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Row generalization of the fully frustrated triangular XY model

Wei-min Zhang and W. M. Saslow
Center for Theoretical Physics, Department of Physics, Texas A&M University, College Station, Texas 77843-4242

M. Gabay
Laboratoire de Physique des Solides, Université de Paris–Sud, 91405 Orsay, France
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We have considered the phase diagram, in mean-field theory, of a generalization of the fully frustrated triangular lattice (FFTR) of XY spins. This may be relevant to otherwise isotropic spin systems subject to unidirectional strain along one of the lattice directions. There are two exchange constants, $-J$ and $-\eta J$, where the latter apply only to bonds in the horizontal direction; for $\eta=1$ this row model reduces to the usual FFTR model. We find two ordered phases at low temperatures. For $\eta<0.5$ the system goes into an antiferromagnetic state with ferromagnetic rows whose direction alternates as one moves vertically. For $\eta>0.5$, the system goes into a spiral state. The line $\eta=0.5$ marks a second-order phase transition.

I. INTRODUCTION

In analogy to the generalization by Berge *et al.*[1,2] of Villain's fully frustrated model of XY spins on a square lattice,[3] we have recently generalized the fully frustrated model of XY spins on a triangular lattice (FFTR).[4] Every third horizontal bond is given a bond strength of $-\eta J$ instead of $-J$, as in the pure AF case. Thus one-third of the sites have six $-J$ bonds, and two-thirds of the sites have one $-\eta J$ and five $-J$ bonds. This leads to a unit cell with three spins and the system is separated into three sublattices, A, B, and C.

In this paper we consider a generalization of the FFTR that does not change the size of the unit cell. Rather than change only one-third of the horizontal bonds, we change all of them, to the value $-\eta J$. See Fig. 1. This is the situation that would occur for a FFTR system subjected to uniaxial stress along the horizontal direction. For uniaxial stress along an arbitrary direction, one would have to include three, rather than two, values for the bonds along the three nearest-neighbor directions.

We will study this "modified row" version of the FFTR model in the framework of mean-field theory. So long as $\eta\neq1$, we expect this to give a reasonable representation of the physics. For $\eta=1$, due to the special symmetry of the problem, Monte Carlo calculations[5,6] in an external field H give an additional, collinear, phase that does not occur in mean-field theory.[7,8] We consider only the case $H=0$. The resultant phase diagram, given in Fig. 2, lies in the $\eta-T$ plane. We briefly summarize it.

At low temperatures, there are two ordered phases, according to the value of η. For $\eta>0.5$, the system goes into a spiral phase (Sp), which for $\eta=1$ (the usual FFTR model) is commensurate with the periodicity of the lattice. For $\eta<0.5$ the system goes into an antiferromagnetic state with ferromagnetic rows whose direction alternates as one moves vertically. At high temperatures, both ordered phases give way to the paramagnetic phase. The line $\eta=0.5$ separates the two ordered phases at all temperatures, and marks a second-order phase transition.

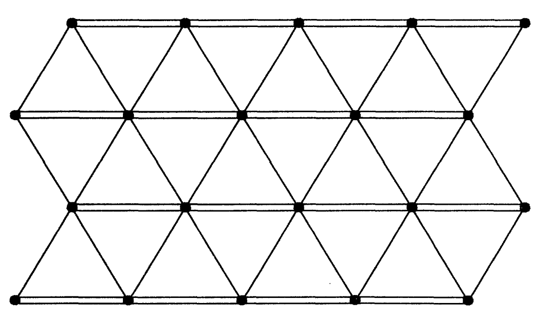

FIG. 1. Bond configuration for the row generalization of the fully frustrated triangular lattice. The single lines represent bonds of strength $-J$; the double lines (along the horizontal) represent bonds of strength $-\eta J$.

