Antiferromagnetic XY model on a triangular lattice: ordered states in a magnetic field

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The structure of ordered states of a two-dimensional planar antiferromagnet (with a triangular lattice) in a magnetic field is analyzed. Incorporating the free energy of spin waves lifts the continuous degeneracy. A phase diagram is constructed. It contains (in contrast with that in the absence of a magnetic field) four distinct ordered phases.

A planar antiferromagnet on a triangular lattice can be described in the exchange approximation by the Hamiltonian

$$H = J\sum_{(jj')} \mathbf{m}_j\mathbf{m}_{j'} - \mathbf{h}\sum_j \mathbf{m}_j = J\sum_{(jj')}\cos(\varphi_j - \varphi_{j'}) - h\sum_j \sin\varphi_j, \quad (1)$$

where the unit planar vectors $\mathbf{m}_j = (\cos\varphi_j, \sin\varphi_j)$ are specified at lattice sites, $\mathbf{h}$ is the magnetic field, and the summation in the first term is over pairs of nearest neighbors. For $h < h_{c2} \equiv 9J$, the ground state of (1) is a three-sublattice structure. For $h = 0$, the magnetic moments (spins) in the different sublattices are rotated 120° from each other. In addition to the continuous degeneracy resulting from the simultaneous rotation of all spins, this state has a discrete twofold degeneracy.

An interesting property of model (1) is that the continuous degeneracy of the ground state persists even at $0 < h < h_{c2}$. A minimum of (1) is reached under the conditions

$$\sum_{l=1}^{3} \cos\phi_l = 0\,; \qquad \sum_{l=1}^{3} \sin\phi_l = h/(3J) \quad (2)$$

which leave one free parameter (see Ref. 1, for example). Here the ϕ_l are the values of φ_j in each of the three sublattices. Analytic studies[2,3] of the phase diagram of model (1) have ignored the important circumstance that at a finite temperature this random degeneracy is lifted when the free energy of spin waves is taken into account.

The simplest calculation (in the harmonic approximation) shows that a minimum of the free energy of the spin waves corresponds to a maximum of the quantity

$$S(\phi_1, \phi_2, \phi_3) = \cos^2(\phi_1 - \phi_2) + \cos^2(\phi_2 - \phi_3) + \cos^2(\phi_3 - \phi_1) \quad (3)$$

[ϕ_1, ϕ_2, and ϕ_3 are assumed to satisfy (2)]. Incorporating this anisotropy leads to the appearance of a gap for a previously gapless mode and to a strict long-range order. We wish to emphasize that in continuously degenerate, two-dimensional systems an arbitrarily slight anisotropy is important if the temperature is low in comparison with the scale gradient energy.[4,5]

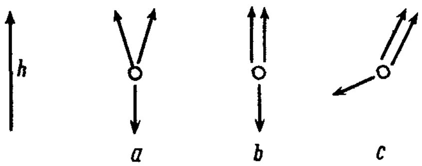

FIG. 1. Those spin directions in the three different sublattices which correspond to a minimum of the free energy of spin waves. a—$h < h_{c1}$; b—$h = h_{c1}$; c—$h_{c1} < h_{c2}$.

Just which states correspond to minima of the free energy? Figure 1 shows the spin directions in the three different sublattices which maximize S. For $h < h_{c1} \equiv 3J$, the three sublattices are all nonequivalent; the spins in one of them are antiparallel to the field, while those in the two others have components, differing in sign, perpendicular to the field (Fig. 1a). The degeneracy of this state is six, corresponding to interchanges of all the sublattices.

At $h = h_{c1}$, the spin directions in two of the sublattices become the same and become parallel to the field (Fig. 1b). The degeneracy drops to three. At $h_{c1} < h < h_{c2}$, an asymmetry arises in the direction perpendicular to the field (Fig. 1c), and this asymmetry raises the degeneracy back up to six. When anharmonicities are taken into account, the average magnetic moment in this state turns out to be not parallel to the field.

As the temperature is raised, these ordered states are disrupted. At a value of h only slightly above h_{c1}, an Ising phase transition should be the first to occur as the temperature is raised. This transition restores the symmetry between states which are mapped into each other by a mirror reflection of the spin positions. Above this transition the asymmetry disappears in the direction perpendicular to the field, and the degree of degeneracy drops to three. The temperature of this transition should vanish at the point $h = h_{c1}$, at which the difference between states due to a projection of the spins onto the axis perpendicular to the field disappears.

Analogously, if the field lies only slightly below h_{c1}, the first phase transition that should occur is an Ising transition. This transition restores the equivalence of the two

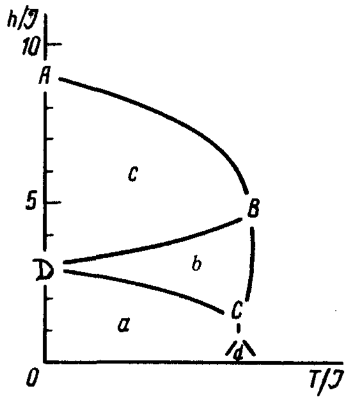

FIG. 2. Phase diagram of a planar antiferromagnet on a triangle lattice. Phases a and c—With sixfold degeneracy; b—with threefold degeneracy; d—with twofold degeneracy. Here N is a disordered (paramagnetic) phase.

sublattices in which the spins are nearly parallel to the field. The temperature of this transition also vanishes at the point $h = h_{c1}$.

Figure 2 shows the phase diagram which follows from the analysis of this letter and from the results of a numerical simulation.[1,6] In phases a, b, and c, the directions of the average spins in each of the sublattices are the same as in Figs. 1a, 1b, and 1c, respectively. The Ising transitions described above occur on lines BD and CD. Phase b is a commensurate $\sqrt{3}\times\sqrt{3}$ crystal of spins which are antiparallel to the field against the background of parallel spins. This structure melts on line BC.

At $h = 0$ a Berezinskiĭ-Kosterlitz-Thouless phase transition, associated with the continuous degeneracy, occurs at a temperature lower than that of the Ising transition, which is associated with the discrete degeneracy.[6] Incorporating the field-induced anisotropy indicates that the point of the Berezinskiĭ-Kosterlitz-Thouless transition should be the termination of the phase-transition line which separates the phases with sixfold and twofold degeneracy (cf. Ref. 5). In phase d (with a twofold degeneracy), the three sublattices are all equivalent (in terms of their average spin), but there is an "antiferromagnetic" ordering in terms of the alternation of the signs of the vorticities (circulations) calculated in the various unit cells of the lattice.

A triangular lattice is typical of an adsorbed monolayer forming a two-dimensional crystal. Experimental confirmation of the properties described here can be expected,[7] in particular, from dense monolayers of molecular oxygen adsorbed on graphite.

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