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Test of the coherent-anisotropy-field approximation for a lattice model of a random-axis ferromagnet in a high magnetic field

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We report the results of a numerical test of the coherent-anisotropy-field approximation (CAFA) for characterizing the high-field limit of the magnon spectrum for a lattice model of a ferromagnet with random anisotropy axes. The CAFA reproduces the downward shift in the ferromagnetic resonance frequency and accounts for the modification of the density of states induced by the disorder. The agreement confirms the analogy between the random-axis model in the high-field limit and the potential fluctuation model for the random-alloy problem.

I. INTRODUCTION

In a recent paper,[1] an approximate treatment of the magnon excitations in a lattice model of a ferromagnet with random-axis anisotropy was outlined. The analysis pertained to the high-field limit where the applied magnetic field was large in comparison with the exchange and anisotropy fields. It was pointed out that there was a formal analogy between the random anisotropy problem in the high-field limit and the problem of the electronic states in a model alloy with random potential fluctuations. This analogy was utilized to develop an approximate theory for the magnons based on the concept of a coherent anisotropy field which is the magnetic counterpart of the coherent potential that plays a central role in the coherent-potential approximation for random alloys. The purpose of this paper is to report the results of a test of the coherent-anisotropy-field approximation (CAFA) against exact results for finite arrays of spins that are obtained utilizing matrix diagonalization and equation-of-motion techniques. In Sec. II we review the random-axis model and the CAFA, Sec. III is devoted to a discussion of the numerical techniques, and Sec. IV summarizes the comparison between the CAFA and the numerical calculations.

II. RANDOM-AXIS FERROMAGNET AND THE CAFA

The Hamiltonian for a ferromagnet with random-axis anisotropy takes the form

$$\mathcal{H} = -\sum_{(i,j)} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j - \mathcal{D}\sum_i(\hat{\mathbf{n}}\cdot\mathbf{S}_i)^2 + H\sum_i S_i^z . \quad (1)$$

In Eq. (1), the first and third terms denote the exchange and Zeeman interactions, respectively. The second term is the random anisotropy and is characterized by an anisotropy axis $\hat{\mathbf{n}}_i$ which varies randomly throughout the system. One can develop a harmonic theory for the excitations by carrying out a Holstein-Primakoff expansion about the equilibrium spin orientations.

In the high-field limit, the spins are lined up along the applied field. In this limit the harmonic approximation to the magnon Hamiltonian takes the form

$$\mathcal{H}_0 = \sum_i\sum_j SJ_{ij}a_i^\dagger a_i - \sum_{(i,j)} SJ_{ij}(a_i^\dagger a_j + a_j^\dagger a_i) + 3SD\sum_i(\cos^2\theta_i - \tfrac{1}{3})a_i^\dagger a_i + H\sum_i a_i^\dagger a_i , \quad (2)$$

where S is the spin, $a_i(a_i^\dagger)$ obey Bose commutation relations, and $D = \mathcal{D}[1-1/(2S)]$ is the renormalized anisotropy constant. The symbol θ_i denotes the angle between the anisotropy axis and the applied field.

In our analysis we will assume that the spins occupy sites on a simple cubic lattice and that the exchange interaction, limited to nearest neighbors, is the same for all nearest-neighbor pairs. With these assumptions, the first and fourth terms in Eq. (2) can be combined leading to the result

$$\mathcal{H}_0 = \sum_i(6SJ+H)a_i^\dagger a_i - SJ\sum_{(i,j)}{}'(a_i^\dagger a_j + a_j^\dagger a_i) + 3SD\sum_i(\cos^2\theta_i - \tfrac{1}{3})a_i^\dagger a_i , \quad (3)$$

where the prime signifies that the sum is limited to nearest neighbors.

In the alloy analogy, the first and third terms in Eq. (3) play the role of the uniform and fluctuating terms in the potential, while the second term corresponds to the electron transfer or hopping term. The influence of the disorder depends on the ratio D/J and on the distribution of $\cos\theta$. We will consider cases of moderate to strong disorder corresponding to $D/J = 3$, 6, and 9. We also make the assumption that $\cos\theta$ is uniformly distributed between -1 and $+1$ so that the average value of the potential fluctuation is zero.

In testing the CAFA, we will focus on the ferromagnetic resonance, or uniform mode, frequency, and the density of states. Both of these are obtained from the CAFA propagator $\langle G\rangle$ defined by

$$\langle G\rangle[\mathbf{k}, E - H_a^c(E)] = [E - H_a^c(E) - E(\mathbf{k})]^{-1} , \quad (4)$$

where $E(\mathbf{k})$ is the magnon energy in the absence of disorder

$$E(\mathbf{k}) = H + 2JS(3 - \cos k_x - \cos k_y - \cos k_z), \quad (5)$$

and $H_a^c(E)$ is the frequency-dependent coherent anisotropy field whose calculation is outlined in Ref. 1. The uniform mode frequency ω_0 is determined by the peak in the imaginary part of $\langle G\rangle[0,\omega_0 - H_a^c(\omega_0)]$, whereas the density of states $\rho(E)$ is given by the sum

$$\rho(E) = -(1/\pi)\sum_{\mathbf{k}} \mathrm{Im}\langle G\rangle[\mathbf{k}, E - H_a^c(E)]. \quad (6)$$

