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Phase Locking in Heisenberg Helimagnets

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Abstract

We consider a Heisenberg model with ferromagnetic nearest-neighbor and competing further-neighbor exchange interactions in a small applied magnetic field at low temperature T. As a function of the exchange constants, the modulation vector is shown to have devil's staircase behavior. We consider the effects of nonzero temperature and quantum effects. We find a special modulation wave vector at which the incommensurability energy vanishes for the classical system at $T=0$.

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We consider a Heisenberg model with ferromagnetic nearest-neighbor and competing further-neighbor exchange interactions in a small applied magnetic field at low temperature T. As a function of the exchange constants, the modulation vector is shown to have devil's staircase behavior. We consider the effects of nonzero temperature and quantum effects. We find a special modulation wave vector at which the incommensurability energy vanishes for the classical system at $T = 0$.

I. INTRODUCTION

Magnets with competing interactions often have quite a rich phase diagram. For instance, in the ANNNI model,[1,2] which is an Ising model with competing interactions along only one direction (labeled the z direction), one studies the phase diagram in the T-J_2 plane, where the nearest-neighbor interaction is assumed to be ferromagnetic and of unit magnitude, J_2 is the next-nearest antiferromagnetic interaction, and T is the absolute temperature in energy units. The phase diagram at low temperature[2] shows (a) for small J_2 a ferromagnetic phase, (b) for large J_2 an antiferromagnetic phase in which the spins along the z direction form a periodic structure with a unit cell in which the sequence of spins is (up, up, down, down), and finally (c) at intermediate values of J_2 an incomplete devil's staircase, in which the modulation vector is constant over small ranges of J_2, which separates regions where the wave vector varies continuously with J_2.

For the Heisenberg model one obtains rather different behavior. Here, in the absence of anisotropy (or with easy plane anisotropy), the modulated phase is a helix of wave vector Q.[1,3] For this model Q is a continuous function of J_2. Basically, the difference between the Ising model and the Heisenberg model is that in the former the entropy depends on the phase of the order parameter modulation, whereas in the latter the spin magnitude (which determines the entropy) is constant over the modulation, and therefore the entropy is independent of the phase of the modulation. However, in the presence of a magnetic field h applied in the plane of the spins, it is clear that the magnitude of the spins does depend to some extent on the orientations, at least at nonzero temperature. If the modulation involves a variation in the magnitude of the order parameter, it is clear that the free energy can depend on the phase of the modulation, so that one gets phase locking as in the ANNNI model.

To study such effects we consider spin models with competing interactions:

$$H = - \sum_{i,j} J_{ij} \mathbf{S}(i) \cdot \mathbf{S}(j) - h \sum_i S_x(i). \qquad (1)$$

We treat spins on a simple tetragonal lattice with interactions within a basal plane given by $J_1 = 1$, J_2, and J_3, respectively between first, second, and third neighbors.[4] Spins i and j which are nearest neighbors in adjacent basal planes are subject to a ferromagnetic interaction J'. We shall treat two

models of the type of Eq. (1), the first a classical x-y model, and the second a quantum Heisenberg model, in which case we carry calculations as an expansion in $1/S$. We restrict ourselves to the limit of small but nonzero field h. The $T = 0$ phase diagram[4] for the classical model for $h = 0$ is shown in Fig. 1.

The phase diagram we find for the model of Eq. (1) for small $h \neq 0$ is similar to that of the Frenkel–Kontorova[5] (FK) model whose phase diagram (for the parameter analogous to h being small) is known to be in the form of an incomplete devil's staircase. The model we treat differs from the FK model in that we allow further-than-nearest-neighbor interactions, and also the competing interactions occur in a plane, rather than along a single direction. Also, because we do not impose any particular chirality, our model would have different critical properties from the chiral x-y model considered by Yokoi et al.,[6] although the ground-state properties are expected to be similar. We should note that in no case have quantum interactions or finite temperature effects been investigated for such a model. A unique result of our analysis is that for modulation with a wavelength equal to three lattice spacings, the commensurability energy vanishes at $T = 0$, i.e., the ground state energy in the classical model is independent of phase.
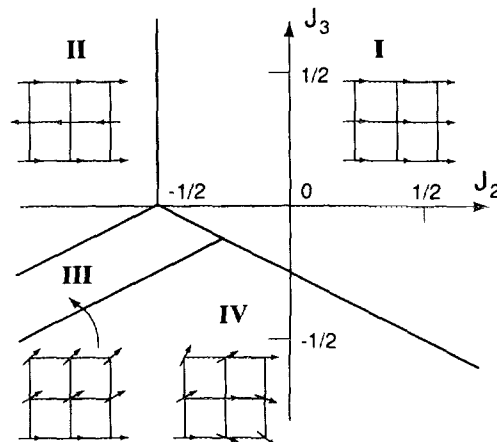

FIG. 1. Phase diagram (Ref. 4) of the classical model for Eq. (1) for $h = 0$. Within region III Q lies along a [1,0] direction and its magnitude is given by $\cos(aQ) = -(1 + 2J_2)/(4J_3)$, where a is the lattice constant.

