

# Phases of a 2D planar antiferromagnet in a uniform field

D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau  
*T. J. Watson IBM Research Center, Yorktown Heights, NY; Department of Physics, Massachusetts Institute of Technology, Cambridge; Department of Physics, University of Georgia, Athens*

(Submitted 15 November 1985)

Pis'ma Zh. Eksp. Teor. Fiz. **43**, No. 1, 51–54 (10 January 1986)

The behavior of a planar antiferromagnet (the  $XY$  model) is reanalyzed on square and triangular 2D lattices in a uniform magnetic field. The phase diagrams recently proposed by Dotsenko and Uimin are then discussed.

Two recent papers<sup>1,2</sup> give mutually contradictory results for the phase diagrams of a planar antiferromagnet (the  $XY$  model) on triangular and square 2D lattices in the presence of a uniform magnetic field  $H$ . The Hamiltonian of the system is given by

$$\beta\mathcal{H} = \frac{1}{T} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos \theta_i, \quad (1)$$

where  $h \equiv H/T$ , and  $T$  is the temperature.

Dotsenko and Uimin<sup>1</sup> proposed the phase diagram shown in Fig. 1a for a square lattice. This diagram evidently includes a (Berezinskii-) Kosterlitz-Thouless (KT) phase-transition boundary, which extends from the critical point in a zero field, and the boundary for an Ising transition, (1), which goes to the origin ( $T = 0$ ) in the limit  $H \rightarrow 0$ . In contrast, the phase diagram in Fig. 1b, which we proposed in Ref. 2, includes only an Ising transition boundary, which is connected to the transition point in a zero field. This result means that in an infinitesimal field  $H$  a long-range order is observed in the system below the critical temperature in a zero field. A difference also arises in the phase diagram for a triangular lattice in a weak magnetic field. Dotsenko and Uimin's phase diagram in Fig. 2a clearly separates the unbinding of the vortices and the Ising transition in a zero field. This result is in accordance with Miyashita and Shiba's suggestion.<sup>3</sup> In contrast, the phase diagram in Fig. 2b, from Ref. 2, determines a single multicritical point for a zero field; this point is associated with an unbinding of vortices which is caused by domain walls. This point cuts off two clearly defined boundaries corresponding to a nonzero field. In the present letter we provide further arguments in favor of the phase structure in Figs. 1b and 2b in view of Dotsenko and Uimin's studies.

We begin with a square lattice. In this case the model of an antiferromagnet in a uniform field is projected onto the equivalent model of a ferromagnet with a stepped field. We thus write

$$\beta\mathcal{H} = - \frac{1}{T} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - h \sum_i \xi_i \cos \theta_i, \quad (2)$$

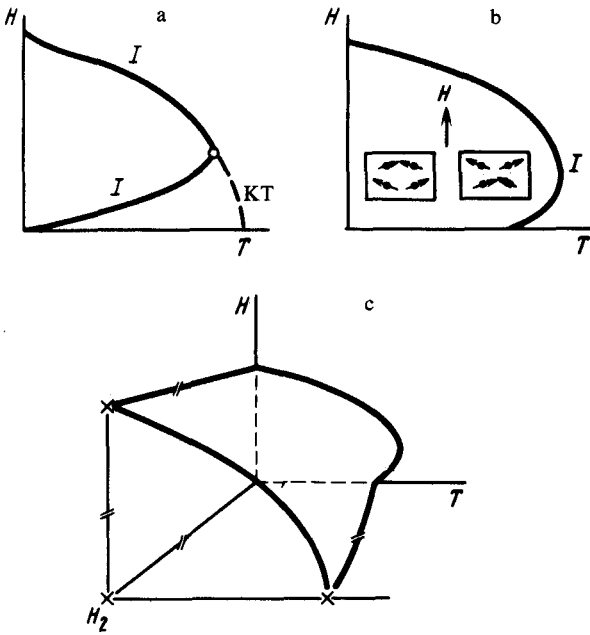


FIG. 1. Schematic phase diagrams for a planar antiferromagnet ( $XY$  model) on a square lattice. a—Diagram proposed in Ref. 1; b—diagram proposed in Ref. 2; c—global structure in the presence of both a uniform magnetic field and a uniaxial anisotropy. Shown in part b are the two realizations of the degenerate ground state for a weak field in the ordered region of the diagram. The labels on the boundaries specify an Ising transition (I) or a Kosterlitz-Thouless transition (KT).

where we have  $\xi_i = 1$  on sublattice I and  $\xi_i = -1$  on sublattice II.