III. NUMERICAL TECHNIQUES

As mentioned in the Introduction, numerical techniques for calculating the magnon excitations involve matrix diagonalization and equation-of-motion techniques. Since the application of the former to the random-axis model is discussed in a recent paper,[2] we will consider in detail only the equation-of-motion approach. Both techniques have as their starting point a classical (Néel) equilibrium configuration obtained by rotating the spins into their local fields, which are the sums of the exchange, anisotropy, and applied fields, viz.,

$$\mathbf{H}_i^{\mathrm{loc}} = J\sum_j{}' \mathbf{S}_j + 2D\hat{\mathbf{n}}_i(\hat{\mathbf{n}}_i \cdot \mathbf{S}_i) + H\hat{\mathbf{z}}. \quad (7)$$

Since the rotation of the ith spin affects the local fields at the other sites, the process must be iterated until the total energy stabilizes (to one part in 10^8).[3]

Having obtained a local equilibrium configuration by this method, one can develop a harmonic theory for the magnon dynamics by treating deviations of the spin from their equilibrium orientations as small quantities. The effect of this step is to generate a set of linear equations for the local spin operators. By integrating the equations of motion, one can obtain the zero-temperature dynamic structure factor $S(\mathbf{k},\omega)$. Since the calculation is similar to an analogous calculation of the dynamic structure factor of a Heisenberg spin glass,[3] we will only point out the changes involved in applying the formalism of Ref. 3 to an anisotropic system. The major modification entails replacing Eqs. (2.4) and (2.5) of Ref. 3 by the corresponding equations

$$R_{jk} = -\tfrac{1}{2} SJ_{jk}\mathbf{u}_j^+ \cdot \mathbf{u}_k^+ - \delta_{jk} SD(\hat{\mathbf{n}}_j \cdot \mathbf{u}_j^+)^2, \quad (8)$$

$$S_{jk} = -\tfrac{1}{2} SJ_{jk}\mathbf{u}_j^+ \cdot \mathbf{u}_k^- + \delta_{jk}\left[S\sum_n J_{jn}\hat{\gamma}_j \cdot \hat{\gamma}_n + 2SD(\hat{\mathbf{n}}_j \cdot \hat{\gamma}_j)^2 - SD(\mathbf{u}_j^- \cdot \hat{\mathbf{n}}_j)(\mathbf{u}_j^+ \cdot \hat{\mathbf{n}}_j) + H\gamma_j^z\right], \quad (9)$$

where the symbols have the same meaning as in that reference.

By using the fluctuation-dissipation theorem, one can show that the response to a spatially uniform, oscillating field is proportional to $S(0,\omega)$. Thus we are led to identify the ferromagnetic resonance frequency with the location of the peak in $S(0,\omega)$.

IV. COMPARISON

In making the comparison between the CAFA and the numerical simulations, units were chosen such that $J = S = 1$. The high magnetic field limit was ensured by taking H large enough that $|\langle S_z\rangle| \approx 1$. With $|\langle S_z\rangle| \geq 0.99$ as a criterion, we used $H = 12.3$, 28.4, and 46.5 for $D/J = 3$, 6, and 9, respectively.

The results for the density of states are shown in Figs. 1 and 2. Energies are measured relative to H since in the absence of anisotropy, the application of a field shifts the energies of all of the modes by this amount. Figure 1 is a histogram showing the distribution of modes obtained by diagonalizing the dynamical matrices derived from six configurations, each with $8\times8\times8$ spins. Figure 2 is the density of states in the CAFA. From these figures, it is evident that the CAFA accounts reasonably well for the modification of the density of states by disorder, reproducing the peak that develops at low energies as the distribution approaches the large-D limit

$$\rho(E) = [(E-H)/3D + \tfrac{1}{3}]^{-1/2}, \quad -D \leq E - H \leq 2D, \quad (10)$$

appropriate when $D/J \gg 1$.

The corresponding comparison for the ferromagnetic resonance frequencies is shown in Fig. 3, where the solid curve is the CAFA and the circles (triangles) denote data obtained by integrating the equations of motion of arrays of $16\times16\times16$ ($12\times12\times12$) spins. Again, the CAFA is seen to do a credible job of reproducing the numerical data.

The negative shift in the frequency of the uniform mode can be interpreted as an energy shift coming from the cou-

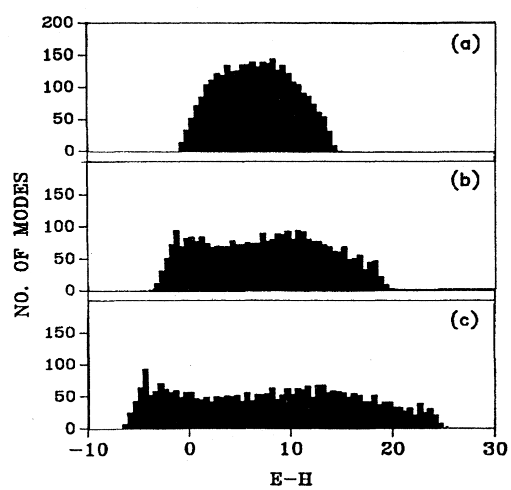

FIG. 1. Histogram showing distribution of magnon energies in a saturating field H. Results from six configurations, each with 512 spins: (a) $D=3$, $H=12.3$; (b) $D=6$, $H=24.4$; (c) $D=9$, $H=46.5$. $J=S=1$.