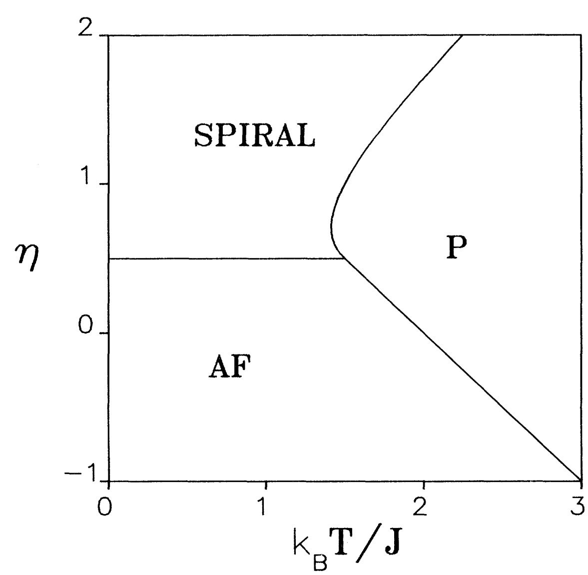

FIG. 2. Mean-field phase diagram in the $\eta-J$ plane.

We give the ground state solution in the next section and obtain the mean-field phase diagram in η-T space in Sec. III. Section IV provides a brief summary.

II. GROUND STATE

The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \ . \tag{2.1}$$

The brackets in the subscript indicate a sum over nearest neighbors only, with no double counting. The lattice constant is taken to be unity. We take spin i to have an orientation angle

$$\theta_i = \Delta_1(\hat{\mathbf{x}} \cdot \mathbf{r}_i) + \Delta_2(\hat{\mathbf{y}} \cdot \mathbf{r}_i) \ , \tag{2.2}$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ are the unit vectors in the x and y directions and Δ_1, Δ_2 are quantities to be determined by minimizing the energy. For simplicity we write Δ_y for $(\sqrt{3/2})\Delta_2$.

It is sufficient to look at the energy per spin, given by

$$\varepsilon = 2\eta J \cos(\Delta_1) + 4J \cos(\Delta_1/2)\cos(\Delta_y) \ . \tag{2.3}$$

Minimizing this with respect to Δ_1 and Δ_y gives the conditions

$$0 = \sin(\Delta_1/2)[2\eta \cos(\Delta_1/2) + \cos(\Delta_y)] \ , \tag{2.4}$$

$$0 = \cos(\Delta_1/2)\sin(\Delta_y) \ . \tag{2.5}$$

There are three solutions to these equations: a spiral solution (SP), a solution with ferromagnetic rows that are aligned antiferromagnetically relative to one another (AF), and one with antiferromagnetic rows that are totally decoupled from one another. This last solution is never favored.

The spiral solution is determined by the conditions

$$\begin{aligned} &\sin(\Delta_y) = 0 \ , \\ &2\eta \cos(\Delta_1/2) + \cos(\Delta_y) = 0 \ . \end{aligned} \tag{2.6}$$

This leads to the conditions

$$\cos(\Delta_y) \equiv s = \pm 1, \quad 2\eta \cos(\Delta_1/2) = -s \ , \tag{2.7}$$

which can only be satisfied for $|\eta| > 0.5$ The energy per spin for this state is (for s taking either sign)

$$\varepsilon_{\mathrm{Sp}} = -2J \left[\eta + \frac{1}{2\eta} \right] \ . \tag{2.8}$$

In Fig. 3 we plot Δ_1 versus η. In Fig. 4 we display the spin configuration for $\eta = 2$. For later comparison note that for $s = 1$ (so that $\Delta_y = 0$), if $\eta \to \frac{1}{2}$ then $\Delta_1/2 \to \pi$. As a consequence, $\Delta_1/2 + \Delta_y \to \pi$, so that each row is ferromagnetically aligned ($\Delta_1 + 2\pi \equiv 0$), and the rows align with alternating directions as one moves vertically ($\Delta_1/2 + \Delta_y \to \pi$). The same conclusion holds for $s = -1$.

