Spin Waves in Thin Films; Dipolar Effects*

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We have examined the spin-wave eigenfrequencies and eigenfunctions for a model ferromagnetic film, in the presence of both exchange and magnetic dipole interactions. A detailed computer study of spin waves in a thirty-layer film is presented for the case where the exchange and dipole interactions are of comparable strength. We discuss in detail both surface and "bulk" modes for this case. Also, the symmetry properties of the eigenvectors are discussed, along with a method for converting certain two-dimensional dipole sums to a rapidly converging form.

I. INTRODUCTION

N this paper, we present a detailed theoretical study of the magnetic excitations of a thin, uniform ferromagnetic film. The purpose of the work is to examine in detail the effect of dipolar interactions between the spins on the spin-wave eigenfunctions and eigenfrequencies.

There have been a number of other studies of the effect of free surfaces on the properties of magnetic materials in the spin-wave regime.¹⁻⁵ Glass and Klein¹ have computed the temperature dependence of the magnetization of thin films by noting that in this instance one must replace the integration over the wave-vector component perpendicular to the surface by a discreet sum. Corciovei² has also examined this problem for a simple cubic lattice with (100) surfaces and nearest-neighbor exchange interactions. In his calculation, an anisotropy field was introduced, and he included the fact that a spin in the surface layer interacts with fewer spins than a spin in the interior.

Recently Wallis, Maradudin, Ipatova and Klochikhin³ pointed out the existence of surface spin waves associated with a (100) free surface of a semi-infinite simple cubic lattice, in the presence of nearest and nextnearest neighbor exchange interactions. In the presence of exchange interactions only, it appears that such modes will be present whenever bonds non-normal to the surface are broken in forming the surface.⁴ In the work of Corciovei,² the surface modes do not appear, because he did not include the next-nearest neighbor exchange.

For the model employed in Ref. 3, it has been possible to find analytical expressions for the surface contribution to the magnon specific heat, as well as the variation of the mean sublattice deviation with temperature, and distance from the surface.⁴

In Refs. 1-4, the dipolar interactions between spins have been ignored, except for the introduction of an effective anisotropy field in one case. The anisotropy field enters this theory in the same manner as an externally applied magnetic field.

Damon and Eshbach⁵ have demonstrated that in the limit of long wavelengths, surface magnons exist in the presence of dipolar interactions between the spins. Their approach is a macroscopic one, which considers the demagnetizing field generated by the spin motion. Exchange interactions are not included, so the results are valid for very long wavelengths, where the dominant contribution to the spin-wave energy comes from the Zeeman energy, and the macroscopic demagnetizing fields.

In this paper, we consider a ferromagnetic film, with each atomic layer saturated. We derive the equations of motion in the presence of both exchange and dipolar interactions. In the presence of the surfaces, the translational invariance in the two directions parallel to the surface is not destroyed. The eigenvectors thus have the Bloch form for these spatial directions. The eigenfrequencies and eigenvectors associated with a given wave vector parallel to the surface can be found by solving a $2N \times 2N$ eigenvalue problem, where N is the number of layers in the film.

In Sec. II, the equations of motion are placed in the form convenient for the present calculations. The symmetry properties of the eigenvectors are discussed and compared to the analogous problem in lattice dynamics.⁶ In Sec. III, a transformation is applied to the dipolar sums encountered in Sec. II, so rapidly converging series are obtained for these quantities. In Secs. IV and V, we discuss results of numerical calculations for a film of 30 atomic layers. Both surface and "bulk" modes are examined, with emphasis placed on those features of the eigenfunctions that illustrate the general points made in Sec. II.

The computations described below have been carried out for the situation in which the dipolar interactions are comparable in strength with the exchange interactions, in order to emphasize the qualitative effect of the dipolar coupling on the eigenfunctions and eigenfrequencies. In metallic ferromagnets, where the Curie

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⁵ R. Damon and J. W. Eshbach, J. Phys. Chem. Solids 19, 308 (1961).

⁶S. Y. Tong and A. A. Maradudin (to be published).

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temperature may be several hundred degrees Kelvin, the exchange interactions are very large compared to the dipolar interactions. However, in insulating compounds (such as EuS) the Curie temperature is quite low, and the dipole moment associated with the magnetic ion is large, so that these two interactions are comparable in strength.

II. GENERAL CONSIDERATIONS

We consider an array of spins S arranged on a simple cubic lattice with lattice constant a. The crystal is supposed to be a thin film constructed of N atomic layers of spins, semi-infinite in two directions, and with two free (100) surfaces. The magnetization is directed parallel to the film surface, parallel to a principle axis of the crystal. We choose a coordinate system with the magnetization parallel to the z axis, and the surfaces of the film parallel to the x-z plane. The y axis is thus perpendicular to the surfaces. Also, we ignore the effect of finite temperatures on the spin-wave spectrum by supposing the film is at temperature T=0, with the magnetization M equal to the saturation value M_s .

The Hamiltonian for the model film is taken in the form

$$\mathcal{K} = \mathcal{K}_Z + \mathcal{K}_{\mathrm{EX}} + \mathcal{K}_D$$

where \mathcal{K}_{Z} describes the interaction of the spins with an externally applied field H, $\mathfrak{K}_{\mathrm{EX}}$ and \mathfrak{K}_{D} are the dipolar and exchange terms. Explicitly, one has

$$\Im \mathcal{C}_{Z} = -g\mu_{B}H \sum_{\mathbf{l}} S_{Z}(\mathbf{l})$$
$$\Im \mathcal{C}_{\mathrm{EX}} = -\frac{1}{2} \sum_{\mathbf{l}\mathbf{l}'} J(\mathbf{l} - \mathbf{l}') \mathbf{S}(\mathbf{l}) \cdot \mathbf{S}(\mathbf{l}')$$

(S(I), S(I'))

and

$$3C_{D} = g^{2} \mu_{B}^{2} \sum_{II'} \left\{ \frac{S(I) - S(I)}{|I - I'|^{3}} - 3 \frac{[(I - I') \cdot S(I)][(I - I') \cdot S(I')]}{|I - I'|^{5}} \right\}$$

The prime indicates that the case l = l' is excluded from the sums.

