel}G_s(z;l_yl_y')-d_{\perp}G_s(z;l_y+1,l_y')+d_{\perp}G_s(z;l_y-1,l_y')=-\delta_{l_yl_y'} . \tag{2.18}$$

while for $l_y=0$, assuming $l_y'>0$ for the moment, we have

$$zG_s(z;0l_y')-d_{\parallel}^{(s)}G_s(z;0l_y')-d_{\perp}G_s(z;1,l_y')=0 . \tag{2.19}$$

We divide the line $0\le l_y\le\infty$ into two segments, $l_y\ge l_y'$ and $0\le l_y<l_y'$. We then introduce $\kappa_{\perp}(z)$, determined by

$$\cos[\kappa_{\perp}(z)]=\frac{(d_{\parallel}-z)}{2d_{\perp}} , \tag{2.20}$$

where $\kappa_{\perp}(z)$ is chosen always so that $\mathrm{Im}(\kappa_{\perp})>0$. For $l_y\ge l_y'$, we have

$$G_s(z;l_yl_y')=A^{>}e^{i\kappa_{\perp}l_y} , \tag{2.21a}$$

while for $0\le l_y\le l_y'$ we have

$$G_s(z;l_yl_y')=A_{+}^{\le}e^{i\kappa_{\perp}l_y}+A_{-}^{\le}e^{-i\kappa_{\perp}l_y} , \tag{2.21b}$$

The two forms for G_s must agree at $l_y=l_y'$, and must also satisfy Eq. (2.18) and Eq. (2.19). From these, we may determine the three coefficients $A^{>}$, $A^{<}$, and $A_{-}^{\le}$. When this is done, one finds

$$G_s(z;l_yl_y')=\frac{i}{2d_{\perp}\sin(\kappa_{\perp})}\left[e^{i\kappa_{\perp}|l_y-l_y'|}-\left[\frac{\Delta d_{\parallel}+d_{\perp}e^{i\kappa_{\perp}}}{\Delta d_{\parallel}+d_{\perp}e^{-i\kappa_{\perp}}}\right]e^{i\kappa_{\perp}(l_y+l_y')}\right] . \tag{2.22}$$

We have defined

$$\Delta d_{\parallel}(\mathbf{k}_{\parallel})=d_{\parallel}^{(s)}(\mathbf{k}_{\parallel})-d(\mathbf{k}_{\parallel}) . \tag{2.23}$$

Our interest is in the full Green's function $G(z;l_yl_y')$ evaluated at $l_y'=l_y$. This may be expressed compactly in terms of

$$g_{\infty}(z)=\frac{i}{2d_{\perp}\sin[\kappa_{\perp}(z)]} \tag{2.24}$$

and

$$g_s(z)=\frac{1}{\Delta d_{\parallel}+d_{\perp}\exp[-i\kappa_{\perp}(z)]} . \tag{2.25}$$

One finds, after a bit of algebra,

$$G(z;l_yl_y)=[1-\exp(i2\kappa_{\perp}l_y)]g_{\infty}(z)+g_s(z)\exp(i2\kappa_{\perp}l_y)\times\left[1+\tfrac{1}{2}H_s\frac{g_s(z)}{1-\frac{1}{2}H_s[g_s(z)+g_s(-z)]}\right] . \tag{2.26}$$

Upon noting $\mathrm{Im}(\kappa_{\perp})>0$, one sees that as $l_y\to\infty$, $G(z;l_yl_y)\to g_{\infty}(z)$ independent of l_y. Thus, $g_{\infty}(z)$ is the bulk Green's function from which the spin deviation deep in the crystal is determined. With $H_s=0$, at $l_y=0$ $G(z;00)$ reduces to $g_s(z)$. This function thus controls the spin deviation at the surface of the ferromagnet, in the absence of surface anisotropy.

The result in Eq. (2.26) is an exact solution of the problem, in the spin-wave limit. At this point, we have made no assumptions about the relative order of magnitude of the various terms in the Hamiltonian. This will be done is Sec. III, when we extract explicit results from the Green's functions.

We conclude with a few general remarks on the behavior of the function $\kappa_{\perp}(z)$, whose analytic structure controls that of the Green's function.

We begin with remarks on the bulk properties of the model. The crystal admits bulk spin waves of plane wave character. Their dispersion relation can be expressed in terms of the quantities introduced above. In the bulk, the wave vector $\mathbf{k}=\mathbf{k}_{\parallel}+\hat{\mathbf{y}}k_{\perp}$ is a three-dimensional wave vector, of course. The frequency $\Omega_B(\mathbf{k}_{\parallel}k_{\perp})$ of a spin wave of wave vector $\mathbf{k}$ is easily shown to be

$$\Omega_B(\mathbf{k}_{\parallel}k_{\perp})=d_{\parallel}(\mathbf{k}_{\parallel})-2d_{\perp}(\mathbf{k}_{\parallel})\cos(k_{\perp}d) , \tag{2.27}$$

where d is the spacing between adjacent planes parallel to the surface. We assume both $d_{\parallel}(\mathbf{k}_{\parallel})$ and $d_{\perp}(\mathbf{k}_{\parallel})$ are positive, as they will be in the long-wavelength limit appropriate to our subsequent discussion of thermally excited spin waves.

Then for fixed $\mathbf{k}_{\parallel}$, the band of bulk frequencies is bounded from below by $\Omega_m(\mathbf{k}_\parallel)$ and above by $\Omega_M(\mathbf{k}_\parallel)$, where

$$\Omega_m(\mathbf{k}_\parallel)=d_\parallel(\mathbf{k}_\parallel)-2d_\perp(\mathbf{k}_\parallel)\ , \tag{2.28a}$$

$$\Omega_M(\mathbf{k}_\parallel)=d_\parallel(\mathbf{k}_\parallel)+2d_\perp(\mathbf{k}_\parallel)\ . \tag{2.28b}$$

Then Eq. (2.20) becomes

$$\cos[\kappa(z)]=1-2\left[\frac{z-\Omega_m(\mathbf{k}_\parallel)}{\Omega_M(\mathbf{k}_\parallel)-\Omega_m(\mathbf{k}_\parallel)}\right]\ . \tag{2.29}$$

Now let $z\to\Omega+i\eta$, with η infinitesimal. There are three frequency regimes, and $\kappa_\perp(z)$ behaves as follows.

(i) $\Omega_M<\Omega<\infty$: Here $\kappa_\perp(z)\to i\pi+\gamma^>(\Omega)$, where

$$\cosh(\gamma^>)=2\left[\frac{\Omega-\Omega_m}{\Omega_M-\Omega_m}\right]-1\ . \tag{2.30}$$

(ii) $\Omega_m<\Omega<\Omega_M$: One has $\kappa_\perp$ real, with

$$\cos(\kappa_\perp)=1-2\left[\frac{\Omega-\Omega_m}{\Omega_M-\Omega_m}\right]\ . \tag{2.31}$$

(iii) $-\infty<\Omega<+\Omega_m$: In this regime, $\kappa_\perp$ is pure imaginary, $\kappa_\perp=i\gamma^<$, where

$$\cosh(\gamma^<)=1+2\left[\frac{\Omega_m-\Omega}{\Omega_M-\Omega_m}\right]\ . \tag{2.32}$$

In our Green's function, we also encounter $\kappa_\perp(-z)$, where $z=\Omega+i\eta$. For this quantity we have the following.