The AF state is determined by the conditions

$$\sin(\Delta_1/2) = 0, \quad \sin(\Delta_y) = 0 \ . \tag{2.9}$$

This leads to the conditions

$$\cos(\Delta_1/2) \equiv r = \pm 1, \quad \cos(\Delta_y) \equiv s = \pm 1 \ . \tag{2.10}$$

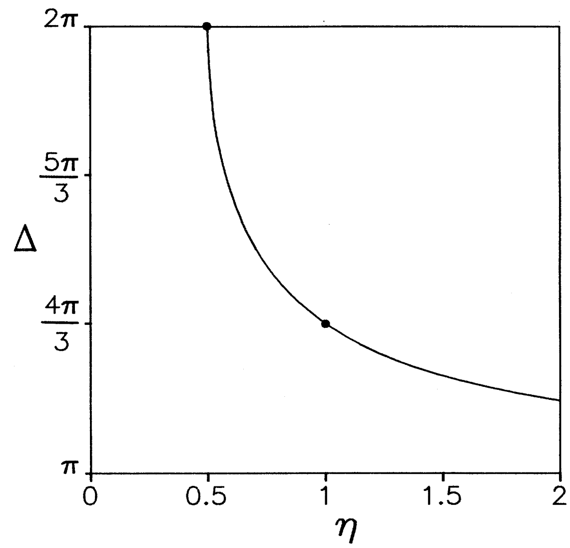

FIG. 3. Mean-field calculation of Δ_1 vs η. The dot at $\eta = 1$ represents the fully frustrated triangular lattice solution, and the dot at $\eta = 0.5$ represents the limit where the spiral state goes into the AF state.

The energy per spin for this solution is

$$\varepsilon = 2J(\eta + 2rs) \ . \tag{2.11}$$

This is minimized for $rs = -1$. Both $r = 1$, $s = -1$ and $r = -1$, $s = 1$ lead to an antiferromagnetic state with ferromagnetic rows that alternate direction as one moves vertically. The energy per spin for the AF state is

$$\varepsilon_{\mathrm{AF}} = 2J(\eta - 2) \ . \tag{2.12}$$

The third solution of Eqs. (2.4) and (2.5) is given by

$$\cos(\Delta_1/2) = 0, \quad \cos(\Delta_y) = 0 \ . \tag{2.13}$$

This corresponds to antiferromagnetic rows. Because the mean field due to interrow coupling is zero, the rows are completely decoupled from one another. The energy per spin for this state is

$$\varepsilon_{\mathrm{AF\ rows}} = -2J\eta \ . \tag{2.14}$$

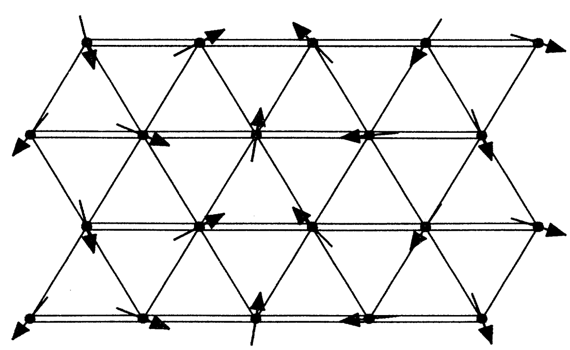

FIG. 4. Spiral spin configuration for $\eta = 2$. Note that in the spiral phase the vertical repeat distance is two units, so that the system remains commensurate in the vertical direction.

Comparison of the energies of these three states shows that the spiral state is lowest in energy for $\eta > 0.5$, whereas the AF state is lowest in energy for $\eta < 0.5$. Because, by the discussion following (2.8), the Sp phase approaches the AF phase as $\eta \rightarrow 0.5$, the transition at $\eta = 0.5$ is continuous, so the AF-Sp line is second order.

III. MEAN-FIELD EQUATION FOR FINITE TEMPERATURE

Because there is only one spin per unit cell, the analysis hardly changes at finite temperatures. Assuming that the solutions at $T=0$ are modified only by a factor representing the effect of thermal fluctuations, the energies of the spiral and AF states can then be obtained by setting the magnetization equal to

$$R(\beta H_i), \quad R(u) = I_1(u)/I_0(u) , \tag{3.1}$$

where $\beta = (k_B T)^{-1}$, H_i is the local field, and $I_n(u)$ is the modified Bessel function of order n. We henceforth set the Boltzmann constant k_B to unity.