In each sum, the position vectors I range over the sites of the slab described above. In this work, we neglect surface anisotropy fields, since it has been found that in high quality metallic films the surface spins behave as if they are unpinned.⁷ Also, we ignore changes in the exchange constants near the film surfaces. At this moment, we know of no experimental information relating to this question. A crude argument suggests that for S-state ions, changes in exchange constants near the surface may be small.⁸ Actually, while we have neglected anisotropy fields in the surface, as well as

changes in the exchange constants near the surface in this work, it is a straightforward matter to include these changes in our programs, if this proves of interest.

We next consider the equations of motion for the operators $S_X(\mathbf{l})$ and $S_Y(\mathbf{l})$. With $\hbar = 1$, one has

$$i\dot{S}_X(\mathbf{l}) = [S_X(\mathbf{l}), \mathcal{H}]$$

$$i\dot{S}_Y(\mathbf{l}) = [S_Y(\mathbf{l}), \mathcal{K}].$$

It is a straightforward manner to compute the commutators from the Hamiltonian given above. We then linearize the equations of motion by invoking the spinwave approximation, valid for small deviations of the spins from the equilibrium alignment parallel to the z axis. The linearization is carried out by discarding terms quadratic in the small quantities $S_X(\mathbf{l})$ and $S_Y(\mathbf{l})$, and also replacing $S_Z(\mathbf{l})$ by the *c* number plus S wherever it appears. It is convenient to write the position vector **l** in the form $\mathbf{l} = a(l_X, l_Y, l_Z)$, where l_X , $l_Y l_Z$ are integers. It will also be useful to introduce quantities $D_{ii}(l_X l_Y l_Z)$ defined by

$$D_{ij}(l_X l_Y l_Z) = \frac{1}{(l_X^2 + l_Y^2 + l_Z^2)^{3/2}} \bigg[\delta_{ij} - 3 \frac{l_i l_j}{(l_X^2 + l_Y^2 + l_Z^2)} \bigg].$$

The linearized equations of motion may then be written in the form

$$\dot{S}_{X}(\mathbf{l}) = \sum_{\mathbf{l}'} \Gamma_{XY}(\mathbf{l} - \mathbf{l}') S_{Y}(\mathbf{l}') + \sum_{\mathbf{l}'} \Gamma_{XX}(\mathbf{l} - \mathbf{l}') S_{X}(\mathbf{l}') \quad (1a)$$

$$\dot{S}_{Y}(\mathbf{l}) = \sum_{\mathbf{l}'} \Gamma_{YX}(\mathbf{l}-\mathbf{l}') S_{X}(\mathbf{l}') + \sum_{\mathbf{l}'} \Gamma_{YY}(\mathbf{l}-\mathbf{l}') S_{Y}(\mathbf{l}'), \quad (1b)$$

where the quantities $\Gamma_{ij}(\mathbf{l}-\mathbf{l}')$ are given by

$$\Gamma_{XY}(\mathbf{l}-\mathbf{l}') = g\mu_B H(\mathbf{l})\delta_{11'} + g\mu_B M_S D_{YY}(l_X - l_{X'}, l_Y - l_{Y'}, l_Z - l_{Z'}) -SJ(\mathbf{l}-\mathbf{l}')$$

$$\Gamma_{XX}(\mathbf{l}-\mathbf{r}) = g\mu_B M_S D_{XY}(l_X - l_{X'}, \cdots)$$

$$\Gamma_{YX}(\mathbf{l}-\mathbf{l}') = -g\mu_B H(\mathbf{l})\delta_{1l'} - g\mu_B M_S D_{XX}(l_X - l_{X'}, \cdots)$$

$$+ SJ(\mathbf{l}-\mathbf{l}')$$

$$\Gamma_{YY} = -g\mu_B M_S D_{XY}(l_X - l_{X'}, \cdots).$$

The quantity $H(\mathbf{l})$ that appears in the definition of the Γ 's is an effective field that acts on the spin **l**. $H(\mathbf{l})$ includes both exchange and dipolar contributions. Explicitly, one has

$$H(\mathbf{l}) = H + (g\mu_B)^{-1}S \sum_{\mathbf{l}'} J(\mathbf{l} - \mathbf{l}') - M_S \sum_{\mathbf{l}'} D_{ZZ}(l_X - l_X' \cdots).$$

In these equations, we have introduced the saturation magnetization per unit volume $M_S = (g\mu_B S)/a^3$. In order to obtain the equations of motion in the form of Eqs. (1), it is necessary to recognize that for the film

⁷ P. E. Wigen, C. F. Kooi, and M. R. Shanabarger, J. Appl-Phys. **35**, 3302 (1964). ⁸ D. L. Mills, Phys. Rev. Letters **20**, 18 (1968).

geometry employed here,

$$\sum_{\mathbf{l}'} \frac{(l_z - l_z')(l_Y - l_{Y'})}{|\mathbf{l} - \mathbf{l}'|^5} = \sum_{\mathbf{l}'} \frac{(l_z - l_z')(l_X - l_{X'})}{|\mathbf{l} - \mathbf{l}'|^5} \equiv 0$$

since inhomogeneous terms proportional to these quantities appear in the equations of motion. In a geometry in which these sums are nonvanishing, one must question the stability of the ferromagnetic ground state.

We shall look for solutions of Eqs. (1) which vary harmonically in time. Since translational invariance is present with respect to translations parallel to the slab surfaces, the solutions will satisfy the Bloch conditions with respect to translations in these two directions. Thus, we seek solutions of the form

$$S_{X,Y}(\mathbf{l}) = \exp[i\Omega t - i\phi_X l_X - i\phi_Z l_Z] S_{X,Y}(l_Y)$$

Inserting this form into Eqs. (1) gives a set of $2N \times 2N$ equations for the coefficients $S_X(l_Y)$, $S_Y(l_Y)$ and the frequency Ω . One has

$$i\Omega S_{X}(l_{Y}) = \sum_{l_{Y'}} \gamma_{XY}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{Y}(l_{Y'}) + \sum_{l_{Y'}} \gamma_{XX}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{X}(l_{Y'}) \quad (2a)$$

$$i\Omega S_{Y}(l_{Y}) = \sum_{l_{Y'}} \gamma_{YX}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{X}(l_{Y'}) + \sum_{l_{Y'}} \gamma_{YY}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{Y}(l_{Y'}), \quad (2b)$$

where

$$\gamma_{ij}(\phi_X\phi_Z, l_Y - l_Y') = \sum_{l_X' l_Z'} \Gamma_{ij}(\mathbf{l} - \mathbf{l}')$$
$$\times e^{i\phi_X(l_X - l_X')} e^{i\phi_Z(l_Z - l_Z')}$$

In the definition of $\gamma_{ij}(\phi_X,\phi_Z; l_Y-l_Y')$, one must note that when $l_Y = l_{Y'}$, the term with $l_X' = l_X$, $l_Z' = l_Z$ must be excluded.

