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Excitation Spectrum of Magnetic Domain Walls

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The eigenvalue equation for the normal modes of excitation of a moving infinite planar magnetic domain wall in an infinite material having the most general second-rank tensor anisotropy is presented. The eigenvalues and eigenfunctions of both the spin waves in the presence of the moving wall and the excitation of the wall itself are given to first order in velocity. Cylindrical-domain resonance experiments are proposed to test for the existence of the excitation modes and their effect on domain propagation. The dispersion relation for the wall excitation modes is found to imply a new material requirement for high mobility.

I. INTRODUCTION

The excitation spectrum of an infinite planar 180° domain wall in an infinite magnetic material having a constant magnetization magnitude M_s is treated here in the continuum approximation. For the description of this system, Cartesian tensors in a right-handed coordinate system and Euler angles will be used. The position in the material is denoted by x_j , and only the polar (θ) and azimuthal (φ) Euler angles are used. The polar axis is the x_3 direction, and φ is zero in the x_1 direction. Vectors as well as their components will be denoted by symbols of the form v_j and, similarly, tensors will be denoted by symbols of the form T_{jk} . Repeated indices are understood to be summed from 1 to 3. The totally antisymmetric unit tensor is denoted by e_{kjp} .

II. MAGNETIC ENERGY DENSITY

The material is taken to have the most general second-rank tensor anisotropy. When the coordinate system is properly oriented with respect to the crystalline axes and when the arbitrary zero

of energy is chosen so that the lowest value of the anisotropy energy is zero, the anisotropy energy density may be written

$$\rho_K = (1/M_s^2) K_{jk} M_j M_k, \quad (1a)$$

where M_j is the magnetization vector and

$$K_{jk} \equiv \begin{bmatrix} K_u & 0 & 0 \\ 0 & K_u + K_o & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad K_u > 0, \quad K_o > 0 \quad (1b)$$

(u for uniaxial and o for orthorhombic). The anisotropy energy is minimized when $M_j = [0, 0, \pm M_s]$. In a bubble domain device, such a material would be oriented with the plate normal along the polar (3) axis and the domain-wall normals in the 1,2 plane. Attention will subsequently be restricted to a planar domain wall whose wall normal lies in the 1, 2 plane, for which the local demagnetizing energy density between two regions having $M_3 = \pm M_s$ is

$$\rho_d = 2\pi(n_j M_j)^2 \quad (2a)$$

$$= 2\pi n_j n_k M_j M_k. \quad (2b)$$

In (2) n_j is the unit wall normal ($n_3 = 0$).

Since $2\pi n_j n_k$ is a tensor of the same rank as (1b), it may be added to the anisotropy tensor. The resulting tensor is diagonalized by a rotation of the coordinate system used in (1b) about the polar axis by

$$\varphi_d = \frac{1}{2} \tan^{-1} \left(\frac{\sin 2\varphi_n}{\cos 2\varphi_n - q_o} \right) + N \frac{\pi}{2}, \quad (3a)$$

where N is an appropriate integer, φ_n is the orientation angle of the wall normal with respect to the original coordinate system, and

$$q_o = K_o / 2\pi M_s^2. \quad (3b)$$

When this composite anisotropy-demagnetizing tensor is normalized by dividing by $2\pi M_s^2$, the anisotropy energy density becomes $2\pi K'_{jk} M_j M_k$, where

$$K'_{jk} = \begin{bmatrix} q_1 & 0 & 0 \\ 0 & q_1 + q_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (3c)$$

in which

$$q_1 = q_u + \frac{1}{2} (1 + q_o - q_2), \quad (3d)$$

$$q_2 = [(1 + q_o)^2 - 4q_o \cos^2 \varphi_n]^{1/2}, \quad (3e)$$

and

$$q_u = K_u / 2\pi M_s^2. \quad (3f)$$

Finally, after adding an isotropic exchange term, the total energy density becomes

$$\rho_E = \frac{A}{M_s^2} \frac{\partial M_j}{\partial x_k} \frac{\partial M_j}{\partial x_k} + 2\pi K'_{jk} M_j M_k, \quad (3g)$$