(i) $-\infty<\Omega<-\Omega_M$: One has

$$\kappa_\perp(-z)=i\pi+\gamma^>(|\Omega|)\ ,$$

where

$$\cosh[\gamma^>(|\Omega|)]=2\left[\frac{|\Omega|-\Omega_m}{\Omega_M-\Omega_m}\right]-1\ . \tag{2.33}$$

(ii) $-\Omega_M<\Omega<-\Omega_m$: Here we have

$$\kappa_\perp(-z)\to\kappa_\perp(|\Omega|)\ ,$$

where

$$\cos[\kappa_\perp(|\Omega|)]=1-2\left[\frac{|\Omega|-\Omega_m}{\Omega_M-\Omega_m}\right]\ . \tag{2.34}$$

(iii) $-\Omega_m\le\Omega<\infty$: Now

$$\kappa_\perp(-z)\to i\gamma_-(\Omega)$$

where

$$\cosh[\gamma_-(\Omega)]=1+2\left[\frac{\Omega_m+\Omega}{\Omega_M-\Omega_m}\right]\ . \tag{2.35}$$

III. EXPLICIT RESULTS

In the preceding section, we obtained formal results which allow us to analyze the influence of surface anisotropy on the surface magnetization of the Heisenberg model in the spin-wave regime. We now turn to a detailed study of the various contributions. For this purpose, we require explicit expressions for the various functions which enter the formulas of Sec. II. We turn to a specific model for this purpose, the fcc crystal with (100) surface. Within the surface, the exchange interactions assume the value J_s, possibly different from the bulk exchange J. The range of all exchange couplings is confined to nearest neighbors.

It should be emphasized that our conclusions do not depend on this choice of model; one may see that the variation with wave vector and frequency of various characteristic quantities that enter the analysis are similar to those found below for a wide class of models. Only numerical prefactors differ. It is essential that the range of the exchange couplings is microscopic, and that alterations in the strength of exchange couplings near the surface are confined to a microscopic region near the surface for these results to hold. Of course, J_s must not differ so markedly from J that the magnetic structure at the surface differs from that found in the bulk.[16]

We let a_0 be the lattice constant of the fcc crystal; $a_0/2$ is then the distance between adjacent (100) planes. We shall always consider modes whose wavelength is long compared to a lattice constant. Thus, various quantities defined in Sec. II may be approximated by long-wavelength expansions. We let $\mathbf{k}_\parallel=\hat{\mathbf{x}}k_x+\hat{\mathbf{z}}k_z$ to find

$$d_\parallel(\mathbf{k}_\parallel)=H_0+2H_x+\tfrac{1}{8}H_x a_0^2k_\parallel^2-\frac{H_x a_0^4}{384}(k_x^4+6k_x^2k_z^2+k_z^4)+\cdots\ , \tag{3.1a}$$

$$d_\perp(\mathbf{k}_\parallel)=\tfrac{1}{2}H_x\left[2-\tfrac{1}{8}a_0^2k_\parallel^2+\frac{a_0^2}{384}(k_x^4+k_z^4)+\cdots\right]\ , \tag{3.1b}$$

$$d_\parallel^{(s)}(\mathbf{k}_\parallel)=H_0+\tfrac{1}{2}H_x+\tfrac{1}{8}\epsilon H_x a_0^2k_\parallel^2-\frac{\epsilon H_x a_0^4}{384}(k_x^4+6k_x^2k_z^2+k_z^4)\ , \tag{3.1c}$$

and

$$\Delta d_\parallel(\mathbf{k}_\parallel)=H_x-\tfrac{1}{8}(1-\epsilon)H_x a_0^2k_\parallel^2-\frac{H_x(1-\epsilon)a_0^4}{384}(k_x^4+6k_x^2k_z^2+k_z^4)+\cdots\ . \tag{3.1d}$$

We have introduced $H_x=4JS$, which serves as a measure of the strength of the exchange field experienced by a spin in the lattice. Also $\epsilon=J_s/J$.

We now divide the discussion up into subsections.

A. Influence of surface anisotropy on surface spin waves

The surface spin waves of interest here have excitation energies which lie below the minimum bulk spin-wave frequency $\Omega_m(\mathbf{k}_\parallel)$ defined in Sec. II. For the fcc crystal considered here, in the long-wavelength limit, one has

$$\Omega_m(\mathbf{k}_\parallel)=H_0+\tfrac{1}{4}H_x a_0^2 k_\parallel^2-\frac{H_x a_0^4}{192}(k_x^4+3k_x^2k_z^2+k_z^4)+\cdots . \tag{3.2}$$

The surface spin waves appear as poles in the Green's function,[9] in the frequency regime $|\Omega|<\Omega_m$. Such poles may arise only from the terms involving $g_s(z)$ in Eq. (2.26). The implicit dispersion relation is then

$$1-\tfrac{1}{2}H_s[g_s(\Omega_s)+g_s(-\Omega_s)]=0 , \tag{3.3}$$

where $\Omega_s(\mathbf{k}_\parallel)$ is the dispersion relation of the surface mode.

Quite clearly, if $+\Omega_s(k_\parallel)$ is a root of Eq. (3.3), so is $-\Omega_s(\mathbf{k}_\parallel)$. The surface wave gives rise to a pole both on the positive real axis, and the negative real axis of the frequency plane. In earlier work, for a given choice of $\mathbf{k}_\parallel$, the spin-wave Green's function contained a surface wave pole only on the positive real axis.

This new feature is introduced by surface anisotropy, and its physical origin can be appreciated from a study of the equations of motion of the spin system. With $H_s=0$, all bulk and surface spin waves are circularly polarized. Mathematically, if one examines the equation of motion of the operator $S_-(l)$, which creates a single spin deviation on site l in the spin-wave regime [$S_z(l)$ is replaced by $+S$ in the equations of motion in this limit], the operator $S_-(l)$ is coupled only to operators $\{S_-(l')\}$ that describe single spin deviations on the same or nearest-neighbor sites. The equations of motion admit only positive-frequency solutions.

When $H_s\neq 0$, for a site l within the surface layer, the linearized equation of motion for $S_-(l)$ contains terms in $S_+(l)$ also. It is easy to see that this induces elliptical character in both the bulk and surface spin waves. If one launches a circularly polarized bulk wave deep in the crystal in the direction of the surface, the reflected waves will have elliptically polarized character. The residue of the surface spin-wave pole on the negative frequency axis can be viewed as a measure of the degree of ellipticity in the wave; as $H_s\to 0$, this residue vanishes, leaving a contribution to $\Delta(l_y)$ from only the positive frequency pole.

The presence of the surface anisotropy also leads to zero point oscillations in the spin system near the surface, at $T=0$. The fully aligned state, with spins along the external magnetic field, is no longer an exact eigenstate of the Hamiltonian, when $H_s\neq 0$. Mathematically, one sees how the zero-point contributions to $\Delta(l_y)$ enter within the present formalism by noting the identity

$$n(-\Omega)=-1-n(\Omega) ,$$

and that

$$\mathrm{Im}[G(\mathbf{k}_\parallel\Omega+i\eta;l_y l_y)]$$

is negative when $\Omega<0$. The negative frequency pole at $-\Omega_s$, along with the branch cut on the negative frequency axis in the range $-\Omega_M<\Omega<-\Omega_m$ both contribute to the zero point motion of the spins near the surface, at $T=0$. We shall estimate its amplitude below, to find it quite small under the conditions of primary interest to the present study.