Eqs. (2) define a $2N \times 2N$ eigenvalue problem. For a given value of ϕ_X and ϕ_Z , upon solving the eigenvalue problem one obtains the frequencies of all spin-wave modes which are characterized by wave-vector components (ϕ_X/a) , and (ϕ_Z/a) parallel to the surface. Also, the eigenfunctions may be found. The purpose of this paper is to present the results of such calculations. Before discussing the details of our computations, it is useful to examine the symmetry properties of the equations.

For our geometry, it is easy to see that $\gamma_{XY}(\phi_X\phi_Z; l_Y - l_{Y'})$ and $\gamma_{YX}(\phi_X\phi_Z; l_Y - l_{Y'})$ are even functions of ϕ_X , ϕ_Z and $(l_Y - l_{Y'})$. Furthermore, these two quantities are real. On the other hand, both $\gamma_{XX}(\phi_X\phi_Z; l_Y - l_{Y'})$ and $\gamma_{YY}(\phi_X\phi_Z; l_Y - l_{Y'})$ are even functions of ϕ_Z , but are odd functions of both ϕ_X and $(l_Y - l_{Y'})$. Also, note that γ_{XX} and γ_{YY} are pure imaginary. These statements may be verified by direct examination of the definitions of the quantities, noting that the sums on l_X' and l_Z' run from $+\infty$ to $-\infty$.

Let us next consider the symmetry operations that leave the slab invariant. There are three operations that have useful consequences for our purposes.

First, consider a reflection in a plane placed parallel to the x-z plane at the midpoint of the film. Under such a reflection, the z components and x components of the spin vectors change sign. Also, the external magnetic field H changes sign. Consequently, this reflection is not a good symmetry operation since both H and M_s change sign. However, when this reflection is combined with a time reversal, H and M_s are restored to their original direction. Thus, the product of the time reversal combined with the reflection is a good symmetry operation. Given an eigenvector $\{S_X(l_Y), S_Y(l_Y)\}$ of frequency Ω , the symmetry operation applied to the eigenvector yields a new eigenmode of frequency $-\Omega$ and amplitude $\{S_X'(l_Y), S_Y'(l_Y)\}, \text{ where } S_X'(l_Y) = S_X(-l_Y), \text{ and } S_Y'(l_Y)$ $= -S_Y(-l_Y)$. By direct insertion of $\{S_X', S_Y'\}$ into the equations of motion, and then employing the properties of the γ_{ij} 's described above, one may indeed verify that this object is an eigenvector of frequency $-\Omega$. Thus, given an eigenvector $\{S_X, S_Y\}$ of frequency Ω , we have a prescription for constructing an eigenvector of the same ϕ_X and ϕ_Z that is associated with frequency $-\Omega$. Thus, for a given ϕ_X and ϕ_Z , this implies half of the eigenfrequencies of the $2N \times 2N$ matrix will be positive, and half negative. Thus, there are only N distinct values of the excitation energy $|\Omega|$ for a given ϕ_X and ϕ_Z . This observation provides a check on the computer program, since correct diagonalization of the properly constructed matrix must produce eigenvalues and eigenvectors related in the above manner.

Additional relations between eigenvectors and eigenfrequencies may be obtained from the remaining reflections, combined with time reversal. For example, reflection in the y-z plane combined with time reversal is a good symmetry operation. From this fact, one deduces that given an eigenvector $\{S_X(l_Y), S_Y(l_Y)\}$ of frequency Ω and wave vector $\{\phi_X, \phi_Z\}$, the vector $\{\mathfrak{S}_{X}'(l_{Y}),\mathfrak{S}_{Y}'(l_{Y})\} \quad \text{with} \quad \mathfrak{S}_{X}'(l_{Y}) = -\mathfrak{S}_{X}(l_{Y}), \quad \mathfrak{S}_{X}'(l_{Y})$ $=+S_{Y}(l_{Y})$ is an eigenvector associated with wave vector $\{-\phi_X, \phi_Z\}$ and frequency $-\Omega$. Finally, reflection in the x-y plane, without time reversal, shows that $\{S_X'(l_Y), S_Y'(l_Y)\}$ with $S_X'(l_Y) = -S_X(l_Y),$ $S_Y'(l_Y)$ $= -S_Y(l_Y)$ is an eigenvector of frequency $+\Omega$ and wave vector $\{\phi_X, -\phi_Z\}$. These rules were also employed to check the numerical calculations.

It is interesting to note that there is no symmetry operation which may be invoked to prove that for general ϕ_x and ϕ_z , the functions $S_x(l_Y)$ and $S_Y(l_Y)$ may be chosen to have well-defined parity. For the special case $\phi_x = \phi_z = 0$, the first two arguments allow this to be demonstrated. For then applying a reflection in the x-z plane, followed by one in the y-z plane, one finds that given an eigenvector $S_1 = \{S_x(l_Y), S_Y(l_Y)\}$ of frequency $+\Omega$, and wave vector $\phi_x = \phi_z = 0$, the vector $S_2 = \{S_x(-l_Y), S_Y(-l_Y)\}$ is also an eigenvector of frequency $+\Omega$ and wave vector $\phi_x = \phi_z = 0$. Then the linear combinations (S_1+S_2) and (S_1-S_2) are both eigenvectors of frequency Ω . One eigenvector has even parity, and one has odd parity. It is clear that for general ϕ_X and ϕ_Z , the proof breaks down.⁹

The behavior in the last section contrasts with the corresponding problem in lattice dynamics. For crystalline films with reflection symmetry, one may see that the analogous eigenfunctions $\{U_X(l_Y), U_Y(l_Y), U_Z(l_Y)\}$ can be constructed from components $U_i(l_Y)$ with welldefined parity.¹⁰ The difference between our magnetic problem and the theory of lattice dynamics lies in the pseudovector character of the spin operators, combined with their behavior under time reversal.