where A is the isotropic exchange constant. From this point onward, as well as in (3g), the components of all vectors and tensors and the angles θ and φ are assumed to be specified with respect to the coordinate system in which K'_{ij} is diagonal. Note that when $K_o = 0$, $q_2 = 1$ and $q_1 = q_u = K_u / 2\pi M_s^2$, so that q_1 then reduces to the q defined in Sec. IV of Ref. 1. The q_1 and q_2 used by Hagedorn² do not depend on φ_n since he chose a particular φ_n in order to simplify his presentation. Equation (3e) is equivalent to Eq. (6.5) of Ref. 3. In (3g) there is no applied-field term and all global (from the surface of the infinite magnetic medium) demagnetizing effects have been neglected.

III. EIGENVALUE EQUATION

In the absence of damping, the equation of motion of the magnetization is

$$\frac{\partial M_j}{\partial t} = -|\gamma| e_{jhp} M_k H_p, \quad (4)$$

where t is time, γ is the gyromagnetic ratio, and

the equivalent field H_j is the negative of the functional derivative of (3g), $-\delta\rho_E/\delta M_j$, as usual. The exact solution for the steady-state domain-wall motion obtained by Walker⁴ (originally obtained for the case of $K_o = 0$, nonzero damping, and nonzero applied field) applies here with little more than a change of notation. In terms of the orientation angles, this solution, when oriented so that the wall normal is along the x_1 axis, is

$$\varphi = \varphi_0, \quad (5a)$$

$$\cos\theta = \tanh[(\pi/l_w) n_j (x_j - v_j t)], \quad (5b)$$

where the orientation angle φ_0 , the wall width l_w , and the velocity v are constants. (Since only motion normal to the wall has significance here, the velocity will henceforth be written as a scalar $v = v_i n_i$.) When the solution (5a), (5b) is substituted into the equation of motion (4), the resulting consistency equations are the azimuthal-angle torque equation

$$\frac{v}{|\gamma|} \frac{\pi}{l_w} = -2\pi M_s q_2 \sin 2\varphi_0 \quad (5c)$$

and wall-width equation

$$A(\pi/l_w)^2 = 2\pi M_s^2 q_d. \quad (5d)$$

In (5d)

$$q_d \equiv q_1 + q_2 \sin^2 \varphi_0 \quad (5e)$$

and is defined as the dynamic q value. Any set of parameters for which these equations are simultaneously solved represents a possible moving-wall state of the system. The velocity corresponding to the φ_0 value for which the azimuthal-angle torque magnitude is maximized, $\varphi_0 = \frac{1}{4}\pi + N(\frac{1}{2}\pi)$, will be termed the Walker breakdown velocity. Note that $q_d \sin^2 \theta$ is the normalized anisotropy energy density of the system when φ is constrained to φ_0 . Thus (5d) is the usual wall-width expression with q replaced with q_d . The energy of the moving wall is similarly

$$\sigma_w = 4(A 2\pi M_s^2 q_d)^{1/2}. \quad (5f)$$

When (5c) is solvable there are generally four solutions, $0 \leq \varphi_0 < 2\pi$. The stable solutions, which are the only ones of interest here, are the ones nearest $\varphi_0 = 0$ or $\varphi_0 = \pi$. Note that in order for wall-motion solution of the Walker form to exist q_1 and q_2 must be nonzero.

The next step in obtaining the eigenvalue equation is to transform the components of M_j (but not the position coordinates) so that the moving-wall solution becomes $M'_j = (0, 0, M_s)$. This is a generalization of the procedure used previously⁵⁻⁹ in the special case, $v = 0$. The time- and space-dependent orthogonal transformation which accomplishes this is

$$M'_j = W_{jk} M_k, \quad (6a)$$

$$M_j = W_{kj} M'_k, \quad (6b)$$

where

$$W_{jk} = \begin{bmatrix} \cos\theta \cos\varphi & \cos\theta \sin\varphi & -\sin\theta \\ -\sin\varphi & \cos\varphi & 0 \\ \sin\theta \cos\varphi & \sin\theta \sin\varphi & \cos\theta \end{bmatrix}, \quad (6c)$$

