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Ground state of a model with competing interactions and spin anisotropy

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Recent experiments on rare-earth multilayers have led to its being important to understand in detail the phase diagrams of models with competing interactions and spin anisotropy. Therefore we study the ground state of the XY model with competing first- and second-neighbor interactions and sixfold anisotropy, D. Infinite series of long-period phases are found to be stable. Particular attention is given to the evolution between the continuous spin and the discrete spin limits as D is increased from zero to infinity.

Systems with spatially modulated magnetic phases are surprisingly common in nature. The canonical examples are the rare-earth elements and their compounds which display a fascinating variety of periodic configurations, many with long wavelengths which can be commensurate or incommensurate with the underlying lattice.[1,2] These structures originate from the competition between exchange interactions which peak at a nonzero wave vector and spin anisotropy terms in the energy.

Considerable insight into the physics underlying the formation of modulated structures has been obtained by studying models with short-range competing interactions where tiny entropic differences between the different spin states lead to infinite sequences of commensurate and incommensurate phases.[3,4] Spin anisotropy and magnetic-field terms have also been introduced into the Hamiltonian but work has tended to be limited to values of the interactions chosen with the purpose of modeling specific rare-earth compounds.[5–7] Because of the current experimental interest in the fabrication of rare-earth multilayer structures,[8,9] it is now also important to understand the models of the bulk rare-earth solids throughout the ranges of their parameters.

Therefore in this paper we study in detail the ground state of a model with competing interactions and spin anisotropy as the anisotropy is varied from zero to infinity. The phase structure is determined by solving the equations which minimize the energy by iteration and then comparing the energies of the resulting solutions.[10] This is a powerful way of investigating the details of the ground-state phase diagram and is easily generalized to give the mean-field approximation to the finite-temperature behavior of the system.

The particular model we consider is the classical XY model with competing first- and second-neighbor axial interactions and sixfold anisotropy, D. For zero anisotropy the ferromagnetic ground state is replaced by a helical structure with continuously varying wave vector as the ratio of the competing interactions increases. For infinite D the model reduces to the six-state clock model with competing interactions where a small number of short-wavelength phases are stable. Our aim is to understand the evolution between these structures as the anisotropy is reduced.

The answer is surprisingly complex: an infinite number of long-period phases are stable in the ground state for any noninfinite anisotropy. One set of these springs from a multiphase point at $D=\infty$ where the ground state is infinitely degenerate. As D is decreased each phase becomes wider, then narrower (in the ratio of the competing interactions), until they hit the XY axis at a point which corresponds to the expected value of the wave vector (see Fig. 1). Two further sequences of phases spring from metastable multiphase points at infinite anisotropy and only appear as stable phases for small values of D. Hence the inverse anisotropy acts as a mechanism for generating sequences of long-period phases in a way analogous to the temperature in the *ANNNI* model.[4]

Similar features are seen in the chiral XY model with twofold anisotropy.[10] This is however a special case because the model maps onto a system with convex interactions and hence all phases are stable for all values of the spin anisotropy.[11] Mailhot *et al.*[12] studied the Heisenberg model with competing axial interactions and biquadratic exchange. They suggested the existence of modulated phases but were unable to resolve them. Sasaki[13] considered the model studied here in a magnetic field in the limit of large anisotropy.

We study an XY model with competing interactions along the z axis in the presence of a sixfold spin anisotropy term. Each classical XY spin vector lies in a plane perpendicular to z and has unit magnitude. The Hamiltonian is

$$H=-\frac{1}{2}J_0\sum_{ijj'}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i,j'}-J_1\sum_{i,j}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i+1,j}-J_2\sum_{i,j}\mathbf{S}_{i,j}\cdot\mathbf{S}_{i+2,j}+D\sum_{i,j}[1-\cos(6\theta_{i,j})]\ , \qquad (1)$$

where i labels the planes of spins perpendicular to the z direction and j and j' are nearest-neighbor spins within each plane. It will be useful to define $\theta_{i,j}$ as the angle between the spin located at the site (i,j) and, say, the x axis. The in-plane coupling is chosen to be ferromagnetic ($J_0>0$) and hence for zero temperature all the spins within a given plane are parallel. Competition is introduced along the z direction by taking the first- and second-neighbor interactions to be ferromagnetic and antiferromagnetic, respectively ($J_1>0$, $J_2<0$). $x=|J_2|/J_1$ will prove an important variable in the description of the phase diagram.