Finally, in the absence of dipolar interactions for any ϕ_x and ϕ_z , one may also show the eigenvectors can be chosen with well-defined parity.

We conclude this section by writing the equations of motion in a slightly different form. Introduce quantities $d_{ij}(\phi_X \phi_Z; l_Y - l_Y')$ related to the γ 's by

$$\gamma_{XX}(\phi_X\phi_Z; l_Y - l_Y') = id_{XX}(\phi_X\phi_Z; l_Y - l_Y')$$

$$\gamma_{YY}(\phi_X\phi_Z; l_Y - l_Y') = id_{YY}(\phi_X\phi_Z; l_Y - l_Y')$$

$$\gamma_{XY}(\phi_X\phi_Z; l_Y - l_Y') = d_{XY}(\phi_X\phi_Z; l_Y - l_Y')$$

$$\gamma_{YX}(\phi_X\phi_Z; l_Y - l_Y') = d_{YX}(\phi_X\phi_Z; l_Y - l_Y').$$

From our earlier remarks, one sees the d_{ij} 's are real numbers. Also, let $S_X(l_Y) = S_X(l_Y)$, and $S_Y(l_Y)$ $=-iS_{\mathbf{Y}}(l_{\mathbf{Y}})$. Then the equations become

$$\Omega S_{X}(l_{Y}) = \sum_{l_{Y'}} d_{XY}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{Y}(l_{Y}) + \sum_{l_{Y'}} d_{XX}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{X}(l_{Y})$$
(3a)

$$\Omega S_{Y}(l_{Y}) = \sum_{l_{Y'}} d_{YX}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{X}(l_{Y'}) + \sum_{l_{Y'}} d_{YY}(\phi_{X}\phi_{Z}; l_{Y} - l_{Y'})S_{Y}(l_{Y'}). \quad (3b)$$

Equations (3) provide a convenient form for the equations, because the problem is reduced to one of diagonalizing a real matrix. One may write Eqs. (3) in a convient matrix form by introducing a column vector

$$\mathbf{S} = \begin{bmatrix} S_{\mathcal{X}}(1) \\ \vdots \\ S_{\mathcal{X}}(N) \\ S_{\mathcal{Y}}(1) \\ \vdots \\ S_{\mathcal{Y}}(N) \end{bmatrix}.$$

Then Eq. (3) has the form

 $\Omega S = dS$

with **d** real.

It should be noted that **d** is *not* a symmetric matrix; returning to the symmetry properties of the γ_{ij} , one may see that

$$\mathbf{d} = \begin{pmatrix} a & S_1 \\ S_2 & -a \end{pmatrix},$$

where a is an $N \times N$ antisymmetric matrix, S_1 and S_2 are symmetric with $S_1 \neq S_2$.

It is physically reasonable that we are led to diagonalize a non-Hermitian matrix, in the presence of dipolar interactions. It is well known¹¹ that for a number of geometries, the ferromagnetic state of dipolar coupled spin arrays is unstable. This manifests itself in the appearance of complex spin-wave frequencies, which occur in complex conjugate pairs. If d were Hermitian, then the frequencies would necessarily be purely real. From the work of Cohen and Keffer,¹¹ it is known that for some geometries, complex magnon frequencies must emerge, if the ferromagnetic ground state is assumed. To allow for this possibility, clearly one must encounter a non-Hermitian matrix in the eigenvalue problem. It is readily seen that d becomes symmetric in the absence of dipolar coupling.

Our computer program computed both the real and imaginary parts of the eigenfrequencies. However, for the range of parameters and geometry explored in this work, the spin-wave frequencies were found to be real.

Before discussing the results, we will in Sec. III rearrange the dipole sums into rapidly converging series, employing a method used by Tong and Maradudin.⁶ In their present form, the dipole sums converge slowly, in an oscillatory fashion.

III. DIPOLE SUMS

In the previous section, we encountered certain dipole sums which appear in the elements of the matrix **d**. Since these sums converge very slowly in an oscillatory manner, direct and accurate computation of the sums is exceedingly costly in computer time. In this section, we convert the dipole sums to series that converge very rapidly by a method also employed in Ref. 6. The sums we are concerned with have the form

$$D_{ij}(\phi_X \phi_Z; l_Y) = \sum_{l_X, l_Z = -\infty}^{+\infty} e^{i\phi_X l_X} e^{i\phi_Z l_Z} D_{ij}(l_X l_Y l_Z),$$

$$= \sum_{l_X l_Z} e^{i\phi_X l_X} e^{i\phi_Z l_Z} \left[\frac{\delta_{ij}}{(l_X^2 + l_Y^2 + l_Z^2)^{3/2}} - 3 \frac{l_i l_j}{(l_X^2 + l_Y^2 + l_Z^2)^{5/2}} \right]$$

The prime on the summation indicates that when $l_{Y}=0$, the term $l_{X}=l_{Z}=0$ is to be excluded.

We can express the dipole sums in terms of the quantity

$$S(\phi_X \phi_Z; l_Y) = \sum_{l_X l_Z} \frac{e^{i\phi_X l_X} e^{i\phi_Z l_Z}}{(l_X^2 + l_Y^2 + l_Z^2)^{5/2}}.$$

¹¹ M. H. Cohen and F. Keffer, Phys. Rev. 99, 1135 (1955).

⁹ Actually, for $\phi_Z \neq 0$, the proof works so long as $\phi_X = 0$. ¹⁰ R. Fuchs and K. L. Kliewer, Phys. Rev. 140, A2076 (1965).

For example,

$$D_{XX}(\phi_X\phi_Z; l_Y) = \left[-\frac{\partial^2}{\partial\phi_Z^2} + 2\frac{\partial^2}{\partial\phi_X^2} + l_Y^2\right] S(\phi_X\phi_Z; l_Y).$$

The remaining dipole sums may be expressed in terms of S in a similar manner.

It will be convenient to first consider the case $l_Y \neq 0$, then next examine the sum for $l_Y = 0$ separately.