We need an expression for $g_s(\Omega)$ in Eq. (33). In the low-frequency, long-wavelength regime, in Eq. (2.25) we may replace $\exp[-i\kappa_\perp(z)]$ by $1-i\kappa_\perp(z)$, so that

$$g_s(z)\cong\frac{1}{\Delta d_\parallel(\mathbf{k}_\parallel)+d_\perp(\mathbf{k}_\parallel)-id_\perp(\mathbf{k}_\parallel)_\parallel\kappa_\perp(z)} \tag{3.4}$$

and $d_\perp(\mathbf{k}_\parallel)\kappa_\perp(z)$ may be replaced by $d_\perp(0)\kappa_\perp(z)$. This provides a good approximation when $\Omega_m(k_\parallel)\ll H_x$, and $k_\parallel a_0\ll 1$. When Eq. (2.20) is then used to relate $\kappa_\perp(z)$ to the frequency, for $-\Omega_m\le\Omega\le+\Omega_m$, we find

$$g_s(\Omega)\cong\frac{1}{-H_x\beta(k_\parallel)+H_x^{1/2}(\Omega_m-\Omega)^{1/2}} , \tag{3.5a}$$

where

$$\beta(k_\parallel)=\tfrac{1}{16}[1+2(1-\epsilon)]a_0^2k_\parallel^2 . \tag{3.5b}$$

We shall assume throughout that $\epsilon<\frac{3}{2}$. If this inequality is not satisfied, one may demonstrate that when $H_s=0$, the long-wavelength surface spin waves studied in Refs. 5, 6, and 9 are pushed up into the bulk spin-wave bands by the presence of surface anisotropy.

The frequency of the surface spin waves is then found from the implicit dispersion relation

$$[(\Omega_m-\Omega)^{1/2}-H_x^{1/2}\beta][(\Omega_m+\Omega)^{1/2}-H_x^{1/2}\beta] =\tfrac{1}{2}\frac{H_s}{H_x^{1/2}}[(\Omega_m-\Omega)^{1/2}+(\Omega_m+\Omega)^{1/2}-2H_x^{1/2}\beta] . \tag{3.6}$$

In the absence of surface anisotropy, Eq. (3.6) admits the solutions

$$\lim_{H_s\to 0}\Omega_s(\mathbf{k}_\parallel)=\pm[\Omega_m(\mathbf{k}_\parallel)-H_x\beta^2(\mathbf{k}_\parallel)] . \tag{3.7}$$

These surface waves are identical in character to those studied some years ago, in analyses of the semi-infinite Heisenberg ferromagnet.[5,6,9] They lie lower in frequency than the bulk spin waves, and in the limit $k_\parallel a_0\ll 1$ their frequency differs from that of a bulk spin wave propagating parallel to the surface only by terms in $(k_\parallel a_0)^4$. They are thus very weakly bound compared to other examples of surface waves one encounters. For example, Rayleigh surface acoustic waves propagate with a sound velocity lower than that of any bulk phonon. For surface acoustic waves, the surface mode dispersion relation thus differs from that of any bulk wave to lowest order in $k_\parallel a_o$.

As the wave vector approaches zero, the frequency of all bulk spin waves approaches the Zeeman frequency of an isolated spin, which is H_0 in our units. In the limit $H_s\to 0$, the same statement applies to the surface spin wave. Thus, as $\mathbf{k}_\parallel\to 0$, the surface spin wave becomes degenerate with the very-long-wavelength bulk spin waves.

Addition of even a small amount of surface anisotropy splits the surface spin-wave frequency off below the bulk bands, as $\mathbf{k}_\parallel\to 0$. In this limit, Eq. (3.6) may be solved in closed form:

$$\lim_{k_\parallel \to 0} \Omega_s^2(k_\parallel) = H_0 \left[H_0 - \frac{H_s^2}{2H_x} \lambda \right] \tag{3.8a}$$

with

$$\lambda = \left[\left[1 + \frac{H_s^2}{8H_0 H_x} \right]^{1/2} + \frac{H_s}{2\sqrt{2} H_0^{1/2} H_x^{1/2}} \right]^2 . \tag{3.8b}$$

In the limit of interest in this study, where H_0 and H_s are similar in magnitude and both small compared to $H_x, \lambda \simeq 1$ to good approximation, and

$$\lim_{k_\parallel \to 0} \Omega_s(k_\parallel) \cong \left[H_0 \left[H_0 - \frac{H_s^2}{2H_x} \right] \right]^{1/2} . \tag{3.9}$$

Notice that (when $\lambda \cong 1$) if H_s is so large that

$$H_s > H_s^{(c)} = (2H_0 H_x)^{1/2} ,$$

one finds $\Omega_s^2(0) < 0$. For surface anisotropy fields this large, our assumed ground state, with spins in each layer including the surface layer parallel to the external Zeeman field, becomes unstable. For $H_s > H_s^{(c)}$, spins near the surface will be canted away from the bulk magnetization, in the direction of the easy axis.

Our model system is stabilized by the external field H_0. In its absence, Ω_s^2 is negative at $\mathbf{k}_\parallel = 0$ for any value of H_s. In a real system, where dipolar fields are present, in the limit $H_0 \to 0$, the ground-state spin configuration is stabilized near the surface by dipolar fields generated by canting of the spin array. This question has been studied by the present author recently,[17] and in the limit $H_0 \to 0$ the spins in all layers, including the surface, prefer to align parallel to the surface until

$$H_x > H_s^{(c)} = 4\pi M(\xi + 1) ,$$

where $\xi \cong (H_x / 4\pi M)^{1/2}$ in present notation.

With H_s in the range of a few tesla, and H_0 the order of a tesla or so, the values of $H_s^{(c)}$ lie well above H_s, and the ground state used here is appropriate. This may not be the case in ferromagnetic materials whose Curie temperature lies well below that of Fe or Ni, which are the materials we have in mind in the present analysis.

The dependence of $\Omega_s(\mathbf{k}_\parallel)$ on the wave vector $k_\parallel$ is complicated, and we explore only one limit. This is the character of the surface spin waves important in our upcoming discussion of the thermally excited modes. These have energies the order of $k_B T$, which we assume is large compared to H_o and H_s. The excitation energy of such modes is dominated by exchange. The surface anistropy field H_s may then be viewed as a modest perturbation on the frequency of these waves. In this regime, we show in Appendix A that the dispersion relation of the surface waves is approximated well by the expression

$$\Omega_s(k_\parallel) \cong \Omega_m(\mathbf{k}_\parallel) - H_x \left[\beta + \frac{H_s}{2H_x} \right]^2 . \tag{3.10}$$

We shall use the following result in our study of the surface wave contribution to the mean spin deviation near the surface. Note, as demonstrated in Appendix A that Eq. (3.10) requires for its validity

$$k_\parallel a_0 \gg H_x (H_s / H_x)^2 .$$

As a consequence, it does not reduce to Eq. (3.9) as $k_\parallel \to 0$. As noted in Appendix A, this form is appropriate for our discussion of thermally excited spin waves in a material such as Fe, everywhere but at rather low temperatures.

B. The surface spin-wave contribution to the mean spin deviation

We must evaluate

$$\mathrm{Im}[G(\Omega + i\eta; l_y l_y)] ,$$

for the Green's function displayed in Eq. (2.26). The frequency regime of interest is $-\Omega_m < \Omega < +\Omega_m$ where, as we have seen from the preceding section, there are two surface spin-wave poles at $\pm\Omega_s$.