As Knops<sup>4</sup> and Cardy<sup>5</sup> have shown, the stepped field is an unimportant variable in this case. However, it does generate a uniaxial anisotropy field  $h_2$  upon renormalization.

Specifically, we take the continuum limit of Eq. (2), determine the fields  $\theta_I$  and  $\theta_{II}$  on the two sublattices, and get rid of the integration of the field  $\theta_I - \theta_{II}$ . We then find that for a sufficiently small field  $h$  the renormalized Hamiltonian, which depends

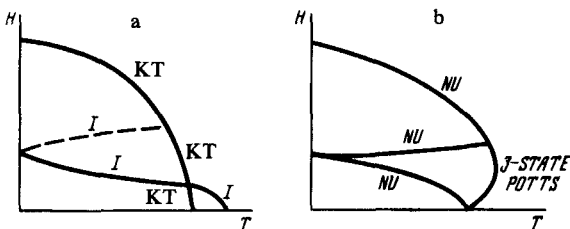


FIG. 2. Schematic phase diagrams for a planar antiferromagnet ( $XY$  model) on a triangular lattice. a—Proposed in Ref. 1; b—proposed in Ref. 2. The labels on the boundaries specify a nonuniversal transition (NU) or a three-state Potts transition.

on the variable  $\theta = \theta_I + \theta_{II}$ , corresponds to the continuum limit to the Hamiltonian

$$\beta \mathcal{H} = - \frac{1}{T_{eff}} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - h_2 \sum_i \cos 2\theta_i + O(h^4) \dots, \quad (3)$$

where

$$\begin{aligned} T_{eff} &= T - AT^2 h^2, \\ h_2 &= -BTh^2, \end{aligned} \quad (4)$$

$A$  and  $B$  are positive, and  $h_2 = H_2/T_{eff}$ .

Equation (3) describes a planar ferromagnet (the  $XY$  model) with a uniaxial anisotropy field. Since we have  $h_2 < 0$ , there are two realizations of the ground state with magnetization perpendicular to the applied field  $H$ . The renormalization-group equations for  $T_{eff}$  and  $h_2$ , derived by Jose *et al.*<sup>6</sup> and Elitsur *et al.*,<sup>7</sup> are

$$\begin{aligned} \frac{dT_{eff}}{d \ln a} &= -cT_{eff}^2 h_2^2, \\ \frac{dh_2}{d \ln a} &= (2 - T_{eff}/\pi)h_2, \end{aligned} \quad (5)$$

where  $c > 0$ , and  $a$  is the lattice constant, which changes upon the renormalization. At  $T_{eff} \leq T_{KT} = \pi/2$ , the field  $h_2$  is an *important* variable, so that at  $h_2 = 0$  the ordinary KT phase is replaced by a phase with a *long-range order* at a nonzero  $h$ . Working from inequalities for correlation functions, Elitsur *et al.*<sup>7</sup> showed rigorously that only two phases are possible for Hamiltonian (3): a phase with a long-range order and a paramagnetic phase, separated by an Ising transition.

Since the temperature  $T$  was brought to  $T_{eff}$  after the stepped field was removed by the renormalization (the situation is equivalent to the suppression of fluctuations by the stepped field), we conclude that the system has a long-range order at  $T < T_{KT}$ . This conclusion contradicts the phase diagram in Fig. 1a.

The analysis above leads to the global phase diagram in Fig. 1c. At nonzero  $H_2$ , there exists a surface of Ising transitions, which reduces to a fixed point ( $T = T_I$ ,  $H = 0$ ,  $H_2 = \infty$ ) upon renormalization. The structure of this phase diagram is also supported by Monte Carlo calculations.