in which the angles are those given by (5a) and (5b). Again it must be emphasized that W_{jk} is to be applied to M_k only and not to x_k . The problem is now formally reduced to the usual spin-wave problem, except that the wave equation has time- and space-dependent coefficients. The magnetization may be written

$$M'_j = [m_x, m_y, (M_s^2 - m_x^2 - m_y^2)^{1/2}], \quad (7)$$

so that the excitations of the system may be written in terms of the two-component object

$$m = \frac{1}{\sqrt{2}} \begin{bmatrix} m_x + im_y \\ m_x - im_y \end{bmatrix}, \quad (8)$$

where $i = \sqrt{-1}$. Finally, the excitation equation is written in terms of a normalized time and normalized coordinates attached to the wall. These coordinates are defined by

$$\tau = 4\pi M_s |\gamma| q_d t, \quad (9a)$$

$$s_1 = (\pi/l_w)(n_j x_j - vt), \quad (9b)$$

$$s_2 = (\pi/l_w) e_{jhp} \xi_j n_h x_p, \quad (9c)$$

and

$$s_3 = (\pi/l_w) \xi_j x_j, \quad (9d)$$

where ξ_j is a unit polar vector having the components

$$\xi_j = [0, 0, 1]. \quad (9e)$$

Here s_1 is the normalized distance from an arbitrary point to the plane at the center of the domain wall; s_2 and s_3 are normalized transverse distances.

From (3), (4), and the definitions given above,

$$m = \frac{\text{sech } s_1}{2[4\kappa^2(\kappa^2 + 2\mathfrak{C})]^{1/4}} \left\{ \left(1 \pm i s \frac{[\kappa^2(\kappa^2 + 2\mathfrak{C})]^{1/2}}{2(\kappa^2 + \mathfrak{C})} (s_1) \right) \begin{bmatrix} \pm \kappa + (\kappa^2 + 2\mathfrak{C})^{1/2} \\ \mp \kappa + (\kappa^2 + 2\mathfrak{C})^{1/2} \end{bmatrix} \right. \\ \left. + i s \frac{\kappa^2}{4(\kappa^2 + \mathfrak{C}) r(r+1)} [\tanh s_1 F_s(r+1, s_1) + r F_a(r+1, s_1)] \begin{bmatrix} \pm \kappa - (\kappa^2 + 2\mathfrak{C})^{1/2} \\ \pm \kappa + (\kappa^2 + 2\mathfrak{C})^{1/2} \end{bmatrix} \right\} \exp[i(\kappa_j s_j + \Omega \tau)], \quad \kappa_1 = 0. \quad (13b)$$

The spin-wave eigenvalues are (see Appendix B)

$$\Omega_s = \pm [(1 + \kappa^2)(1 + \kappa^2 + 2\mathfrak{C})]^{1/2} - s \kappa_1 \quad (13c)$$

it can be shown that the linearized equation for the excitations is (see Appendix A)

$$\left(\frac{\partial}{\partial s_j} \frac{\partial}{\partial s_j} I - i s \frac{\partial}{\partial s_1} \sigma_x - (2 \tanh^2 s_1 - 1 + \mathfrak{C}) I \right. \\ \left. + \mathfrak{C} \sigma_x + s \tanh s_1 \sigma_y - i \frac{\partial}{\partial \tau} \sigma_z \right) m = 0, \quad (10a)$$

where σ_x , σ_y , and σ_z are the Pauli spin matrices, I is the 2×2 unit matrix,

$$s \equiv \frac{1}{2} \frac{q_2}{q_d} \sin 2\varphi_0, \quad (10b)$$

and

$$\mathfrak{C} \equiv \frac{1}{2} \frac{q_2}{q_d} \cos 2\varphi_0. \quad (10c)$$

Note again that (10a) is valid only in the approximation that the demagnetizing field is represented by (2), as discussed by Winter.⁵

IV. EIGENVALUES AND EIGENFUNCTIONS

The eigenvalues and eigenfunction for the translation and spin-wave modes^{5,9} to first order in the velocity parameter s are now presented. The wall excitation modes are normalized according to

$$\int_{-\infty}^{\infty} m^\dagger \sigma_z m ds_1 = \pm 1 \quad (11a)$$

and the spin-wave states are normalized according to

$$m^\dagger \sigma_z m = \pm 1, \quad |s_1| = \infty, \quad (11b)$$

where the dagger superscript denotes complex conjugate transpose.