The parameter $D>0$ models a sixfold anisotropy in the (x,y) plane. The two limits $D=0$, $D=\infty$ are well understood. For $D=0$ the ground state is ferromagnetic for $x<\frac{1}{4}$. For $x>\frac{1}{4}$ it exhibits helical order with a wave vector $\mathbf{q}=q\mathbf{z}$ which is, in general, incommensurate with the underlying lattice. The magnitude of the wave vector is determined by the exchange energies through the relation $\cos q=(4x)^{-1}$.

For $D=\infty$, however, the spin angles $\theta_{i,j}$ are constrained to take one of the discrete set of values $\pi k_{i,j}/3$, where $k_{i,j}=0,1,2,3,4,5$ will be used to label the different spin states. The Hamiltonian (1) then reduces to the six-state clock model with competing interactions.[14] The ground state now has a very different character: only a few short-period commensurate phases are stable as x is varied. For $x<\frac{1}{3}$ the ground state is ferromagnetic. For $\frac{1}{3}<x<1$ the order along the z axis is helical with a sequence $k_i\equiv k_{i,j}=\ldots 01234501\ldots$, with spins in adjacent planes differing by an angle $(\pi/3)$. For $x>1$ there are two degenerate states at zero temperature $\ldots 01340134\ldots$ and $\ldots 00330033\ldots$. Following Ref. 14 we use a notation, described more fully below, which distinguishes the two ground states degenerate for $x>1$ as $\langle 2\rangle$ and $\langle\bar{2}\rangle$, respectively.

At $x=1$ itself there is a multiphase point where infinitely many phases coexist. These are all states for which $|k_{i+1}-k_i|=1$ or 2, with the proviso that two neighboring jumps of 2, $|k_{i+2}-k_{i+1}|=|k_{i+1}-k_i|=2$, are forbidden. If $|k_{i+1}-k_i|=2$ we shall say that there is a wall between i and $i+1$. A band is defined as the sequence of spins between two walls. A given state can be labeled by $\langle l_1,l_2,l_3,\ldots\rangle$ where the repeating sequence comprises bands of length $l_1,l_2,l_3,\ldots$. For example, $\ldots 01|345|12|450\ldots$, where walls are denoted by vertical lines, will be labeled $\langle 23\rangle$.

The aim is to elucidate the ground state of the Hamiltonian (1) as a function of x and D to understand the crossover between the two very different types of ordering at $D=0$ and $D=\infty$. We use a method which is analogous to the exact $T=0$ limit of the mean-field theory for discrete spin models with competing interactions at finite temperatures. Our results are then checked by high D expansions[15] and an effective potential approach.[11]

The ground-state energy E_0 for the Hamiltonian (1) on an $N\times N\times N$ three-dimensional lattice can be written

$$\frac{E_0}{N^2}=-\frac{1}{2}\sum_i \mathbf{F}_i\cdot\mathbf{M}_i+D\sum_i[1-\cos(6\alpha_i)]\ , \tag{2}$$

where $\mathbf{F}_i$ is a local field defined by

$$\mathbf{F}_i=J_1(\mathbf{M}_{i-1}-\mathbf{M}_{i+1})+J_2(\mathbf{M}_{i-2}+\mathbf{M}_{i+2})+q_\perp J_0\mathbf{M}_i\ . \tag{3}$$

$q_\perp$ is the number of nearest neighbors in a plane and $\mathbf{M}_i$ is the average magnetization per spin in a plane, a vector with unit magnitude which makes an angle α_i with the x axis.

For a given choice of x and D the stable phase corresponds to a minimum of E_0. Minimizing (2) with respect to the α_i gives a set of N coupled nonlinear equations which can be solved numerically by iteration. In general there are many metastable states corresponding to phases with spin configurations similar to that of the ground state. Typically the solution found by iteration has the same wave vector as the input configuration. In principle the true ground state can be found by comparing the energies of all possible solutions. However, this is a tedious procedure and the possibility always exists that the ground state has not been included in the trial configurations.

To avoid these problems we use a systematic approach first proposed by Selke and Duxbury in their study of the mean-field phase diagram of the *ANNNI* model.[16,17] They built up the phase diagram step by step by assuming that the first phase which may appear between two phases $\langle\nu_1\rangle$ and $\langle\nu_2\rangle$ is $\langle\nu_1\nu_2\rangle$; between $\langle\nu_1\rangle$ and $\langle\nu_1\nu_2\rangle$ is $\langle\nu_1^2\nu_2\rangle$ and so on. This pattern has never been violated in the phase diagram of models of this type, the pattern held in several cases checked for this model and it is confirmed by high D expansions. Once such ordering of the phases is assumed, phase boundaries follow easily from a comparison of the energies.