(i) Case
$$l_Y \neq 0$$

We begin with the identity

$$\frac{1}{\alpha^{5/2}} = \frac{4}{3\sqrt{\pi}} \int_0^\infty dt \ t^{3/2} e^{-\alpha t}.$$

Thus, S may be written

$$S(\phi_X \phi_Z; l_Y) = \frac{4}{3\sqrt{\pi}} \int_0^\infty dt \ t^{3/2} e^{-l_y^2 t} \{ \sum_{l_Z = -\infty}^{+\infty} e^{-l_Z^2 t} e^{i\phi_Z l_Z} \} \\ \times \{ \sum_{l_X = -\infty}^{+\infty} e^{-l_X^2 t} e^{i\phi_X l_X} \}.$$

We next employ the identity¹²

$$\sum_{l_1=-\infty}^{+\infty} e^{-tl_1^2} e^{il_1\phi_1} = \frac{\pi^{1/2}}{t^{1/2}} \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{1}{t}(\pi n + \frac{1}{2}\phi_1)^2\right].$$
 (4)

Thus,

$$S(\phi_X \phi_Z; l_Y) = \frac{4\pi^{1/2}}{3} \sum_{nm} \int_0^\infty dt \ t^{1/2} e^{-t l_Y^2} \\ \times e^{-(1/t)[(\pi n + \frac{1}{2}\phi_X)^2 + (\pi m + \frac{1}{2}\phi_Z)^2]}.$$
(5)

The integral may be evaluated in closed form:

$$\int_{0}^{\infty} dx \, x^{1/2} e^{-ax} e^{-b/x} = \frac{1+2(ab)^{1/2}}{2a} \left(\frac{\pi}{a}\right)^{1/2} \exp[-2(ab)^{1/2}].$$

We then obtain

$$\begin{split} \mathbb{S}(\phi_{X}\phi_{Z};l_{Y}) &= \frac{2}{3|l_{Y}|^{3}} \sum_{nm} \left[1 + 2l_{Y}\gamma_{nm}(\phi_{X}\phi_{Z})\right] \\ &\times \exp[-2|l_{Y}|\gamma_{nm}(\phi_{X}\phi_{Z})], \quad (6) \end{split}$$

where

$$\gamma_{nm}(\phi_X\phi_Z) = \left[(\pi n + \frac{1}{2}\phi_X)^2 + (\pi m + \frac{1}{2}\phi_Z)^2 \right]^{1/2}.$$

The sum in Eq. (4) converges extremely rapidly. Even for $\phi_X = \phi_Z = 0$, the term with n=1, m=0 is proportional to $\exp(-2\pi |l_Y|)$. Thus, even for small values of l_Y , excellent convergence is obtained by summing the order of ten terms. From Eq. (4), we may obtain rapidly converging expressions for the dipole sums. We find

. . .

$$D_{XX}(\phi_X\phi_Z; l_Y) = -4\pi \sum_{nm} \frac{(\pi n + \frac{1}{2}\phi_X)^2}{\gamma_{nm}(\phi_X\phi_Z)}$$
$$\times \exp[-2|l_Y|\gamma_{nm}(\phi_X\phi_Z)], \quad (7a)$$
$$D_{YY}(\phi_X\phi_Z; l_Y) = -4\pi \sum_{nm} \frac{(\pi m + \frac{1}{2}\phi_Z)^2}{\gamma_{nm}(\phi_X\phi_Z)}$$

$$\times \exp[-2|l_Y|\gamma_{nm}(\phi_X\phi_Z)], \quad (7b)$$
$$D_{ZZ}(\phi_X\phi_Z; l_Y) = -4\pi \sum_{nm} \gamma_{nm}(\phi_X\phi_Z)$$

$$\times \exp[-2|l_Y|\gamma_{nm}(\phi_X\phi_Z)], \quad (7c)$$

$$D_{XY}(\phi_X\phi_Z; l_Y) = +i4\pi \operatorname{sgn}(l_Y) \sum_{nm} (\pi n + \frac{1}{2}\phi_X)$$

$$\times \exp[-2|l_Y|\gamma_{nm}(\phi_X\phi_Z)]. \quad (7d)$$

For small values of ϕ_X and ϕ_Z , the dominant term in these sums is the term with n=m=0. The expression obtained for the D_{ij} retaining only this term is the result one would find if the sum over l_X and l_Z is replaced by an integration over the two dimensional plane.

(ii) Case
$$l_Y \equiv 0$$

The procedure employed above cannot be used in this case, since the integral in Eq. 5 diverges. Instead, we proceed in the following way. Define

$$S_{X}(\phi_{X}\phi_{Z}) = \sum_{l_{X}l_{Z}}' \frac{l_{X}^{2}}{(l_{X}^{2} + l_{Z}^{2})^{5/2}} e^{il_{X}\phi_{X}} e^{il_{Z}\phi_{Z}}$$
$$S_{Z}(\phi_{X}\phi_{Z}) = \sum_{l_{X}l_{Z}}' \frac{l_{Z}^{2}}{(l_{X}^{2} + l_{Z}^{2})^{5/2}} e^{il_{X}\phi_{X}} e^{il_{Z}\phi_{Z}}.$$

One then has

$$D_{XX}(\phi_X\phi_Z,0) = -2S_X(\phi_X\phi_Z) + S_Z(\phi_X\phi_Z),$$

$$D_{YY}(\phi_X\phi_Z,0) = +S_X(\phi_X,\phi_Z) + S_Z(\phi_X,\phi_Z),$$

$$D_{ZZ}(\phi_X,\phi_Z,0) = -2S_Z(\phi_X,\phi_Z) + S_X(\phi_X,\phi_Z).$$

Consider $S_X(\phi_X, \phi_Z)$. The summation excludes the term with both l_X and $l_Z=0$. For $l_Z\neq 0$, the factor of l_X^2 in the numerator means *all* terms with $l_X=0$ give vanishing contributions to the sum. Thus

$$S_X(\phi_X\phi_Z) = \sum_{l_Z=-\infty}^{+\infty} \sum_{l_X=-\infty}^{+\infty} \frac{l_X^2}{(l_X^2 + l_Z^2)^{5/2}} e^{il_X\phi_X} e^{il_Z\phi_Z}.$$