The normalized angular frequency Ω and wave vector κ_j in a coordinate system parallel to the s_j coordinate system are defined by

$$\omega = 4\pi M_s |\gamma| q_d \Omega \quad (12a)$$

and

$$k_j = (\pi/l_w) \kappa_j. \quad (12b)$$

With the notation $\kappa = |\kappa_j|$, the translation-mode eigenvalues are (see Appendix B)

$$\Omega_t = \pm [\kappa^2(\kappa^2 + 2\mathfrak{C})]^{1/2}, \quad \kappa_1 = 0 \quad (13a)$$

and the translation eigenfunction

and the spin-wave eigenfunctions are

$$\begin{aligned}
m = & \frac{1}{2} [(1 + \kappa^2)(1 + \kappa^2 + 2\mathfrak{C})]^{-1/4} \left(1 + \kappa_1^2 \mp 2s\kappa_1 \frac{(1 + \kappa^2)^{1/2}(1 + \kappa^2 + 2\mathfrak{C})^{1/2}}{2(1 + \kappa^2 + \mathfrak{C})} \right)^{-1/2} \\
& \times \left\{ \left(\kappa_1 + i \tanh s_1 \mp s \frac{(1 + \kappa^2)^{1/2}(1 + \kappa^2 + 2\mathfrak{C})^{1/2}}{2(1 + \kappa^2 + \mathfrak{C})} \right) \left[\frac{\pm(1 + \kappa^2)^{1/2} + (1 + \kappa^2 + 2\mathfrak{C})^{1/2}}{\mp(1 + \kappa^2)^{1/2} + (1 + \kappa^2 + 2\mathfrak{C})^{1/2}} \right] \right. \\
& + s \frac{1}{2(1 + \kappa^2 + \mathfrak{C})} \left[i\kappa_1 \tanh s_1 - 1 + \frac{\kappa^2 - \kappa_1^2}{R(R+1)} \left(-i\kappa_1 \tanh s_1 - R + \frac{1}{2(R-1)} \{ [(R^2 + i\kappa_1(R-1)\tanh s_1 - R \tanh^2 s_1] F_s(R + i\kappa_1, s_1) \right. \right. \\
& \left. \left. - [i\kappa_1 R + R(R-1)\tanh s_1 - i\kappa_1 \tanh^2 s_1] F_a(R + i\kappa_1, s_1) \} \right) \right] \left. \left[\frac{\pm(1 + \kappa^2)^{1/2} - (1 + \kappa^2 + 2\mathfrak{C})^{1/2}}{\pm(1 + \kappa^2)^{1/2} + (1 + \kappa^2 + 2\mathfrak{C})^{1/2}} \right] \right\} \exp[i(\kappa_j s_j + \Omega\tau)]. \quad (13d)
\end{aligned}$$

In (13b) and (13d)

$$r \equiv [1 + 2(\kappa^2 + \mathfrak{C})]^{1/2}, \quad \kappa_1 = 0 \quad (13e)$$

$$R \equiv [2(1 + \kappa^2 + \mathfrak{C}) - \kappa_1^2]^{1/2}, \quad (13f)$$

$$F_s(x, y) \equiv F(x, y) + F^*(x, -y), \quad (13g)$$

$$F_a(x, y) \equiv F(x, y) - F^*(x, -y), \quad (13h)$$

$$F(x, y) \equiv F\left(1, 1; 1 + \frac{1}{2}x; \frac{1}{1 + e^{-2y}}\right), \quad (13i)$$

where $F(a, b; c; z)$ denotes the hypergeometric function and the asterisk denotes complex conjugate.