As can be seen in Fig. 1b, the phase structure for a weak field, originally found through a renormalization-group calculation and later confirmed by Monte Carlo calculations,<sup>8</sup> can be understood physically on the basis of the following simple arguments. In a weak field, the domain wall between the domains with the two possible realizations of the ground state, shown in Fig. 1b, has an energy per unit length  $\epsilon \propto H$  and a thickness  $l \propto 1/H$ . To determine the critical temperature  $T_I$  by equating the energy of the domain wall to the entropy, it is necessary to calculate the entropy of a thick domain wall. Denoting by  $N_L \propto \lambda^L$  the number of configurations for a domain wall of zero width and length  $l$ , we find that the number of configurations of a wall of thickness  $l$  is about  $\lambda^{L/l}$ . This result rules out all configurations for a wall of zero

width with structure with a scale dimension less than  $l$ , and it leads to an entropy which falls off in the appropriate way with increasing  $l$ . The dependence of  $\epsilon$  on  $H$  and that of  $l$  on  $H$  thus cancel out, giving us a nonzero critical temperature in the limit of a zero field:

$$T_I = \frac{L\epsilon}{\ln NL} = \frac{\epsilon}{(1/l)\ln\lambda} \frac{1}{H \rightarrow 0} \frac{1}{\ln\lambda}. \quad (6)$$

In contrast, the suggestion in Ref. 1 that the entropy of the wall is proportional to  $L \ln l$  leads to a nonphysical behavior in that the entropy does not fall off with  $l$ , and it ultimately leads to the result

$$T_I = (\epsilon/\ln l) \xrightarrow{H \rightarrow 0} 0,$$

as shown in Fig. 1a.

We conclude with a brief discussion of the difference between the triangular-lattice phase diagrams shown in Fig. 2. Dotsenko and Uimin<sup>1</sup> predicted two clearly defined transitions in a zero field, while we<sup>2</sup> predicted only a single transition. Recent calculations by the renormalization-group method<sup>9</sup> show that there is only a single transition at  $H = 0$ , as shown in Fig. 2b. Although Yosefin and Domany's analysis<sup>9</sup> does not tell us whether this is a first-order or continuous transition, the existence of a single continuous transition was demonstrated in Ref. 2 by Monte Carlo calculations and a scaling analysis for finite systems. In particular, it was found that the temperature at which the vortices are unbound,  $T_{KT} = 0.505 \pm 0.005$ , and the melting point of the domain walls,  $T_I = 0.510 \pm 0.005$ , are the same, within the statistical error. This result can be explained quite easily on the basis of the physical mechanism for an unbinding of vortices caused by domain walls.

The phase boundaries in a nonzero field have been studied thoroughly through a combination of a symmetry analysis and a scaling calculation by a Monte Carlo method for finite systems; the results contradict those in Fig. 2a. A transition to the universality class of a three-state Potts model has been predicted on the basis of a symmetry analysis and verified through the demonstration that the scaling curves are described exceptionally well by the critical exponents  $\beta = 1/9$ ,  $\gamma = 13/9$ ,  $\nu = 5/6$ , and  $\alpha = 1/3$ . Furthermore, measurements of  $\beta$  at the two interior phase boundaries yield a nonuniversal behavior, so that  $\beta$  varies at least from 0.14 to 0.21. This result is in obvious contradiction of the prediction of the Ising model,  $\beta = 1/8$ .

In summary, a large body of theoretical work, including an analysis by the renormalization-group method, Monte Carlo calculations, symmetry analysis, and qualitative arguments regarding the behavior of domain walls, provides convincing evidence in favor of the phase structure in Figs. 1b and 2b.

<sup>1</sup>Vik. S. Dotsenko and G. V. Uimin, *Pis'ma Zh. Eksp. Teor. Fiz.* **40**, 236 (1984) [*JETP Lett.* **40**, 1009 (1984)]; Landau Institute preprint, 1984-18.

<sup>2</sup>D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, *Phys. Rev. Lett.* **52**, 433 (1984); *Phys. Rev. B* (in press).

<sup>3</sup>S. Miyashita and H. Shiba, *J. Phys. Soc. Jpn.* **53**, 1145 (1984).

<sup>4</sup>H. Knops, *Ann. Phys.* **128**, 5128 (1980).

<sup>5</sup>J. L. Cardy, *Phys. Rev. B* **24**, 5128 (1981).

<sup>6</sup>V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, *Phys. Rev. B* **16**, 1217 (1977).

<sup>7</sup>S. Elitsur, R. Pearson, and J. Shigemitsu, *Phys. Rev. D* **19**, 3698 (1979).

<sup>8</sup>D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, MIT preprint, 1984.

<sup>9</sup>M. Yosefin and E. Domany, *Phys. Rev. B* **32**, 1778 (1985).

Translated by Dave Parsons