Employing an identity used in the earlier discussion,

$$S_{X}(\phi_{X}\phi_{Z}) = \frac{4}{3\sqrt{\pi}} \sum_{l_{Z}=-\infty}^{+\infty} \sum_{l_{X}=-\infty}^{+\infty} l_{X}^{2} e^{il_{X}\phi_{X}} e^{il_{Z}\phi_{Z}}$$

$$\times \int_{0}^{\infty} dt \ l^{3/2} e^{-t(l_{X}^{2}+l_{Z}^{2})} = \frac{4}{3} \sum_{l_{X}=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} l_{X}^{2} e^{il_{X}\phi_{X}}$$

$$\times \int_{0}^{\infty} dt \ t e^{-tl_{X}^{2}} e^{-(1/t)(\pi n + \frac{1}{2}\phi_{Z})^{2}}$$

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¹² This identity is encountered in evaluating lattice sums by Ewald's method. For example, see the discussion by J. M. Ziman, in *Theory of Solids* (Cambridge University Press, London, 1964), Chap. 2.

We have applied Eq. (4) to the sum on l_Z . Then we write

$$S_X(\phi_X\phi_Z) = -\frac{4}{3} \sum_{l_X=1}^{\infty} \sum_{n=-\infty}^{+\infty} \cos(l_X\phi_X) l_X \frac{d}{dl_X}$$
$$\times \int_0^\infty di e^{-il_X^2} e^{-(1/i)(\pi n + \frac{1}{2}\phi_Z)^2}.$$

The integral may be evaluated at this point:

$$\int_0^\infty dt e^{-bt} e^{-a/t} dt = 2 \left(\frac{a}{b}\right)^{1/2} K_1 [2(ab)^{1/2}],$$

where K_1 is the modified Bessel function of order unity. Then,

$$S_{X}(\phi_{X}\phi_{Z}) = -(8/3) \sum_{l_{X}=1}^{\infty} \sum_{n=-\infty}^{\infty} l_{X} \cos(l_{X}\phi_{X}) \\ \times \frac{d}{dl_{X}} \left\{ \frac{|\pi n + \frac{1}{2}\phi_{Z}|}{l_{X}} K_{1}(2l_{X}|\pi n + \frac{1}{2}\phi_{Z}|) \right\}.$$

Using

$$K_2(x) = (2/x)K_1(x) + K_0(x)$$

combined with $K_{1}'(x) = -\frac{1}{2} [K_{2}(x) + K_{0}(x)]$, we find

$$S_{X}(\phi_{X}\phi_{Z}) = (16/3) \sum_{l_{X}=1}^{\infty} \sum_{n=-\infty}^{+\infty} |\pi n + \frac{1}{2}\phi_{Z}| \cos(l_{X}\phi_{X})$$
$$\times [(\pi n + \frac{1}{2}\phi_{Z})K_{0}(2l_{X}|\pi n + \frac{1}{2}\phi_{X}|) + (1/l_{X})K_{1}(2l_{X}|\pi n + \frac{1}{2}\phi_{X}|)]. \quad (8a)$$

A similar treatment applied to S_Z gives

$$\begin{split} S_{Z}(\phi_{X}\phi_{Z}) &= (16/3) \sum_{l_{Z}=1}^{\infty} \sum_{n=-\infty}^{+\infty} |\pi n + \frac{1}{2}\phi_{X}| \cos(l_{Z}\phi_{Z}) \\ &\times \{ |\pi n + \frac{1}{2}\phi_{X}| K_{0}(2l_{Z}|\pi n + \frac{1}{2}\phi_{X}|) \\ &+ (1/l_{Z})K_{1}(2l_{Z}|\pi n + \frac{1}{2}\phi_{X}|) \}. \end{split}$$
(8b)

We have employed the forms in Eq. (7) to compute the dipole sums for the case $l_Y=0$. Since for large values of $x, K_n(x) \sim (e^{-x}/\sqrt{x})$, the series in Eqs. (8) are rapidly convergent.

It is also useful to explicitly exhibit the limit of S_x and S_z as ϕ_x , $\phi_z \rightarrow 0$. One has

$$\lim_{\phi_X \to 0} \lim_{\phi_Z \to 0} S_X(\phi_X \phi_Z) = \lim_{\phi_X \to 0} \lim_{\phi_Z \to 0} S_Z(\phi_X \phi_Z),$$

with

$$s_X(0,0) = \frac{4\pi^2}{9} + \frac{32\pi^2}{3} \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} n^2 K_2(2\pi ln).$$
(9)

We have employed the results of Eqs. (7)-(9) to compute the elements of **d**.

IV. BULK EIGENMODES

By employing the technique of transforming the dipole sums described in Sec. III, we have solved on a computer the eigenvalue problem described in Sec. II for films ranging from 10–50 atomic layers in thickness. In this section, we discuss some of the results for bulk modes in a film of 30 atomic layers. The qualitative behavior of the eigenfrequencies and eigenvectors is similar to the results exhibited in the present section, for the range of thickness investigated.

For the numerical computations, we have chosen units so that $g\mu_B H=1$. The results in this section assumed that in these units, the product of the spin Sand the nearest-neighbor exchange $SJ_1=1$, with the next-nearest neighbor exchange $J_2=\frac{1}{2}(J_1)$. We have chosen the parameter $4\pi g\mu_B M_S$ as a measure of the strength of the dipolar interactions.

We first discuss the modes with $\phi_X = \phi_Z = 0$. These are the modes excited by a microwave field incident normally on the film.

First, consider the lowest frequency mode with $\phi_X = \phi_Z = 0$. This mode in the film corresponds to the uniform precession mode in infinitely extended crystals. In a macroscopic disc, with the magnetization parallel to the surface, the frequency of the mode is given by Kittel's relation¹³ $\hbar\omega_0 = g\mu_B [H(H+4\pi M_S)]^{1/2}$. When the mode is excited, in the macroscopic theory the spin deviation is uniform throughout the sample, with the ratio of the spin deviation S_X (parallel to the surface) and S_Y (normal to the surface) given by $[(H+4\pi M_S)/H]^{1/2}$.