In the $s = 0$ ($v = 0$) case these functions are seen to reduce to the functions of Refs. 5-7. Note that $\Omega_i = 0$ at $\kappa_i = 0$ since this mode is associated with uniform translation of the domain wall. Note also that in first order the moving domain wall remains reflectionless to propagating spin waves since

$$\frac{\partial}{\partial s_1} [e^{-i\kappa_1 s_1} m(\kappa_1)] = 0, \quad |s_1| = \infty \quad (14a)$$

and

$$m(s_1 = \infty) = -m^*(s_1 = -\infty). \quad (14b)$$

In the general case it may be shown from symmetry that Ω_i is an even function of s . Also, since (10a) becomes a constant-coefficient equation at points far removed from the wall, the exact spin-wave eigenvalues are easily computed. They are

$$\Omega_{s_0} = \pm [(1 + \kappa^2)(1 + \kappa^2 + 2\mathfrak{C}) - s^2]^{1/2} - s\kappa_1. \quad (15)$$

Checking back through the many changes of variable shows that this expression is identical to the normal spin-wave dispersion relation for the material considered here. By using these modes (upper signs only) and transforming back to the original coordinate system (or at least a stationary one), it should be possible to form an occupation-number representation in the usual way. The major difference between this representation and the usual spin-wave representation is that the time and space

dependences of the modes do not appear in separate factors.

V. EXPERIMENTAL IMPLICATIONS

If it is assumed that the translation-mode dispersion relation (13a), although derived for an infinite planar wall, remains approximately true for a curved wall of finite extent, then the vibrational modes of this two-dimensional membrane may be computed and checked against experiment. A particularly simple example is a right-circular cylindrical domain in a thin plate of magnetic material. In this case k_ϕ clearly obeys cyclic boundary conditions. The situation at the surface of the plate is complicated but will be approximated here by a zero-derivative boundary condition on k_3 . The components of the wave vector of a wave bound to the domain wall thus may be specified as

$$k_\phi = N_\phi / r_0 \quad (16a)$$

and

$$k_3 = \pi N_3 / h, \quad (16b)$$

where r_0 and h are the domain radius and plate thickness, respectively; N_ϕ and N_3 are integers. Of these modes the one most easily treated is that for which

$$N_\phi = 1, \quad (17a)$$

$$N_3 = 0, \quad (17b)$$

$$\pi r_0 > h. \quad (17c)$$

Condition (17c) is imposed to ensure that the mode considered is the one with the smallest nonzero k vector. This mode has the advantage of being related to the translation of the domain in such a way that wall stretching and magnetostatic interactions are minimized (Ref. 10, Sec. IV. 2. 4). In materials where the damping is sufficiently small that the mode is not critically damped this mode might be observed in one of two ways. A test in which static stability effects are minimized is the observation of translation amplitude resonances at the mode

frequency when a static (on the average) domain is driven by a spatially uniform field gradient varying sinusoidally in time. Another test would be to look for an irregularity in the velocity-drive curve at the velocity for which the principal spin-flipping frequency within the wall ($f_p = v/2l_w$) is equal to the $N_\phi = 1$, $N_3 = 0$ frequency. In order for this test to be valid, this frequency must occur at a sufficiently small velocity so that the quadratic and higher correction terms to the domain-wall excitation frequency are unimportant.

VI. DEVICE IMPLICATIONS

The wall excitation dispersion relation has several implications affecting the choice of materials applicable for high-speed-device applications. One effect which is evident from (13a) is that increasing q_2 decreases the density of low-lying wall excitation states available to act as intermediaries in the dissipation of energy. If the Gilbert damping is very high, the excitation states surely have no great importance since the wall motion and excitations are both well damped by direct processes. However, in materials with small damping (an essential requirement for a high-mobility material), decreasing the density of the wall excitation states will decrease the amount of power coupled into the spin waves (the wake¹¹) by material inhomogeneities such as phonons, so that increasing q_2 will increase the domain mobility. The effect of increasing q_2 may be considered from another point of view by noting that the stiffness of the domain wall with respect to a perturbation at some point on the domain wall generally increases with increasing q_2 .