In this frequency regime, $\kappa_\perp$ is pure imaginary. We let

$$\kappa_\perp = i\gamma(\Omega) \tag{3.11a}$$

where, within the framework of the low-frequency, long-wavelength limit of the previous paragraph, we have

$$\gamma(\Omega) = \frac{(\Omega_m - \Omega)^{1/2}}{H_x^{1/2}} . \tag{3.11b}$$

It will also be convenient to let

$$D(z) = [g_s(z)]^{-1} ,$$

so in the frequency regime of interest,

$$D(\Omega) = H_x^{1/2} (\Omega_m - \Omega)^{1/2} - H_x \beta(k_\parallel) .$$

The first term in the Green's function in Eq. (2.26),

$$[1 - \exp(i 2\kappa_\perp l_y)] g_\infty ,$$

is purely real, as is g_s itself. We can then write

$$\mathrm{Im}[G(l_y l_y; \Omega + i\eta)] = e^{-2\gamma(\Omega) l_y} \mathrm{Im} \left[\frac{N(\Omega)}{F(\Omega)} \right] , \tag{3.12}$$

where, letting $\eta \to 0$ in the numerator,

$$N(\Omega) = D(-\Omega) - \tfrac{1}{2} H_s \tag{3.13a}$$

and

$$F(\Omega) = D(\Omega + i\eta) D(-\Omega - i\eta) - \tfrac{1}{2} H_s [D(\Omega + i\eta) + D(-\Omega - i\eta)] . \tag{3.13b}$$

The discussion in Sec. III A shows $F(\Omega)$ has zeros at $\pm\Omega_s$, and consequently $G(l_y l_y; \Omega + i\eta)$ has poles there. We can perform a Taylor series expansion about each pole, noting they are responsible for the nonvanishing imaginary part of G. If $F'(\Omega) = dF/d\Omega$, we then have

$$\frac{1}{i\pi}\text{Im}[G(l_y l_y;\Omega+i\eta)]=\exp[-2\gamma(\Omega)l_y]\left[\frac{N(\Omega_s)}{F'(\Omega_s)}\delta(\Omega-\Omega_s)+\frac{N(-\Omega_s)}{F'(-\Omega_s)}\delta(\Omega+\Omega_s)\right]. \tag{3.14}$$

After a few lines of computation, one finds

$$F'(\Omega)=\tfrac{1}{2}H_x^{1/2}\left\{(\tfrac{1}{2}H_s+H_x\beta)[(\Omega_m-\Omega)^{-1/2}-(\Omega_m+\Omega)^{-1/2}]-H_x^{1/2}\left[\left[\frac{\Omega_m+\Omega}{\Omega_m-\Omega}\right]^{1/2}-\left[\frac{\Omega_m-\Omega}{\Omega_m+\Omega}\right]^{1/2}\right]\right\}. \tag{3.15}$$

We define

$$\gamma_+=\frac{(\Omega_m-\Omega_s)^{1/2}}{H_x^{1/2}} \tag{3.16}$$

and

$$\gamma_-=\frac{(\Omega_m+\Omega_s)^{1/2}}{H_x^{1/2}} \tag{3.17}$$

to find

$$F'(\Omega)=\tfrac{1}{2}\left[(H_x\beta+\tfrac{1}{2}H_s)\left[\frac{1}{\gamma_+}-\frac{1}{\gamma_-}\right]-H_x\left[\frac{\gamma_-}{\gamma_+}-\frac{\gamma_+}{\gamma_-}\right]\right] \tag{3.18}$$

and $F'(-\Omega_s)=-F'(\Omega_s)$.

Under the conditions of interest, we may show that $\gamma_-\gg\gamma_+$. We may use Eq. (3.10) to evaluate γ_+ and little error is involved if we replace Ω_s by Ω_m in the evaluation of γ_-. This gives

$$\gamma_+\cong\frac{H_s}{2H_x}+\beta(k_\parallel) \tag{3.19a}$$

and

$$\gamma_-\cong\frac{1}{\sqrt{2}}k_\parallel a_0\ . \tag{3.19b}$$

One sees $k_\parallel a_0 \gg \beta(k_\parallel)$ by noting β is of order $(k_\parallel a_0)^2$. The remarks at the end of Appendix A establish that $k_\parallel a_0$ is larger than H_s/H_x in the thermal spin-wave regime, for a material such as Fe.

We then have

$$F'(\Omega_s)\cong\frac{1}{2\gamma_+}(\tfrac{1}{2}H_s+H_x\beta-H_x\gamma_-)=\frac{H_x}{2\gamma_+}(\gamma_+-\gamma_-)\cong-\tfrac{1}{2}H_x\frac{\gamma_-}{\gamma_+}\ . \tag{3.20}$$

Thus, we have

$$\frac{1}{i\pi}\text{Im}[G(l_y l_y;\Omega+i\eta)]=\frac{2}{H_x}\frac{\gamma_+}{\gamma_-}[N(\Omega_s)e^{-2\gamma_+l_y}\delta(\Omega-\Omega_s)-N(-\Omega_s)e^{-2\gamma_-l_y}\delta(\Omega+\Omega_s)]\ . \tag{3.21}$$

For $N(\Omega_s)$, one sees

$$N(\Omega_s)=H_x^{1/2}(\Omega_m+\Omega_s)^{1/2}-H_x\beta-\tfrac{1}{2}H_s=H_x(\gamma_--\gamma_+)\cong H_x\gamma_-\ . \tag{3.22}$$

Upon noting the (exact) identity

$$N(\Omega_s)N(-\Omega_s)=\tfrac{1}{4}H_s^2\ ,$$

we have

$$N(-\Omega_s)=\frac{H_s^2}{4H_x\gamma_-}\ . \tag{3.23}$$

When these results are assembled, in the frequency regime $-\Omega_m\le\Omega\le+\Omega_m$, one finds

$$\frac{1}{i\pi}\text{Im}[G(l_y l_y;\Omega+i\eta)]=2\gamma_+e^{-2\gamma_+l_y}\delta(\Omega-\Omega_s)-\frac{H_s^2}{2H_x^2}\frac{\gamma_+}{\gamma_-}e^{-2\gamma_-l_y}\delta(\Omega+\Omega_s)\ . \tag{3.24}$$

From Eq. (2.7), and the identity

$$n(-\Omega)=-1-n(\Omega)\ ,$$

we have the surface wave contribution to the mean spin deviation, $\Delta_s(l_y)$, given by

$$\Delta_s(l_y)=\frac{1}{N_s}\sum_{\mathbf{k}_\parallel}2\gamma_+(\mathbf{k}_\parallel)\exp[-2\gamma_+(k_\parallel)l_y]n(\Omega_s(k_\parallel))+\frac{1}{N_s}\frac{H_s^2}{2H_x^2}\sum_{\mathbf{k}_\parallel}\frac{\gamma_+(\mathbf{k}_\parallel)}{\gamma_-^2(k_\parallel)}\exp[-2\gamma_-(k_\parallel)l_y]\times[1+n(\Omega_s(k_\parallel))]\ . \tag{3.25}$$

We shall turn to the contribution from the bulk spin waves next. Before we do, some general comments are in order.

As the temperature $T\rightarrow 0$, the right-hand side of Eq. (3.25) remains finite. The surface anisotropy has induced zero-point motions in the spin system, in the near vicinity of the surface. Mathematically, this contribution has its origin in the pole which resides on the negative axis of the frequency plane. While the presence of this contribution is surely interesting in principle, at least in the parameter regime we explore it is also quite small in magnitude, as one sees from the prefactor and our earlier conclusion that $\gamma_-\gg\gamma_+$.

The spatial dependence of Δ_s contains two distinct decay constants γ_+ and γ_-. One sees from an analysis of the equations of motion of the spin system that when $H_s \neq 0$, the surface spin wave eigenfunction contains these two decay constants, γ_+ and γ_-. When $H_s \equiv 0$, and we have the simple Heisenberg ferromagnet, the surface spin waves are circularly polarized, with a single decay constant, for models in the class explored here.[5,6] As soon as $H_s \neq 0$, the wave becomes elliptically polarized; one has a superposition of right and left circularly polarized waves, each with its own decay constant. As demonstrated in earlier papers,[13,14] if dipolar interactions are incorporated into the theory, the surface wave eigenfunction contains three decay constants, not just two. The discussion then becomes quite complex.