We have found the frequency of this mode lies quite close to the macroscopic value, for the range of thicknesses and parameters investigated. For example, when $4\pi g\mu_B M_S = 2.5$ and H = 1.0, Kittel's relation gives 1.8708 for the frequency. For the thirty-layer film, with the exchange interactions assuming the values stated above, we find 1.8725 for the frequency of the lowest mode.

The eigenvectors are plotted in Fig. 1 for various values of $4\pi M_s$, in a thirty-layer film. It is interesting to note that even though no surface pinning fields have been explicitly included in the calculations, the spin deviation is significantly larger in the middle of the film than near the surfaces, when $4\pi M_s$ is large. From Fig. 1, one sees that when $4\pi g\mu_B M_S = 5.0$, the spin deviation in the center of the film is about 6% larger than near the surfaces. This comes about because even in the absence of surface pinning fields, the dipolar field seen by a spin near the surface is significantly different than that seen by an interior spin. For example, in the effective field $H(\mathbf{I})$ introduced in Sec. II, the quantity $-M_s \sum' {}_{\mathbf{l}'} D_{\mathbf{z}\mathbf{z}}(\mathbf{l}-\mathbf{l}')$ occurs. For a spin in the interior of a infinite sample, this quantity equals $\frac{1}{3}(4\pi M_s)$. For a spin in the surface layer, this effective

¹³ See C. Kittel, Introduction to Solid State Physics (J. Wiley & Sons, Inc., New York, 1956), 2nd ed., p. 412.



Ω =1.9I35 Ω=2.0297 0.20 0.20 sx sx 0.10 0.10 30 N 0.0 0.0 30 10 20 20 -0.10 -0.10 -0.20 -0.20 Ω= 2.218I 0.20 s. 0.10 0.0 iċ 20 30 -0.10 -0.20

 $\phi_x = \phi_z = 0.0$

FIG. 1. The spin-wave eigenfunctions for the lowest eigenmode with $\phi_X = \phi_Z = 0$. The eigenfunctions are plotted for various values of $4\pi M_S$, with H=1.0, $SJ_1=1.0$ and $SJ_2=0.5$.

field is about 4% larger than this value. This change in the effective field has a slight pinning effect on the surface spins. There are also other dipolar field terms in the matrix **d** which differ for a surface spin, compared to a spin in the middle of the film.

Since there is curvature in the wave functions of the lowest mode, there will be a contribution to the excitation energy from the exchange interactions, in contrast to the case in the infinitely extended medium. We have found the magnitude of the exchange contribution by comparing the frequency of the lowest eigenmode for the case with $SJ_1 = 1 = 2SJ_2$ with the frequency computed with $SJ_1=SJ_2=0$. When $4\pi g\mu_B M_S=2.5$, the change in frequency is $\Delta\Omega = 0.0638$ for the thirty-layer film. Thus the frequency of the mode suffers a 3%upward shift from the exchange interactions, when the parameters assume the value given above. Thus, it seems that the close agreement between the frequency of the lowest mode of the film and the macroscopic Kittel relation is somewhat fortuitous. There is a decrease in the dipolar contribution to the energy of the mode which for the parameters we examined is offset by a positive exchange contribution.

In Fig. 2, we have plotted the x component of the spin deviation for the three modes with $\phi_X = \phi_Z = 0$ closest in frequency to the "uniform" mode, for the case $4\pi g\mu_B M_S = 2.5$. It can be seen from inspection that the eigenvectors have a well-defined parity with respect to reflections through the midpoint of the film,

FIG. 2. The component of spin deviation S_X parallel to the surface for the three modes closest in frequency to the lowest frequency mode when $\phi_X = \phi_Z = 0.0$. The curves are plotted for $4\pi M_S = 2.5$, with the remaining parameters the same as in Fig. 1.

as required for $\phi_X = \phi_Z = 0$ by the symmetry arguments described earlier. The wave functions are quite similar in form to the functions $\cos[(\pi/N)ny]$, where n=0, 1, 2 In the long-wavelength limit, and in the absence of surface pinning fields, the continuum theory¹⁴ yields wave functions of the form $\cos[(\pi/N)ny]$, where n is an integer. From Fig. 2, one sees that there are deviations from this simple ideal form. For example, it is clear that the slope $(\partial S_X | \partial y)$ is finite at both ends of the film. This is presumably a consequence of the effective pinning fields that result from the influence of the surfaces on the dipolar fields, as we discussed in the previous paragraph. If the eigenfunctions were strictly given by $\cos[(\pi/N)ny]$, then for $n=1, 2, \dots$, the total transverse moment associated with excitation of a spin wave vanishes identically. For the mode of frequency $\Omega = 2.0292$ in Fig. 2, we find the transverse moment associated with the mode is finite but small, with a value of $\approx 2\%$ of that of the "uniform" mode.

In Fig. 3, we have plotted the x component of spin deviation for the four lowest modes with $\phi_X = 0.1\pi$, $\phi_Z = 0.0$, and with $4\pi g\mu_B M_S = 2.5$ in our units. The most striking feature of these results is the strong asymmetry of the eigenfunction with respect to reflection through the midpoint of the film. Recall the discussion of Sec. II, where we pointed out that for $\phi_X \neq 0$, the eigenfunctions do not have well-defined parity in the presence of dipolar coupling between the spins. The deviation from simple

¹⁴ C. Kittel, Phys. Rev. 110, 1295 (1958).



FIG. 3. The x component of spin deviation associated with the four lowest eigenmodes with $\phi_X=0.1\pi$ and $\phi_Z=0.0$, where H, $4\pi M_S$, SJ_1 and SJ_2 have the values employed in Fig. 2.

behavior is especially apparent in the two lowest frequency modes. The two highest frequency modes of Fig. 3 have the appearance of cosine waves, with the argument phase shifted so the maxima do not occur at the film surfaces. It should be noted, however, that the maxima are not of uniform height, so representation of even the highest frequency mode illustrated in Fig. 3 by a simple cosine is a considerable oversimplification.



FIG. 4. The surface mode and the lowest frequency bulk mode, as a function of ϕ_X for $4\pi M=0$ and $4\pi M=2.5$. The curves are plotted for the case H=1, $SJ_1=1$ and $SJ_2=0.5$.

We have inspected the modes of higher frequency and found that they have an appearance qualitatively similar to phase shifted cosine waves of the form $\cos\lceil (\pi/N)ny-\phi(n)\rceil$.