Another related effect is that, when the spin-flipping rate within the domain wall enters the wall excitation spectrum, the opportunity for strong interactions between the domain-wall motion and the excitations exists. If the coupling were sufficiently strong, this could take the form of a limiting-velocity behavior. In a cylindrical domain having the preferred values of diameter and plate thickness defined in Eqs. (6), (31), and (32) of Ref. 1,

$$d = 8l, \quad (18a)$$

$$h = 4l, \quad (18b)$$

$$l = \sigma_w / 4\pi M_s^2, \quad (18c)$$

the mode with $N_\phi = 1$, $N_3 = 0$ has the lowest frequency. For these conditions the domain velocity at which the principal spin-flipping frequency within the wall becomes equal to the frequency of the lowest excitation frequency from (5e), (5f), (12b), (13a), and (16a) is

$$v_m = 4\pi M_s |\gamma| \frac{l_w}{\pi} \frac{1}{8} \left(\frac{q_2 \cos 2\phi_0}{q_a} + \frac{1}{(8q_a)^2} \right)^{1/2}, \quad (19)$$

where the dynamic wall energy has been computed from (5) by using the domain velocity for the wall velocity. The ratio of this velocity to Walker's breakdown velocity, defined previously, is

$$(v_w/v_m) = 4(q_1 q_2)^{1/2} \quad (20a)$$

when

$$q_1 \gg q_2 \sin^2 \phi_0. \quad (20b)$$

Since under condition (20b) s is small, the wall excitation dispersion relation on which (20a) is based should be valid. For devices in which the domain spacing is $24l$ (three times the preferred diameter), the operating frequency consistent with the velocity [(19)] is

$$f_m = 4\pi M_s |\gamma| \frac{1}{384} q_1^{-3/2} q_2^{1/2} \quad (21a)$$

when

$$q_1 \gg q_2 \sin^2 \phi_0. \quad (21b)$$

Although definitive experimental evidence for these modes has not been reported, some comparisons with experiment can be made. The measured static parameters for $\text{PbAl}_4\text{Fe}_3\text{O}_{19}$ are $A = 1.1 \times 10^{-7}$ erg cm⁻¹, $q_1 = 110$, and $q_2 = 1$ ($K_o = 0$).^{2,12} By using these values, the Walker breakdown velocity is ~ 1400 cm/sec and v_m is ~ 30 cm/sec. These values bracket the observed limiting velocity of 100 cm/sec.¹³ The measured static parameters for YFeO_3 are $A = 4.7 \times 10^{-7}$ erg cm, $q_1 = 630$, $q_2 = 320$.^{2,12} (Since $K_o \gg 2\pi M_s^2$ here q_2 need not be specified as a function of angle.) In this case the Walker breakdown velocity is 3.5×10^5 cm/sec, and v_m is 2.2×10^2 cm/sec. The observed velocity-drive relation for this material is linear up to the maximum observed value of 9×10^4 (Ref. 14). The attainment of such high velocities (and mobilities) in YFeO_3 is probably attributable to the high value of q_2 in this material, reducing the density of low-lying translation states.

The preceding indicates that the high-speed-device-material requirements of low damping ($\alpha \ll 1$) and the widest possible wall width (Ref. 1, Sec. IV) remain valid, but that an additional requirement is that q_2 be as high as possible. Consider now a material in which $q_2 = 1$ arising only from the local demagnetizing field. In such a material the entire domain wall is nearly a Bloch wall at low velocity. If $0 < K_o \ll 2\pi M_s^2$ then the domain wall remains a Bloch wall, but now q_1 and q_2 vary around the perimeter of the domain in accordance with (3). This has two detrimental effects: The value of q_2 is reduced below 1 at some locations on the domain perimeter, reducing the Walker breakdown velocity; the variation in q_1 causes the wall energy to vary, which reduces device margins by producing elliptical domains as discussed in Ref. 1, Sec. II.4. The situation is most complex and most damaging at $K_o = 2\pi M_s^2$, in which case planar wall motion

breaks down immediately in some directions.