We now present our results. For a given phase, as D is reduced from infinity, the orientation θ_i of each spin may deviate from the easy axes. This happens in such a way as to close the gaps $|k_{i+1}-k_i|=2$. As $D\to 0$ the angles between successive spins tend to the same value as expected for the XY model. The wavelength of the resulting helical phase is the same as that of the original configuration at $D=\infty$. We use the same notation as for $D=\infty$ bearing in mind that a sequence of clock variables k_i does not necessarily mean that the spins are parallel to the easy axes.

The ground-state phase diagram is shown schematically in Fig. 1. Within the limits of the method all phases which only contain bands of length ≥ 3 and which obey the branching rules, spring from the multiphase point at $x=1$ as D is decreased. All phases containing 2 and 3 bands then appear between $\langle 2\rangle$ and $\langle 3\rangle$ as D is decreased. It was possible to check for the existence of phases with periods of up to 100 lattice spacings. Higher-order phases occupy extremely narrow regions of the phase diagram.

The solid phase boundaries shown in Fig. 1 follow the numerical results. As $D\to 0$ we also show by dotted lines the expected behavior, that the phase widths decrease and a given phase touches the XY axis at a single point corresponding to the appropriate value of q. For example, the $\langle 4\rangle$ phase, which is dominant for large D, meets the $D=0$ axis at the point $x=[\sqrt{2}(\sqrt{3}-1)]^{-1}$ corresponding to $q=(5\pi/12)$. The $\langle 2\rangle$ phase meets the axis at $x=\infty$. It is not possible to follow the low anisotropy behavior numerically because an infinite number of phases would have to be considered.

The phases generated from the $(x=1,\ D=\infty)$ multiphase point correspond to commensurate phases on the $D=0$ axis which lie at $x\geq\frac{1}{2}$. Therefore we still need to understand how commensurate structures with $q<\pi/6$

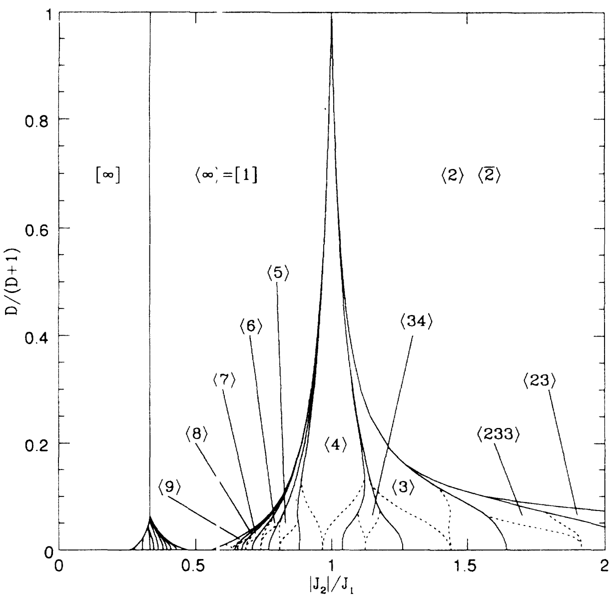

FIG. 1. Ground-state phase diagram of the XY model with competing axial interactions and sixfold spin anisotropy, D. The method of labeling the phases is described in the text. Bold lines depict the numerical results; the dotted boundaries show the expected behavior of the phase boundaries as the XY limit is approached.

which lie between $\frac{1}{4} < x < \frac{1}{2}$ are generated as the value of D is reduced.

For $D = \infty$ the ferromagnetic and helical phases coexist for $x = \frac{1}{3}$. However, this is not a multiphase point and there is a first-order transition between the phases for large D. Decreasing D neither the ferromagnetic nor the helical phases change their energy as the spins remain along an easy axis. Consequently the transition remains at $x = \frac{1}{3}$.