V. SURFACE MODES

It will be recalled from Sec. I that the study of surface spin waves, the analog of the Rayleigh waves of elasticity theory, has been of interest. In particular, Wallis *et al.*³ have examined the dispersion relation of these modes for the Heisenberg model, in the absence of dipolar coupling. For a simple cubic lattice of spins, with a free (100) surface, these authors found a surface spin-wave branch exists, provided next-nearest neighbor interactions are included.

We have encountered similar modes in our study. When a well-defined surface mode exists, we found the frequency of the mode clearly split off below the frequencies associated with the remaining modes with the same value of the wave vector (ϕ_X, ϕ_Z) parallel to the surface. Also, examination of the eigenvector showed the associated spin deviation localized near the film surfaces. Some of our results are presented in Figs. 4–6.

In Fig. 4, the dashed lines show the frequency of the surface mode, compared to that of the lowest "bulk" mode for various values of ϕ_X , with $\phi_Z = 0$, H = 1, $SJ_1=1, J_2=(\frac{1}{2})J_1$, and the dipole strength parameter $4\pi g\mu_B M_S = 0$. With $4\pi g\mu_B M_S = 0$, we have the case considered in Ref. 3, except we have a finite slab of 30 atomic layers, while Wallis and co-workers considered the semi-infinite geometry. Actually, there are two surface modes for a given value of (ϕ_X, ϕ_Z) in the slab, with a slight splitting between them that vanishes as the slab thickness increases. For 30 atomic layers, this splitting is very small, so we show only a single branch in the figure. Also shown in Fig. 4 we have the lowest "bulk" branch and the surface branch for the case $4\pi g\mu_B M_S = 2.5$. Even for this rather large value of the dipole strength parameter, one notices that the splitting between the two modes is affected little by the dipolar interactions. (In Fig. 4, the frequencies have been normalized so that the maximum bulk frequency is unity, for both values of M_s). To see this more clearly, in Fig. 5, we plot the frequency of the surface and the lowest bulk mode, and the surface mode at $\phi_X = \pi$ as a function of the coupling parameter $4\pi g\mu_B M_S$, for the same value of J_1 and J_2 as we used in Fig. 4. We find that the principal effect of the dipolar coupling is to "stiffen" all of the modes of low frequency. The relative position of the surface mode and the bulk manifold is not greatly affected.

We have also explored the properties of the surface modes when the exchange is very small, to see if modes exist in the presence of dipolar interactions only. With $SJ_1=SJ_2=0$, we found no surface modes, for the values of H and $g\mu_BM_S$ employed, however, for very small values of the J's, surface waves make their appearance.



FIG. 5. The frequency of the lowest bulk mode and the surface mode at $\phi_X = \pi$, $\phi_Z = 0$ plotted as a function of $4\pi M$. The remaining parameters are the same as for Fig. 4.

We have illustrated this point in Fig. 6 by plotting S_X as a function of position in the film for the lowest eigenmode associated with $\phi_Z=0$, $\phi_X=\pi$ for $4\pi g\mu_B M_S=2.5$, $g\mu_B H=1$, and various values of J_1 , always taking $J_2=(\frac{1}{2})J_1$. It can be seen that when



FIG. 6. The component of spin deviation (S_X) parallel to the surface for the lowest eigenvalue associated with $\phi_X = \pi$, $\phi_X = 0$ and $4\pi M = 2.5$. We have taken H = 1.0, and various values of SJ_1 with $J_2 = \frac{1}{2}J_1$.

 $J_1=0$, [see Fig. 6(a)], this has a cosinelike spatial variation throughout the film, with the spin deviation large in the center, and small at both surfaces. When $SJ_1=0.08$, the slope of the wave function at the surfaces of the film decreases to a value near zero, as can be seen in Fig. 6(a). Also, the value of S_X at the surfaces is considerably larger than for the case $J_1=0$. When SJ_1 is increased to 0.09, the slope at the surface changes sign, and although the maximum is near the center of the film, there is a strong flattening of the wave function.

As one can see from Fig. 6(b), by the time $SJ_1=0.12$, the maximum is depressed well below the value at the film surfaces, and the mode appears to have the form of a surface mode. As J_1 is increased more, the mode becomes more tightly bound to the surfaces. This may be seen in Fig. 6(b), where we plot S_X for the mode with $SJ_1=0.15$. In these two figures, arbitrary units for S_X have been used.

It should be mentioned that when two modes are very nearly degenerate, the computer tended to produce an eigenvector that was a linear combination of the two nearly degenerate vectors. This difficulty was encountered for the modes illustrated in Fig. 6(b), since the splitting between the symmetric and the antisymmetric modes is small.¹⁵ The curves plotted were obtained by assuming only the two surface modes are mixed, so the eigenvector for the symmetric mode may be extracted as proportional to the sum $S_X(l_Y)+S_X(-l_Y)$.

All of the surface modes found in this work had frequencies split off below the bulk modes of the same (ϕ_X, ϕ_Z) as the surface mode in question. It is interesting that in the absence of exchange, and in the long-wavelength limit, Damon and Eshbach⁵ found surface modes with frequencies greater than the maximum frequency $g\mu_B[H(H+4\pi M_S)]^{1/2}$ for bulk modes. For small values of (ϕ_X, ϕ_Z) where our numerical work might be expected to overlap with Damon and Eshbach's theory, we were unable to find evidence of surface modes above the lowest bulk frequency. Of course, in this region, the penetration length of the Damon-Eshbach modes becomes long compared to our slab thickness, so it is not surprising for us to encounter difficulty in passing from the short-wavelength modes of the type considered by Wallis and co-workers3 to the Damon-Eshbach regime. Indeed, for small ϕ_X and ϕ_Z , one encounters low-lying modes that are geometrical resonances of the slab, with no clear surface character.

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¹⁵ One may show from the symmetry arguments of Sec. II that at the special point $\varphi_X = \pi$, $\varphi_Z = 0$, the modes again have welldefined parity. This follows upon noting that the points $(\pi,0)$ and $(-\pi,0)$ are in fact the same points in reciprocal space, since they differ by a reciprocal lattice vector of the two dimensional Brillouin zone.