As $H_s \to 0$, the expression for $\Delta_s(l_y)$ in Eq. (3.25) reduces to $\Delta_s^{(0)}(l_y)$, where

$$\Delta_s^{(0)}(l_y)=\frac{1}{N_s}\sum_{\mathbf{k}_\parallel} 2\beta(\mathbf{k}_\parallel)\exp[-2\beta(\mathbf{k}_\parallel)l_y]n(\Omega_s(k_\parallel)) \ . \tag{3.26}$$

This result is identical in form to that derived many years ago by Maradudin and the present author.[9]

C. The bulk spin-wave contribution to the mean spin deviation

We are here concerned with the frequency regimes $\Omega_m \le \Omega \le +\Omega_M$, and also when $H_s \neq 0$, $-\Omega_M \le \Omega \le -\Omega_m$. We write

$$G(z;l_y l_y)=g_\infty(z)+\Delta G(z;l_y) \ , \tag{3.27}$$

and consider first the contribution from $g_\infty(z)$, which is independent of l_y.

As $\eta \to 0, \kappa_\perp(\Omega+i\eta)$ approaches a real positive number, for Ω in the range $\Omega_m \le \Omega \le \Omega_M$, and it is pure imaginary everywhere outside this range. It follows that $\mathrm{Im}[g_\infty(\Omega+i\eta)]$ is nonzero only for $\Omega_m \le \Omega \le \Omega_M$. In this frequency range

$$\frac{1}{i\pi}\mathrm{Im}[g_\infty(\Omega+i\eta)]=\frac{1}{2\pi}\frac{1}{d_\perp(k_\parallel)\sin[\kappa_\perp(\Omega)]} \ . \tag{3.28}$$

Then calling this contribution to the mean spin deviation $\Delta(\infty)$,

$$\Delta(\infty)=\frac{1}{2\pi N_s}\sum_{\mathbf{k}_\parallel}\int_{\Omega_m}^{\Omega_M}\frac{d\Omega\, n(\Omega)}{d_\perp(k_\parallel)\sin[\kappa_\perp(\Omega)]} \ . \tag{3.29}$$

One changes the integration on frequency to one on the variable $k_\perp = 2\kappa_\perp(\Omega)/a_0$ to find

$$\Delta(\infty)=\frac{a_0}{2\pi}\frac{1}{N_s}\sum_{\mathbf{k}_\parallel}\int_0^{2\pi/a_0} dk_\perp n(\Omega(\mathbf{k})) \ , \tag{3.30}$$

where $\Omega(\mathbf{k})$ is the frequency of a bulk spin wave of wave vector $\mathbf{k}=\mathbf{k}_\parallel+\hat{\mathbf{z}}k_\perp$.

The expression in Eq. (3.30) may be shown to be identical to the mean spin deviation in the bulk of the crystal, as provided by spin-wave theory. The Brillouin zone employed is different in shape (but not in volume) to the first Brillouin zone commonly used in solid-state physics; this is because our analysis is based on the surface Brillouin zone for the network of $\mathbf{k}_\parallel$ values. Periodicity of $\Omega(\mathbf{k})$ in the reciprocal lattice ensures that our expression is identical to that which employs the conventional first Brillouin zone. At low temperatures, for Δ_∞ we have the well-known Bloch $T^{3/2}$ law

$$\Delta(\infty)=C_\infty T^{3/2} \ , \tag{3.31a}$$

where for our model

$$C_\infty=\frac{\zeta(\frac{3}{2})}{2\pi^{3/2}}\left[\frac{k_B}{H_x}\right]^{3/2} \ . \tag{3.31b}$$

The contribution from $\Delta G(z;l_y)$ describes the contribution from bulk spin waves to the spatial variation of the magnetization near the surface. We separate the discussion of the regime $\Omega_m \le \Omega \le \Omega_M$ from $-\Omega_M \le \Omega \le -\Omega_m$.

1. *The frequency regime* $\Omega_m \le \Omega \le \Omega_M$

As before, we write $g_s(z)=1/D(z)$, and note that for $\Omega>0, d(-\Omega-i\eta)$ has no branch cut. Consequently, this may be replaced by $D(-\Omega)$. Then one has

$$\mathrm{Im}[\Delta G(\Omega+i\eta;l_y)]\mathrm{Im}\left[e^{i2\kappa_\perp l_y}\left[\frac{1}{2id_\perp\sin\kappa_\perp}+\frac{1}{D(\Omega+i\eta)-\Gamma(\Omega)}\right]\right] \ , \tag{3.32}$$

where

$$\Gamma(\Omega)=\frac{1}{2}\frac{H_s D(-\Omega)}{D(-\Omega)-\frac{1}{2}H_s} \tag{3.33}$$

is purely real. Upon recalling that

$$D(\Omega+i\eta)=\Delta d_\parallel + d_\perp e^{-i\kappa_\perp} \ ,$$

a bit of rearrangement gives

$$\mathrm{Im}[\Delta G(\Omega+i\eta;l_y)]=\mathrm{Im}\left[\frac{e^{i2\kappa_\perp l_y}}{2id_\perp\sin(k_\perp)}\times\left[\frac{\Delta d_\parallel-\Gamma+d_\perp e^{i\kappa_\perp}}{\Delta d_\parallel-\Gamma+d_\perp e^{-i\kappa_\perp}}\right]\right] \tag{3.34}$$

from which it follows that

$$\frac{1}{2\pi}\text{Im}[\Delta G(\Omega+i\eta;l_y)]=\frac{1}{2\pi}\frac{\cos(2\kappa_\perp l_y+2\psi)}{d_\perp\sin(\kappa_\perp)} \quad (3.35)$$

The angle ψ is found from the relation

$$\tan(\psi)=\frac{\Gamma-\Delta d_\parallel-d_\perp\cos(\kappa_\perp)}{d_\perp\sin(\kappa_\perp)} . \quad (3.36)$$

The results in Eqs. (3.35) and (3.36) are exact, within the spin-wave limit.

The contribution to the mean spin deviation from the contribution in Eq. (3.35) will be called $\delta\Delta_c^{(+)}$. We find, when the integral on frequency is converted to one on $k_\perp$, where $k_\perp=2\kappa_\perp/a_0$,

$$\delta\Delta_c^{(+)}(l_y)=\frac{a_0}{2\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^{2\pi/a_0}dk_\perp\cos(a_0k_\perp l_y+2\psi)n(\Omega(\mathbf{k})) \quad (3.37)$$

when

$$\Omega(\mathbf{k})=d_\parallel(\mathbf{k}_\parallel)-2d_\perp(\mathbf{k}_\parallel)\cos(a_0k_\perp/2)$$

is the bulk spin-wave frequency. If we set $\psi\equiv 0$ in this expression, we recover Rado's early result.[10]

When $\Omega>0$, our long-wavelength low-frequency approximations allow us to write

$$D(-\Omega)=-H_x\beta(k_\parallel)+H_x^{1/2}(\Omega+\Omega_m)^{1/2} \quad (3.38a)$$

$$\cong H_x^{1/2}(\Omega+\Omega_m)^{1/2} \quad (3.38b)$$

in the regime of interest. Hence,

$$\Gamma(\Omega)=\frac{H_s}{2}\frac{H_x^{1/2}(\Omega+\Omega_m)^{1/2}}{H_x^{1/2}(\Omega+\Omega_m)^{1/2}-\frac{1}{2}H_s}\cong\tfrac{1}{2}H_s \quad (3.39)$$

since, for our thermally excited spin waves,

$$H_x^{1/2}(\Omega+\Omega_m)^{1/2}\cong(H_xk_BT)^{1/2}>>H_s$$

when we have both $H_x>>H_s$, and $k_BT>H_s$. Then when $\Delta d_\parallel+d_\perp\cos(\kappa_\perp)$ is approximated by its long-wavelength form, and we let $\kappa_\perp=a_0k_\perp/2$, one has