II. SUMMARY OF CALCULATIONS

We now briefly describe the calculations. First, we discuss the classical x-y model, in which the orientation of the ith spin is specified by the angle χ_i such that $S_x(i) = \cos\chi_i$ and $S_y(i) = \sin\chi_i$. We calculate the free energy as a perturbation expansion for small h in the form

$$F(h) = F(0) + \tfrac{1}{2!}F_2 h^2 + \tfrac{1}{3!}F_3 h^3 + \cdots. \qquad (2)$$

We focus on F_3, which is given as

$$F_3 = \beta^2 \sum_{i,j,k} \langle X(i)X(j)X(k)\rangle_T \equiv \langle A\rangle_T, \qquad (3)$$

where $\beta = (kT)^{-1}$, $\langle\ \rangle_T$ indicates a thermal average at temperature T, and $h = 0$, and

$$X(i) = \cos(\mathbf{Q}\cdot\mathbf{r}_i + \phi + \theta_i). \qquad (3)$$

Thus, F_3 is evaluated in terms of averages taken with respect to the $h = 0$ undistorted helix whose ground state is given by $\chi_i = \mathbf{Q}\cdot\mathbf{r}_i + \phi$. Note that we have allowed for an arbitrary phase, ϕ, in the modulated spin ground state. The thermal average in Eq. (3) is over the phase space of angular fluctuations θ_i of all spins $i = 1,2,\cdots$ relative to their ground state orientations for which $\theta_i = 0$. In this notation the Hamiltonian at zero magnetic field takes the form

$$H = -\sum_{ij} J_{ij}\cos(\mathbf{Q}\cdot\mathbf{r}_{ij} + \theta_{ij}), \qquad (5)$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and $\theta_{ij} = \theta_i - \theta_j$. Since it is not possible to evaluate F_3 exactly, we have recourse to a spin-wave expansion. Thus, we expand both $X(i)$ and H in powers of θ_i, writing

$$H = H_0 + V, \qquad (6)$$

with

$$H_0 = E_0 + \tfrac{1}{2}\sum_{i,j} J_{ij}\theta_{ij}^2 \cos(\mathbf{Q}\cdot\mathbf{r}_{ij}), \qquad (7)$$

where E_0 is the ground state energy. The value of $\mathbf{Q}$ is determined so as to minimize H when $\theta_{ij} = 0$. Thus, $\mathbf{Q}$ is an implicit function of the J_{ij}'s.

We evaluate Eq. (3) using

$$\langle A\rangle_T = \langle Ae^{-\beta V}\rangle_0 / \langle e^{-\beta V}\rangle_0, \qquad (8)$$

where $\langle\ \rangle_0$ indicates a thermal average with respect to the noninteracting spin-wave Hamiltonian H_0. Note that $\langle\theta_i\theta_j\rangle_0 = kTG_{ij}$, where G_{ij} is the spin-wave Green's function whose spatial Fourier transform is given in terms of the Fourier transform of the exchange integrals as

$$G^{-1}(\mathbf{q}) = 2J(\mathbf{Q}) - J(\mathbf{Q} - \mathbf{q}) - J(\mathbf{Q} + \mathbf{q}). \qquad (9)$$

Thus, $\theta_i \sim \sqrt{T}$ and $\beta V \sim \sqrt{T}$. By expanding X_i in powers of θ_i and $\langle A\rangle_T$ as written in Eq. (8) in powers of βV, we obtain F_3 as an expansion in powers of T. Thereby we find results of the form

$$F_3 = NA_3(T)\sum_{G}\delta(3\mathbf{Q} - \mathbf{G})\cos(3\phi), \qquad (10)$$

where $\mathbf{G}$ is a reciprocal lattice vector and N is the total number of spins. A tedious calculation described elsewhere[7] gives

the result

$$A_3(T) = -\frac{9kT}{2}G(\mathbf{Q})^3\left(\frac{a}{2\pi}\right)^3\int d\mathbf{q}$$
$$\times\left(1 - 2\frac{G(\mathbf{Q}+\mathbf{q})}{G(\mathbf{q})}\right.$$
$$\left. + \frac{G(\mathbf{Q}+\mathbf{q})G(\mathbf{Q}-\mathbf{q})}{G(\mathbf{q})^2}\right) + O(T^2). \qquad (11)$$

The integral is carried over $-\pi < aq_\alpha < \pi$, where a is the lattice constant and α labels components x, y, or z. Note that $A_3(T)$ vanishes at $T = 0$, in agreement with the results of Elliott and Lange.[8] However, for finite temperature $A_3(T)$ is nonzero, as expected in analogy with results for the FK model.