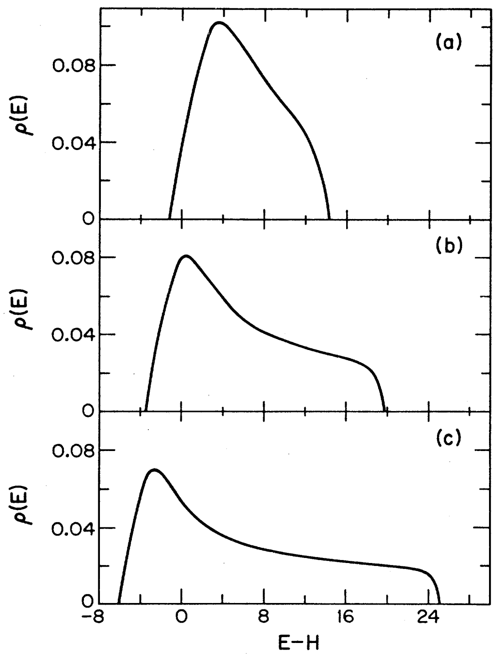

FIG. 2. Density of states in the CAFA: (a) $D=3$, (b) $D=6$, (c) $D=9$. All curves have the same area. $J=S=1$.

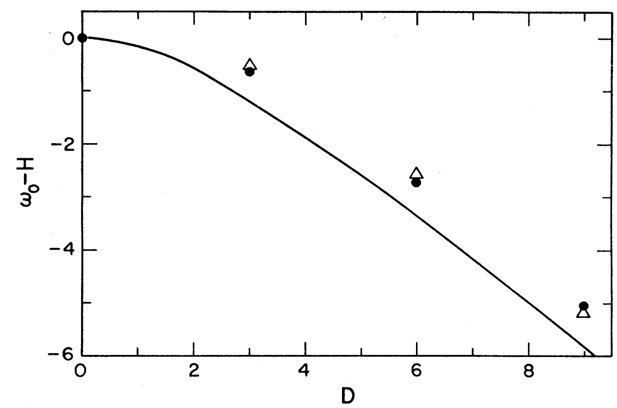

FIG. 3. Frequency of the uniform mode in a saturating field H vs D: curve, CAFA; solid circles, results from $16\times16\times16$ arrays; open triangles, results from $12\times12\times12$ arrays. $J=S=1$.

pling to modes with finite k, which is induced by the perturbation described by the last term in Eq. (3).[4] This result can be seen in a second-order calculation using the one-magnon states

$$|\mathbf{k}\rangle = N^{-1/2}\sum_j \exp(i\mathbf{k}\cdot\mathbf{r}_j)a_j^\dagger|\text{vac}\rangle\,, \qquad (11)$$

as the unperturbed eigenstates. One has

$$\Delta\omega = (3SD)^2 \sum_{\mathbf{k}\neq 0} \frac{|\langle 0|\sum_i(\cos^2\theta_i-\frac{1}{3})|\mathbf{k}\rangle|^2}{E(0)-E(\mathbf{k})} = [(3SD)^2/N^2]\sum_{i,j}\sum_{\mathbf{k}\neq 0}\frac{(\cos^2\theta_i-\frac{1}{3})(\cos^2\theta_j-\frac{1}{3})}{E(0)-E(\mathbf{k})}\,. \qquad (12)$$

Since there is no correlation between the directions of the anisotropy axes at different sites, the cross terms in Eq. (12) vanish leaving

$$\Delta\omega = (3SD)^2\left[N^{-1}\sum_i(\cos^2\theta_i-\tfrac{1}{3})^2\right]N^{-1}\sum_{\mathbf{k}\neq 0}[E(0)-E(\mathbf{k})]^{-1} = (3SD)^2\langle(\cos^2\theta-\tfrac{1}{3})^2\rangle N^{-1}\sum_{\mathbf{k}\neq 0}[E(0)-E(\mathbf{k})]^{-1}\,, \qquad (13)$$

which is negative since $E(0)$ is at the bottom of the bond so that $E(0)-E(\mathbf{k})<0$. In the case of the simple cubic lattice with nearest-neighbor interactions, Eq. (13) reduces to

$$\Delta\omega = -0.20D^2S/J\,, \qquad (14)$$

which matches the solid curve in Fig. 3 over the interval $0\leq D<1$.

In summary, the data displayed in Figs. 1–3 support the use of the CAFA to characterize the harmonic spin dynamics in a lattice model of a random-axis ferromagnet in a high magnetic field. Having established the validity of the alloy analogy, one is in a position to apply various concepts and mathematical techniques developed for the alloy problem to the random-axis model.[5,6]

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