$$\tan(\psi)=\frac{a}{b} , \quad (3.40)$$

where

$$a=H_x\beta+H_s/2+H_x(a_0k_\perp)^2/8 ,$$

and

$$b=H_xa_0k_\perp/2 .$$

We may split $\delta\Delta_c^{(+)}(l_y)$ up into three terms, by expanding $\cos(a_0k_\perp l_y+2\psi)$. We define

$$\delta\Delta_{c1}^{(+)}(l_y)=\frac{a_0}{2\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^{2\pi/a_0}dk_\perp\cos(a_0k_\perp l_y)n(\Omega(\mathbf{k})) , \quad (3.41a)$$

$$\delta\Delta_{c2}^{(+)}(l_y)=-\frac{a_0}{\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^{2\pi/a_0}dk_\perp\cos(a_0k_\perp l_y)\times n(\Omega(\mathbf{k}))\sin^2(\psi) , \quad (3.41b)$$

and

$$\delta\Delta_{c3}^{(+)}(l_y)=-\frac{a_0}{\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^{2\pi/a_0}dk_\perp\cos(a_0k_\perp l_y)n(\Omega(\mathbf{k}))\times\sin(\psi)\cos(\psi) , \quad (3.41c)$$

where

$$\delta\Delta_c^{(+)}(l_y)=\sum_{i=1}^{3}\delta\Delta_{ci}^{(+)}(l_y) .$$

In Appendix B, we evaluate $\delta\Delta_{c2}^{(+)}(l_y)$ and $\delta\Delta_{c3}^{(+)}(l_y)$. It is shown that, in the limit of interest here, one has

$$\delta\Delta_c^{(+)}(l_y)=\frac{a_0}{2\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^\infty dk_\perp\cos(a_0k_\perp l_y)n(\Omega(\mathbf{k}))-\frac{2}{N_s}\sum_{\mathbf{k}_\parallel}\gamma_+(\mathbf{k}_\parallel)\exp[-2\gamma_+(\mathbf{k}_\parallel)l_y]n(\Omega_m(\mathbf{k}_\parallel)) . \quad (3.42)$$

We have now arrived at the cancellation theorem discussed in Sec. I. If we overlook the small difference between $\Omega_m(\mathbf{k}_\parallel)$ and $\Omega_s(\mathbf{k}_\parallel)$ (their difference is small compared to k_BT when our basic assumptions are obeyed), then the second term of Eq. (3.42) precisely cancels the first and dominant term in the surface spin wave contribution to the mean spin deviation described in Eq. (3.25). Only the rather small second term in Eq. (3.25) remains as a residue.

2. *The frequency regime* $-\Omega_M\le\Omega\le-\Omega_m$

We let $z=-|\Omega|+i\eta$, and then

$$\kappa_\perp(z)=+i\gamma_-(-|\Omega|) ,$$

where

$$\gamma_-(-|\Omega|)\cong(\Omega_m+|\Omega|)^{1/2}/H_x^{1/2} .$$

Then note

$$\kappa_\perp(-z)=-\kappa_\perp(|\Omega|)=-(|\Omega|-\Omega_m)^{1/2}/H_x^{1/2} .$$

A useful identity is

$$D(|\Omega|-i\eta)=D^*(|\Omega|+i\eta) .$$

After a bit of algebra,

$$\frac{1}{i\pi}\text{Im}[\Delta G(-|\Omega|+i\eta;l_y)]=-\frac{H_s}{4i\pi}\frac{\exp[-2\gamma_-(-|\Omega|)l_y]}{[D(-|\Omega|)-\frac{1}{2}H_s]^2}\text{Im}\left[\frac{1}{d(|\Omega|+i\eta)-\Gamma(|\Omega|)}\right] . \quad (3.43)$$

We have

$$D(-|\Omega|)\cong H_x^{1/2}(\Omega_m+|\Omega|)^{1/2}-H_x\beta(k_\parallel)\cong H_x^{1/2}(\Omega_m+|\Omega|)^{1/2} ,$$

and this is large compared to $H_s/2$. Also

$$D(|\Omega|+i\eta)-\Gamma(|\Omega|)=-[H_s/2+H_x\beta(k_\parallel)]-iH_x^{1/2}(|\Omega|-\Omega_m)^{1/2} ,$$

following approximations analogous to those used earlier [in essence, in the earlier sections, we introduced the variable $k_\perp$, and wrote $|\Omega|=\Omega_m+H_x(k_\perp a_0)^2/4$]. Then a bit more algebra gives

$$\frac{1}{i\pi}\mathrm{Im}[\Delta G(-|\Omega|+i\eta,l_y)]=-\frac{H_s^2}{8\pi H_x^3}\frac{\exp[-2\gamma_-(-|\Omega|)l_y]}{[\gamma_-(|\Omega|)]^2}\frac{a_0k_\perp(|\Omega|)}{\gamma_+^2+[(a_0/2)k_\perp(|\Omega|)]^2} \tag{3.44}$$

where

$$k_\perp(|\Omega|)=2(|\Omega|-\Omega_m)^{1/2}/a_0H_x^{1/2} ,$$

and γ_+ is given in Eq. (3.19a).

We then have a contribution to the mean spin deviation near the surface we call $\Delta_c^{(-)}(l_y)$. This may be written

$$\Delta_c^{(-)}(l_y)=\frac{H_s^2}{8\pi H_x^3}\frac{1}{N_s}\sum_{\mathbf{k}_\parallel}\int_{\Omega_m}^{\infty}d\Omega[1+n(\Omega)]\frac{\exp[-2\gamma_-(-|\Omega|)l_y]}{[\gamma_-(-|\Omega|)]^2}\frac{a_0k_\perp(|\Omega|)}{\gamma_+^2+[(a_{0/2})k_\perp(|\Omega|)]^2} . \tag{3.45}$$

Because of the factor $a_0k_\perp(|\Omega|)$ in the numerator, the last factor falls off slowly enough with $|\Omega|$ that the regime of principal importance is $a_0k_\perp \gg \gamma_+$. Hence γ_+^2 in the denominator may be ignored, and the integral is converted to an integral on $k_\perp$. One then finds, noting

$$\gamma_-(-|\Omega|)^2=(2\Omega_m+\tfrac{1}{4}a_0^2k_\perp^2)/H_x ,$$

$$\Delta_c^{(-)}(l_y)=\frac{a_0H_s}{4\pi H_x}\frac{1}{N_s}\sum_{k_\parallel}\int_0^\infty\frac{dk_\perp}{2\Omega_m(\mathbf{k}_\parallel)+\frac{1}{4}a_0^2H_xk_\perp^2}[1+n(\Omega(k))]\exp[-2\gamma_-(-|\Omega|)l_y] . \tag{3.46}$$

This completes our analysis of the various contributions to the mean spin deviation near the surface, in the presence of surface anisotropy fields.