From Eq. (10) we see that after minimization with respect to ϕ, one has a result whose general form is

$$F_p = -N|A_p(T)h^p|\sum_{G}\delta(p\mathbf{Q} - \mathbf{G}), \qquad (12)$$

which indicates the presence of a commensurability energy of order $|A_p(T)h^p|$. For $p = 3$ we have the explicit result given in Eq. (11). For higher values of p, i.e., $p = 5$ and $p = 7$ we have verified by numerical calculations that $A_p(T)$ is nonvanishing even at $T = 0$, in contrast to our result for $p = 3$. For such a calculation we set $J_2 = 0$ and fixed J_3 so that $p\mathbf{Q} = \mathbf{G}$. Then we verified that the dependence of the ground state energy on h, and ϕ could be represented as $E_0 + NA_p h^p\cos(p\phi)$. For modulation vectors near rational values, such a phase locking energy will give rise to regions of size $h^{p/2}$ around $\mathbf{Q} = \mathbf{G}/p$, where the modulation vector is constant. To see this we consider a region in $J_2 - J_3$ parameter space centered about the point where the modulation vector which minimizes E_0 assumes the value $\mathbf{Q}^*$. We assume that $\mathbf{Q}^*$ is close to $\mathbf{Q}_p \equiv \mathbf{G}/p$. For $\mathbf{Q}$ in this vicinity we have the free energy per spin $f(\mathbf{Q})$ as

$$f(\mathbf{Q}) = f(\mathbf{Q}^*) + \tfrac{1}{2}(\mathbf{Q} - \mathbf{Q}^*)^2 f''(\mathbf{Q}^*)$$
$$- |A_p(T)h^p|\delta(\mathbf{Q} - \mathbf{Q}_p). \qquad (13)$$

We see that due to the last term describing the commensuration energy, $f(\mathbf{Q})$ is minimized by $\mathbf{Q} = \mathbf{Q}_p$ over a range of J_2 and J_3 corresponding to

$$\Delta\mathbf{Q} = |2A_p(T)h^p f''(\mathbf{Q}^*)|^{1/2}. \qquad (14)$$

III. DISCUSSION

Note that for the model we consider, the modulation vector in zero field is restricted to a symmetry direction,[4] either along a [1,0] direction in region III or a [1,1] direction in region IV of Fig. 1, but has a magnitude which depends on the exchange parameters J_2 and J_3. Thus, well within regions III and IV we need only concern ourselves with $\mathbf{Q}$ values along the appropriate symmetry direction. Around each point in (J_2,J_3) space for which $\mathbf{Q} = \mathbf{G}/p$ (p is the smallest integer of this form), there is an ellipse whose area is of order h^p over which $\mathbf{Q}$ is constant. Between such ellipses $\mathbf{Q}$ is a continuously variable function of J_2 and J_3. Near the boundary between regions III and IV, the situation is more complicated. Exactly on this boundary the ground

state in zero field is infinitely degenerate: Q can assume any orientation but has an orientation-dependent magnitude.[9] Thus, for any point on the phase boundary in $J_2 - J_3$ space, the ground state has a modulation vector which can be anywhere on a curve defined by $|Q| = f(\theta_Q)$, where θ_Q defines the orientation of Q. One can see that now it is necessary to consider the effect of commensurability energies associated with points obeying $pQ = G$, which have any orientation, provided they are within a distance of order $h^{p/2}$ of the curve $|Q| = f(\theta_Q)$. Furthermore, it is not necessary to be exactly on the boundary III-IV for this effect to come into play. Thus, one sees that even for arbitrarily small h, the phase boundary becomes a sort of scalloped curve in which elliptical regions corresponding to Q's not along a symmetry direction are the steps in a generalized devil's staircase. Space does not permit us to discuss this in complete detail.

We make some observations concerning the quantum Heisenberg system having a modulated ground state. Our preliminary results indicate that $A_p(T=0)$ is nonzero for all p, even $p = 3$, where the classical model gives a vanishing commensurability energy at zero temperature. Furthermore, since quantum effects lift the infinite degeneracy of the III-IV phase boundary, the "scallop" effect mentioned above will become less relevant as S decreases. Including further-than-nearest-neighbor interactions[10] also removes the infinite degeneracy along the III-IV boundary and hence would similarly reduce the "scallop" effect.

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