In the case of the spiral phase, from the energy at $T=0$, Eq. (2.8), it is straightforward to obtain the local field

$$H_i = 2J\left[\eta + \frac{1}{2\eta}\right] R(\beta H_i) . \tag{3.2}$$

This has a solution so long as $T < T_{\mathrm{Sp}}$, where T_{Sp} is determined by solving for T in (3.2) in the small magnetization limit, where $R(u) \approx 0.5u$. Thus, one obtains

$$T_{\mathrm{Sp}}/J = \eta + \frac{1}{2\eta} \quad (\eta > 0.5) . \tag{3.3}$$

Note that, in mean-field theory, the phase is independent of temperature, so that Fig. 3 applies at all temperatures for which the spiral phase occurs.

For the AF phase, from the energy at $T=0$ Eq. (2.11), it is straightforward to obtain the local field

$$H_i = 2J(2-\eta) R(\beta H_i) . \tag{3.4}$$

This has a solution so long as $T < T_{\mathrm{AF}}$, where T_{AF} is determined by solving for T in (3.4) in the small magnetization limit, where $R(u) \approx 0.5u$. Thus, one obtains

$$T_{\mathrm{AF}}/J = 2-\eta \quad (\eta < 0.5) . \tag{3.5}$$

The phase diagram in Fig. 2 is constructed on the basis of Eqs. (3.3) and (3.5).

IV. SUMMARY

From the mean-field equations, we have found two ordered phases, a spiral phase, and an AF phase. The transition between Sp and AF is second order, and the transitions to the P state are second order. This model may be relevant to FFTR systems that are subject to strain along the horizontal direction. For small strains, the system would go from a commensurate spiral to an incommensurate spiral. (Note, however, that the system would remain commensurate along the vertical direction.) Only for extraordinarily large strains (enough to weaken the horizontal bonds by more than a factor of 2) would one expect to see the AF phase.

Note added in proof. We have recently learned of work by H. Kawamura (Prog. Theor. Phys. Suppl. to be publishe), which discusses a three-dimensional version of the model considered here.

ACKNOWLEDGMENTS

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[1]B. Berge, H. T. Diep, A. Ghazali, and P. Lallemand, Phys. Rev. B **34**, 3177 (1986).

[2]M. Gabay, T. Garel, G. Parker, and W. M. Saslow, Phys. Rev. B **40**, 264 (1989).

[3]J. Villain, J. Phys. C **10**, 1717 (1977).

[4]G. Parker, W. M. Saslow, and M. Gabay, Phys. Rev. B **43**, 11 285 (1991).

[5]D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. Lett. **52**, 433 (1984).

[6]D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. B **33**, 450 (1986).

[7]S. Miyashita and H. Shiba, J. Phys. Soc. Jpn. **53**, 1145 (1984). This work, employing a 36-state clock model in zero field, found an Ising temperature slightly larger than an XY temperature, a result that may be explained if the statistical uncertainty were larger than originally estimated.

[8]The nature of this Potts-like phase, with spontaneous discrete symmetry breaking of one sublattice relative to the other two, has been discussed by H. Kawamura, J. Phys. Soc. Jpn. **53**, 2452 (1984), on the basis of thermal fluctuations about the highly degenerate mean-field solution [see D. H. Lee, R. G. Caflisch, J. D. Joannopoulos, and F. Y. Wu, Phys. Rev. B **29**, 2680 (1984)]. One can consider this Potts-like phase for the FFTR with XY spins to be the remnant of the Potts-like phase found for the FFTR with Ising spins by B. D. Metcalf, Phys. Lett. **45A**, 1 (1973). Note that a modified Monte Carlo procedure, invoking mean-field theory as part of the statistical decision process, has successfully reproduced the phase diagram found by Metcalf [R. R. Netz and A. N. Berker, Phys. Rev. Lett. **66**, 377 (1991)].