IV. FINAL RESULTS AND DISCUSSION

When the various contributions above are assembled, for the mean spin deviation one has, with $\delta=2H_0/H_x$,

$$\begin{aligned}\Delta(l_y)=&\frac{a_0}{2\pi N_s}\sum_{\mathbf{k}_\parallel}\int_0^\infty dk_\perp[1+\cos(a_0k_\perp l_y)]n(\Omega(\mathbf{k}))+\frac{2}{N_s}\sum_{\mathbf{k}_\parallel}\gamma_+(\mathbf{k}_\parallel)\exp[-2\gamma_+(\mathbf{k}_\parallel)l_y][n(\Omega_s(k_\parallel))-n(\Omega_m(\mathbf{k}_\parallel))]\\&+\frac{1}{2N_s}\left[\frac{H_s}{H_x}\right]^2\sum_{\mathbf{k}_\parallel}\frac{\gamma_+(\mathbf{k}_\parallel)}{\gamma_-^2(\mathbf{k}_\parallel)}\exp[-2\gamma_-(k_\parallel)l_y][1+n(\Omega_s(\mathbf{k}_\parallel))]\\&+\frac{a_0}{4\pi N_s}\left[\frac{H_s}{H_x}\right]^2\sum_{k_\parallel}\int_0^\infty\frac{dk_\perp\exp[-2\gamma_-(-|\Omega|)_y]}{\delta+\frac{1}{2}a_0^2k_\parallel^2+\frac{1}{4}a_0^2k_\perp^3}[1+n(\Omega(\mathbf{k}))] .\end{aligned} \tag{4.1}$$

The first term is the dominant term in the expression. As $l_y\to 0$, in the low-temperature limit, this provides the contribution $2C_\infty T^{3/2}$ to the mean spin deviation. It is possible to convert the integral into a rapidly converging series, if one wishes to explore the dependence of the mean spin deviation on l_y.[9,18] The spin deviation returns to its bulk value in a distance roughly equal to $(H_x/k_BT)^{1/2}$ layers. There is a long tail, which varies like l_y^{-1}.[9,18]

The second term contains the contribution to the mean spin deviation from the thermally excited surface spin waves, and the "hole" produced in the bulk spin-wave bands which nearly cancel it.

Consider first just the contribution of the surface waves to the spin deviation in the outermost layer. This is given by

$$\Delta_s(0)=\frac{2}{N_s}\sum_{\mathbf{k}_\parallel}\gamma_+(\mathbf{k}_\parallel)n(\Omega_s(k_\parallel)) . \tag{4.2}$$

To good approximation, this may be evaluated by replacing $\Omega_s(k_\parallel)$ by

$$\Omega_s(k_\parallel)=H_0+H_x(a_0k_\parallel)^2/4 ,$$

and we have

$$\gamma_+(k_\parallel)=(H_s/2H_x)+\beta(k_\parallel)$$

in the limit of interest, where

$$\beta(k_\parallel)=(\lambda/16)(k_\parallel a_0)^2 ,$$

and $\lambda=1+2(1-\epsilon)$. When $k_BT \gg H_0$, a short calculation gives

$$\Delta_s(0)=\frac{a_0^2}{4\pi}\frac{k_BT}{H_x}\frac{H_s}{H_x}\ln\left[\frac{k_BT}{H_0}\right]+\frac{a_0^2\lambda}{8\pi}\left[\frac{k_BT}{H_x}\right]^2\zeta(2) , \tag{4.3}$$

where $\zeta(s)$ is the Riemann ζ function of argument s.

We may compare the result in Eq. (4.3) with Rado's principle result,[10] displayed in his Eq. (42). The first term of our Eq. (4.3) agrees with his Eq. (42) in the relevant limit. Note that in his treatment,

$$H_K+2\pi M_0-2K_{ss}^2/M_0A ,$$

is the excitation energy of a surface spin wave of wave vector $\mathbf{k}_\parallel=0$. The term $2\pi M_0$ arises from his approximate[19] treatment of dipolar interactions. This must be set to zero to compare the two results. The field H_K is H_0 in our treatment, and K_{ss}^2/M_0A is analogous to our $H_s^2/2H_x$.[20] In our derivation of Eq. (4.3), we have assumed $H_0 \gg H_s^2/H_x$, and that the surface spin-wave gap is small compared to k_BT. In this limit, Rado's expression for the surface magnetization (set his η to zero) becomes $(K_{ss}k_BT/4\pi A^2)\ln(k_BT/g\mu_BH_K)$, a result identical to the result in our Eq. (4.3) when one realizes his parameter K_{ss} and our H_s are proportional, while his A corresponds to our H_x.

We must take cognizance of the cancellation between the surface wave and the "hole" in the bulk spin-wave bands, however. We note

$$\Omega_s(k_\parallel)=\Omega_m(k_\parallel)-H_x\gamma_+^2(k_\parallel) ,$$

and when our assumptions are obeyed, $H_x\gamma_+^2 \ll k_BT$. Thus

$$n(\Omega_s(k_\parallel))-n(\Omega_m(k_\parallel))\cong -H_x\gamma_+^2(\partial n/\partial\Omega) .$$

If we use this expansion, we have

$$\frac{2}{N_s}\sum_{\mathbf{k}_\parallel}\gamma_+(k_\parallel)[n(\Omega_s(k_\parallel))-n(\Omega_m(k_\parallel))] = -\frac{2H_x}{N_s}\sum_{\mathbf{k}_\parallel}\gamma_+^3\frac{\partial n}{\partial\Omega_m} , \tag{4.4}$$

and if we expand this in powers of H_s we find

$$\frac{2}{N_s}\sum_{k_\parallel}\gamma_+(k_\parallel)[n(\Omega_s(k_\parallel))-n(\Omega_m(k_\parallel))] = \frac{3\lambda^3}{128\pi}\left[\frac{k_BT}{H_x}\right]^3\left[1+\frac{2}{\lambda}\frac{H_s}{k_BT}+\cdots\right] , \tag{4.5}$$

a contribution to the mean spin deviation at the surface that is very small compared to the leading term $2C_\infty T^{3/2}$. The cancellation theorem essentially eliminates the surface wave contribution in the spin-wave temperature regime.

One may also show that the third and fourth terms in Eq. (4.1) are quite small. It is interesting in principle that at $T=0$, they lead to zero-point motion of small amplitude near the surface. The zero-point contribution is of the order of $(H_x/H_x)^2$.

Our conclusion is then that in the low-temperature limit, in theory the classical result $2C_\infty T^{3/2}$ describes the mean spin deviation rather well in the surface, when the assumptions stated are obeyed. These assumptions apply to the surfaces of Fe crystals, and the surfaces and interfaces of ultra thin Fe films studied so far, where the anisotropy fields have been directly measured. When $H_s=0$, the surface spin waves are very weakly bound at long wavelengths, and it is indeed the case that the presence of an easy-axis increases their binding energy substantially. However, their contribution to the mean spin deviation near the surface is offset by the "hole" induced by the surface in the density of bulk spin waves, just above $\Omega_m(k_\parallel)$. As emphasized some years ago,[9] one must always consider the two contributions together, when the mean spin deviation near the surface is studied.

The conclusions we have reached do depend on the assumption that, in our notation, one is in the domain $H_s<k_BT<H_x$. If H_s and H_x are comparable in magnitude, or H_s and k_BT are, then the conclusions will be modified. The full machinery required to explore these domains (within spin-wave theory) has been put in place in Sec. II, but to carry through a complete analysis will be rather involved. The limit $H_s\sim k_BT$ will arise at low temperatures (below 10 K, for parameters characteristic of Fe surfaces), and the case $H_s\sim H_x$ will arise at the surface of materials with low Curie temperatures. This latter case may also be appropriate to a situation where the exchange in the surface is highly anisotropic. From the physical point of view, there is little difference between the influence of anisotropic exchange or single site anisotropy on long-wavelength spin waves. It is possible at a complex interface such as that between MnF_2 and Fe that there is substantial exchange anisotropy.

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APPENDIX A: INFLUENCE OF SURFACE ANISOTROPY ON THERMALLY EXCITED SURFACE SPIN WAVES

As discussed in the text, we wish to examine the influence of surface anisotropy on the dispersion relation of surface spin waves in the regime where $\Omega_s(k)\sim k_BT$, and we have $H_0,H_s \ll k_BT \ll H_x$.