When $K_o \gg 2\pi M_s^2$, the Bloch-to-Néel wall alteration around the domain perimeter, which is characteristic of orthoferrites, is obtained. In this case, the q_1 variation again induces a wall energy variation which in turn induces elliptical domains and reduces device margins. In order to offset this effect, K_u must be increased so that q_1 is substantially greater than 1. The consequent reduction in mobility produced by the decreased wall width then tends to offset the advantage of having q_2 greater than one. Consequently, the preferred material would have q_1 be several times greater than 1 and q_2 very much greater than 1. The material must, of course, meet the usual requirements of a Curie temperature above room temperature, the proper M_s for the desired domain diameter, and low damping ($\alpha \ll 1$). Such a material could possibly be produced starting out with a material which instead of the usual easy axis has intrinsically a strong hard axis. ($K_u = 0$, $K_o \gg 2\pi M_s^2$ in the present notation.) The material would be grown epitaxially on a substrate in such a way that the intrinsic hard axis lies in the plane and the required additional anisotropy K_u would be induced by the growth as it is in epitaxially grown garnet films.¹⁵

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APPENDIX A

This appendix is an outline of the derivation of the excitation equation (10a) from the equation of motion (4) and the transformations (5)-(9).

The equivalent field is obtained from the variational derivative of the energy density [(3g)]:

$$H_j = -\frac{\delta \rho_E}{\delta M_j} = \frac{2A}{M_s^2} \frac{\partial^2 M_j}{\partial x_k^2} - 4\pi K'_{jk} M_k. \quad (\text{A1})$$

The effect of the transformations on the equation of motion will now be shown. The procedure used on H_j is exactly the same. The space and time variables in (4) are transformed according to (9) so that the equation becomes

$$\frac{\partial M_j}{\partial \tau} + s \frac{\partial M_j}{\partial s_1} = \frac{-1}{4\pi M_s q_d} e_{jkn} M_k H_n. \quad (\text{A2})$$

The transformation should be regarded as a transformation of the independent variables of a partial differential equation since the components of M_j are not transformed. Next, the components of M_j (the dependent variables) are transformed according to (6). Multiplying by W_{jk} and inserting $W_{nj} W_{nk} = \delta_{jk}$

where appropriate, we have

$$\begin{aligned} W_{jk} \frac{\partial M_k}{\partial \tau} + s W_{jk} \frac{\partial W_{nk} W_{np} M_p}{\partial s_1} \\ = \frac{-1}{4\pi M_s q_d} W_{jk} e_{knp} W_{rn} W_{ru} M_u W_{vp} W_{vw} H_w, \end{aligned} \quad (\text{A3})$$

$$\frac{\partial M'_j}{\partial \tau} + s \frac{\partial M'_j}{\partial s_1} + s W_{jk} \frac{\partial W_{nk}}{\partial s_1} M'_n = \frac{-1}{4\pi M_s q_d} e_{jkn} M'_k H'_n,$$

where

$$H'_j \equiv W_{jk} H_k, \quad (\text{A4})$$

$$\begin{aligned} \frac{\partial M'_j}{\partial \tau} + s \frac{\partial M'_j}{\partial s_1} + s \operatorname{sech} s_1 e_{2jk} M'_k = \frac{-1}{4\pi M_s q_d} \\ \times e_{jkn} M'_k H'_n, \end{aligned} \quad (\text{A5})$$

$$\frac{\partial M'_j}{\partial \tau} + s \frac{\partial M'_j}{\partial s_1} = -\frac{1}{M_s} e_{jkn} M'_k \left(\frac{H'_n}{4\pi q_d} + s \operatorname{sech} s_1 A_n \right), \quad (\text{A6})$$

where

$$A_n = (0, M_s, 0). \quad (\text{A7})$$

When the process is carried through on H'_j it is found that for Walker's solution, $M'_j = [0, 0, M_s]$,

$$\frac{H'_n}{4\pi q_d} + s \operatorname{sech} s_1 A_n = 0, \quad (\text{A8})$$

so that (A6) is solved. When (7) is approximated by $M'_j = (m_x, m_y, M_s)$ it is found that Eq. (A6) is again solved to zero order in m_x and m_y , and that in first order in m_x and m_y there are two coupled equations which may be arranged in the form (10a). There is a one-to-one correspondence between the left-hand terms in (A6) and the σ_z terms in (10a).