However, it is also necessary to consider two sets of phases which in the limit $D = \infty$ are very close in energy to the ferromagnetic and helical phases but which lower their energy as D decreases. To describe these phases a new notation is needed. Consider sequences of spins with $|k_{i+1} - k_i| = 0, 1$. We shall use the terminology that there is a wall between spins i and $i+1$ if $|k_{i+1} - k_i| = 1$ and that an l-band is a sequence of l parallel spins between two walls. A state is labeled by $[l_1 l_2 l_3 \ldots]$ (where the square brackets are introduced to emphasize the difference from the previous notation) if it comprises a repeating sequence of bands of lengths $l_1, l_2, l_3, \ldots$. For example, the state ...001233450012... is labeled by [211]. $[\infty]$ is the ferromagnetic phase and $\langle \infty \rangle \equiv [1]$. At ($x = \frac{1}{4}$, $D = \infty$) all structures obtained by combining 1- and 2-bands are degenerate. At ($x = \frac{1}{2}$, $D = \infty$) all phases comprising $m \geq 2$ bands are degenerate. As D decreases sequences of periodic phases spring from the multiphase points. For large D, however, these are metastable because the phases $[\infty]$ and [1] have lower energies. However, unlike $[\infty]$ and [1] they can decrease their energy by a canting of the spins. For example, in the phase [21] the two parallel spins move apart as D is decreased reaching, for $D = 0$, the uniform arrangement with $q = 2\pi/9$. Therefore we have to consider the possibility of their appearing as stable phases for small D.

Following the energies of the hidden phases sequences using the approach described above we find that this is indeed the case. The results are shown schematically in Fig. 1 and are enlarged in Fig. 2. The structures which originate from $x = \frac{1}{4}$ become stable only for a very low value of D (around 0.065 for $[21^4]$ and 0.03 for [2]). With numerical limitations all states made up from 1- and 2-bands and obeying the usual branching rules appear. These again are expected to meet the XY axis at points providing commensurate wave vectors that lie in the interval $1/(2\sqrt{3}) < x < \frac{1}{2}$ as shown in Fig. 2. The phases originating from $x = \frac{1}{2}$ appear for $D \simeq 0.02$ and close the gap with ferromagnetic phase.

Several other approaches were used to check our results. A high D expansion in the vicinity of the point ($x = 1$, $D = \infty$) was performed $O(1/D^2)$. The exact ground state was calculated for the crossover between the 6- and 24-state clock models with competing interactions. Both calculations gave results consistent with those described here.

To further check the ansatz that each new phase is formed by a combination of its neighbors we used the effective potential method introduced by Chou and Griffiths.[11] In this approach no assumption need be made about which state is stable for a given set of parameters, but the spin angle on each site must be quantized. Within the numerical limitations of the method (each spin quantized to $\pm 1°$) the results agreed with the previous approaches.

An important question is whether incommensurate

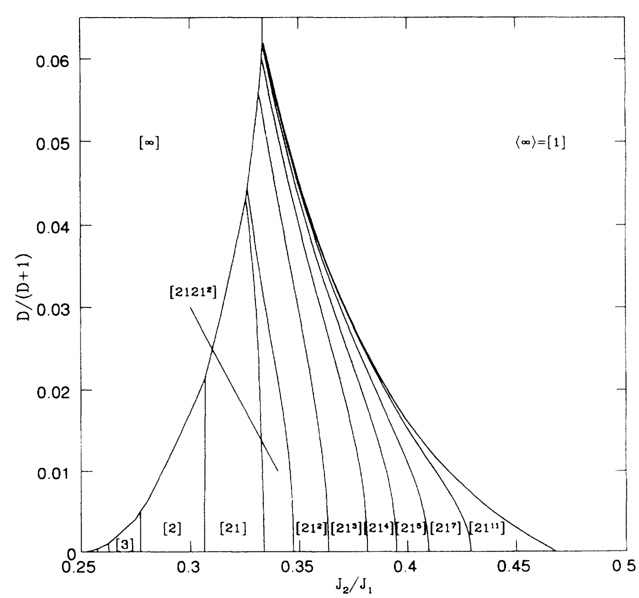

FIG. 2. An enlargement of Fig. 1 for $\frac{1}{4} < J_2/J_1 < \frac{1}{2}$ and small spin anisotropy. To within numerical accuracy all phases between $[\infty]$ and [1] which obey the usual branching rules are stable. They are expected to become narrower and hit the XY axis in a point as $D \rightarrow 0$. However, it is not possible to follow this behavior numerically.

phases persist in the phase diagram for nonzero spin anisotropy. In the continuum limit the Hamiltonian (1) can be mapped onto the Frenkel-Kontorova model.[18] Thus it is expected on the basis of previous work[19] that, for small D, the devil's staircase is incomplete with incommensurate phases appearing between the commensurate ones.

To conclude, we have fully elucidated the ground state of a model with competing interactions and spin anisotropy as the anisotropy is varied from zero to infinity. The method used provides a powerful means of understanding the details of the phase diagram and is easily generalized to give the mean-field approximation to the finite-temperature behavior of the system.

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