In this regime, treat H_s as small. We begin by rewriting Eq. (3.6) in the form

$$\left[(\Omega_m-\Omega_s)^{1/2}-H_x^{1/2}\beta-\frac{H_s}{2H_x^{1/2}}\right][(\Omega_m+\Omega_s)^{1/2}-H_x^{1/2}\beta] = \frac{H_s}{2H_x^{1/2}}[(\Omega_m-\Omega_s)^{1/2}-H_x^{1/2}\beta] \tag{A1}$$

or

$$(\Omega_m-\Omega_s)^{1/2}=H_x^{1/2}\left[\beta+\frac{H_s}{2H_x}\right]+\frac{H_s}{2H_x^{1/2}}\frac{[(\Omega_m-\Omega_s)^{1/2}-H_x^{1/2}\beta]}{[(\Omega_m+\Omega_s)^{1/2}-H_x^{1/2}\beta]} . \quad \text{(A2)}$$

As $H_s \to 0$, the quantity $(\Omega_m-\Omega_s)^{1/2}-H_x^{1/2}\beta$ vanishes, so if we consider an expansion of $(\Omega_m-\Omega_s)^{1/2}$ in powers of H_s, the second term on the right-hand side of Eq. (A2) is of order H_s^2. We examine the magnitude of this term by replacing the numerator by its first approximation, $H_s/2H_x^{1/2}$. Note also that Ω_m and Ω_s are approximately $H_x(k_{\|}a_0)^2/4$ in the thermal spin-wave regime. Hence, in the denominator $H_x^{1/2}\beta$ is smaller than $(\Omega_m+\Omega_s)^{1/2}$ by the factor $k_{\|}a_0$, and may be neglected. Then we have

$$(\Omega_m+\Omega_x)^{1/2}\cong H_x^{1/2}k_{\|}a_0/\sqrt{2} .$$

When these various approximations are combined, we have

$$(\Omega_m-\Omega_s)^{1/2}\cong H_x^{1/2}\left[\beta+\frac{H_s}{2H_x}\right]+\frac{1}{2\sqrt{2}}\frac{H_s^2}{H_x^{3/2}}\frac{1}{k_{\|}a_0}+\cdots . \quad \text{(A3)}$$

The last term may be neglected with respect to the first correction $H_s/2H_x^{1/2}$ from surface anisotropy if $k_{\|}a_0 \gg H_s/H_x$. With $k_BT \sim H_x(k_{\|}a_0)^2$, this requires

$$k_BT \gg H_x\left[\frac{H_s}{H_x}\right]^2 , \quad \text{(A4)}$$

an inequality comfortably satisfied above temperatures in the range of 10 K or so for a material such as Fe. We are led to Eq. (3.10) of the text by neglecting the last term of Eq. (A3).

APPENDIX B: EVALUATION OF TWO CONTRIBUTIONS TO THE SPIN DEVIATION NEAR THE SURFACE

We examine the structure of $\delta\Delta_{c2}^{(+)}(l_y)$ and $\delta\Delta_{c3}^{(+)}(l_y)$ defined in Eqs. (3.41b) and (3.41c) of the text. We begin with $\delta\Delta_{c2}^{(+)}(l_y)$.

Consider first $\sin^2\psi$, with the term in $H_xa_0^2k_\perp^2/8$ in the quantity a ignored for the moment. One has

$$\sin^2(\psi)=\frac{\gamma_+^2}{\frac{1}{4}a_0^2k_\perp^2+\gamma_+^2} , \quad \text{(B1)}$$

where γ_+ is defined in Eq. (3.19a). This function drops off rapidly for $a_0k_\perp > \gamma_+$, and the dominant contribution to the integral comes from the regime $a_0k_\perp \lesssim \gamma_+$. Now if we consider the role of the term $H_xa_0^2k_\perp^2/8$ ignored in Eq. (B1), note that $H_s/2+H_x\beta \equiv H_x\gamma_+$, while when $a_0k_\perp \sim \gamma_+$, one has $H_xa_0^2k_\perp^2/8 \sim H_x\gamma_+^2/8$. Since $\gamma_+ \ll 1$, this term may be ignored. Then noting the upper limit of the $k_\perp$ may be replaced by infinity at low temperatures,

$$\delta\Delta_{c2}^{(+)}(l_y)=-\frac{a_0}{\pi N_s}\sum_{\mathbf{k}_{\|}}\int_0^\infty \frac{dk_\perp\cos(a_0k_\perp l_y)\gamma_+^2}{\gamma_+^2+\frac{1}{2}a_0^2k_\perp^2}n(\Omega(\mathbf{k})) . \quad \text{(B2)}$$

Now when $a_0k_\perp \sim \gamma_+$, one may replace $\Omega(\mathbf{k})$ by simply $\Omega_m(\mathbf{k}_{\|})$. When this is done, the integral on $k_\perp$ may be evaluated in closed form to give

$$\delta\Delta_{c2}^{(+)}(l_y)=-\frac{1}{N_s}\sum_{\mathbf{k}_{\|}}\gamma_+(\mathbf{k}_{\|})\exp[-2\gamma_+(\mathbf{k}_{\|})l_y]n(\Omega_m(\mathbf{k}_{\|})) . \quad \text{(B3)}$$

With the term $H_xa_0^2k_\perp^2/8$ neglected once again, the term $\delta\Delta_{c3}^{+}(l_y)$ becomes, upon writing $\sin(2\psi)=2\sin\psi\cos\psi$,

$$\delta\Delta_{c3}^{(+)}(l_y)=-\frac{a_0^2}{2\pi N_s}\sum_{\mathbf{k}_{\|}}\gamma_+\int_0^\infty \frac{dk_\perp k_\perp\sin(a_0k_\perp l_y)n(\Omega(k_{\|}k_\perp))}{\gamma_+^2+\frac{1}{4}a_0^2k_\perp^2}=+\frac{a_0}{2\pi N_s}\sum_{k_{\|}}\frac{\partial}{\partial l_y}\gamma_+\int_0^\infty \frac{dk_\perp k_\perp\cos(a_0k_\perp l)}{\frac{1}{4}a_0^2k_\perp^2+\gamma_+^2}n(\Omega(\mathbf{k}_{\|}k_\perp)) . \quad \text{(B4)}$$

When the remaining integral is evaluated after replacing $n(\Omega(\mathbf{k}_{\|}k_\perp))$ by $n(\Omega_m(\mathbf{k}_{\|}))$, we have

$$\delta\Delta_{c2}^{(+)}(l_y)=\delta\Delta_{c3}^{(+)}(l_y) . \quad \text{(B5)}$$

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the surface may cause the surface waves to be driven up into the bulk spin-wave bands.

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[18]See Eq. (4.23) of D. L. Mills, in *Surface Excitations,* edited by V. M. Agranovich and R. Loudon (Elsevier, Amsterdam, 1984), p. 379.

[19]In the opening remarks of Sec. II in this paper, we note that earlier authors (Refs. 13 and 14) have established that in the presence of both dipole and exchange couplings (but with $H_s=0$), three (complex) decaying exponentials must be superimposed in the description of the surface wave for all boundary conditions to be satisfied, but in his treatment, Rado has a single exponential only. Note that in the limit of vanishing surface anisotropy and exchange, his calculation fails to yield the Damon-Eshbach surface spin wave known to be present (Ref. 18) in this limit.

[20]With $2\pi M_0$ set to zero, Rado's expression for the gap is somewhat different than ours. We have seen that when $H_s=0$, and in our treatment with dipolar fields ignored, the surface spin wave is a super position of two waves, each with an appropriate decay constant normal to the surface. Rado includes only one of the two waves, not both. Within a similar approximation scheme, our treatment provides $H_0-H_s^2/4H_x$ for the surface spin-wave frequency at $\mathbf{k}_{\parallel}=0$, rather than the correct expression displayed in Eq. (3.8a). Rado's result is a good approximation when $H_s^2 \ll 4H_0H_x$.