APPENDIX B

In this appendix the derivation of the first-order perturbation (in s) eigenvalues of the eigenvalue equation in $f^+(s_1)$ and $f^-(s_1)$, which results when

$$m = \begin{bmatrix} f^+(s_1) \\ f^-(s_1) \end{bmatrix} \exp[i(\kappa_j s_j + \Omega \tau)], \quad j = 2, 3 \quad (\text{B1})$$

is substituted into (10a), is discussed.

The eigenvalue equation is

$$(L_0 + s L_1 + \Omega \sigma_z) m = 0, \quad (\text{B2a})$$

where

$$L_0 = \frac{\partial^2}{\partial s_1^2} - (2 \tanh^2 s_1 - 1 + \kappa_j^2 + \mathcal{C}) I + \mathcal{C} \sigma_x \quad (\text{B2b})$$

and

$$L_1 = -i \frac{\partial}{\partial s_1} \sigma_z + \tanh s_1 \sigma_y, \quad (\text{B2c})$$

where L_0 , L_1 , and $\Omega \sigma_z$ are all self-adjoint. Now if $\Omega = \Omega_0 + s \Omega_1 + \dots$, $f = f_0 + s f_1 + \dots$, and $(L_0 + \Omega_0 \sigma_z) \times f_0 = 0$, then it is a result of first-order perturba-

tion theory that, if f is bound to the wall or reflectionless,

$$\int_{-\infty}^{\infty} f_0^\dagger L_1 f_0 ds_1 + \Omega_1 \int_{-\infty}^{\infty} f_0^\dagger \sigma_x f_0 ds_1 = 0. \quad (\text{B3})$$

Now in the bound case, (13b) for $s=0$, f_0 is even in s_1 and L_1 is odd in s_1 , so that $\Omega_1=0$. In the spin-wave case, $f_0=f_0' e^{ik_1 s_1}$, the form of the envelope function is such that only the term which re-

sults from differentiation of $e^{ik_1 s_1}$ contributes, and therefore

$$\Omega_1 = i \frac{\int_{-\infty}^{\infty} f_0^\dagger (\partial/\partial s_1) \sigma_x f_0 ds_1}{\int_{-\infty}^{\infty} f_0^\dagger \sigma_x f_0 ds_1} = -\kappa_1. \quad (\text{B4})$$

Given the eigenvalues the eigenfunctions may be verified by direct substitution.

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Multiple Ordering in Magnetite

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We present results of a self-consistent band calculation of the ground-state energy and charge orderings based on a tight-binding scheme in magnetite. The calculation is greatly simplified by making use of the large intra-atomic Coulomb interactions between electrons on the Fe ions, previous estimates of the crystal field splittings, and the magnetic ordering. We find that below a critical value (~ 2.2) of the ratio of interatomic Coulomb energy U to bandwidth w the lowest-energy state has no order. Between this critical value and 2.5, the preferred state is multiply ordered (three nonzero order parameters). For larger values of this ratio, the Verwey-symmetry state (one order parameter) is stable, but the value of the order parameter approaches 1 (ionic Verwey order) only in the limit of $U/w \rightarrow \infty$.

INTRODUCTION

For many years, the accepted description of the metal-insulator transition in magnetite was that proposed by Verwey,¹ i.e., that below the transition temperature the Fe^{3+} and Fe^{2+} ions on the B sites are ordered, the likely order being alternate (001) planes of Fe^{3+} and Fe^{2+} ions.

Recently,² we introduced an itinerant-electron one-dimensional model of the extra B -site electrons interacting with each other via interatomic Coulomb repulsions. The model exhibited a phase transition from a "disordered" metallic state above a critical temperature to an ordered insulator below. The charge ordering allowed fractional occupation of sites even at $T=0^\circ\text{K}$. This