LETTER TO THE EDITOR

Frustrated XY model with unequal ferromagnetic and antiferromagnetic bonds

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Abstract. We show that the recent numerical results in this model can be understood in terms of the global phase diagram for coupled XY models.

We consider classical XY spins $S = (\cos \theta, \sin \theta)$ interacting via the following Hamiltonian:

$$H = \sum_{\langle rr'\rangle} J_{rr'} \cos(\theta_r - \theta_{r'}) \tag{1}$$

where the sum is restricted to nearest-neighbour sites of a square lattice. Here $J_{rr'}=-J$ (J>0) on horizontal bonds, $J_{rr'}=-J$ and $J_{rr'}=J\eta$ on alternating columns of the square lattice.

If $\eta=1$ this is the fully frustrated XY model studied by Villain (1975) in the context of the spin glass problem. It can also be realised physically by a Josephson junction array in a transverse magnetic field with half a flux quantum per plaquette which has motivated recent interest in this model (Teitel and Jayaprakash 1983). This model has been studied both analytically (Halsey 1985, Granato and Kosterlitz 1985, Choi and Doniach 1985, Yosefin and Domany 1985) as well as numerically (Teitel and Jayaprakash 1983, Berge et al 1985). The ground state possesses a discrete symmetry Z_2 in addition to the underlying symmetry U(1). Although the result of these papers is not conclusive, there are indications from numerical simulations that a single transition occurs with simultaneous Ising and XY-like behaviour. However, one cannot exclude the possibility of a first-order transition especially in view of the analysis in $4 - \varepsilon$ dimensions (Mukamel 1975).

For $\eta \neq 1$ and >0 each plaquette is still equally frustrated and the ground state is doubly degenerate but the numerical work of Berge *et al* (1985) reveals a double transition with an Ising followed by an XY-like transition as the temperature is increased (figure 1). The Ising transition temperature vanishes at the critical value $\eta_c = \frac{1}{3}$.

In this Letter we show that the numerical results for $\eta \neq 1$ can be understood in terms of the phase diagram of coupled XY models which have been studied before.

To proceed with the analysis we obtain a Landau-Ginzburg-Wilson free energy by considering continuous spins and introducing a weighting factor

$$\prod_{r} \exp(-\frac{1}{2}a|S_r|^2 - u|S_r|^4)$$

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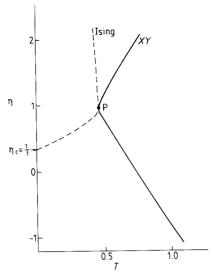


Figure 1. Phase diagram for the frustrated XY model (Berge et al 1985). The nature of the phase transition at P is not determined.

in the partition function. Equation (1) is then rewritten into a Fourier transform and expanded about the modes corresponding to the lowest eigenvalues of the Fourier-transformed coupling matrix J(q, q'). The resulting free energy in the coordinate space is given by

$$F(\psi_{1}, \psi_{2}) = \iint dx \, dy \left(\frac{1}{2} r_{1} |\psi_{1}|^{2} + \frac{1}{2} r_{2} |\psi_{2}|^{2} + \frac{1}{2} e_{1} \left| \frac{\partial}{\partial x} \psi_{1} \right|^{2} + \frac{1}{2} f_{1} \left| \frac{\partial}{\partial y} \psi_{1} \right|^{2} + \frac{1}{2} f_{2} \left| \frac{\partial}{\partial x} \psi_{2} \right|^{2} + \frac{1}{2} f_{2} \left| \frac{\partial}{\partial y} \psi_{2} \right|^{2} + \frac{1}{4} u' (|\psi_{1}|^{2} + |\psi_{2}|)^{2} + v |\psi_{1}|^{2} |\psi_{2}|^{2} + u'' |\psi_{1}|^{2} |\psi_{2}|^{2} \cos 2(\theta_{1} - \theta_{2}) \right)$$

$$(2)$$

where

$$r_{1} = \frac{\lambda(Q_{1})}{kT} + a: \qquad r_{2} = \frac{\lambda(Q_{2})}{kT} + a$$

$$e_{1,2} = \frac{1}{2kT} \frac{\partial^{2}}{\partial q_{x}^{2}} \lambda(q) \Big|_{Q_{1,2}} \qquad f_{1,2} = \frac{1}{2kT} \frac{\partial^{2}}{\partial q_{y}^{2}} \lambda(q) \Big|_{Q_{1,2}}$$

$$\lambda(q) = -J\{(1 - \eta)\cos q_{y} + 2[\cos^{2} q_{x} + \frac{1}{4}(1 + \eta)^{2}\cos^{2} q_{y}]^{1/2}\}$$

and v < 0; u', u'' > 0.

 $\psi_1 = |\psi_1| \exp(\mathrm{i}\theta_1)$ and $\psi_2 = |\psi_2| \exp(\mathrm{i}\theta_2)$ measures fluctuations about the modes $Q_1 = (0,0)$ and $Q_2 = (0,\pi)$ corresponding to the two minimum eigenvalues $\lambda(Q_1)$ and $\lambda(Q_2)$. The mode $(0,\pi)$ ceases to be a minimum at $\eta_c \sim 0.3$ and (2) reduces to the free energy of a single complex field with an expected XY transition. The exact result $\eta_c = \frac{1}{3}$ found in the ground-state analysis of Berge *et al* (1985) is not obtained here because these modes do not satisfy the constraint $|S|^2 = 1$. This constraint, however, is believed to be irrelevant to the critical behaviour.

In two dimensions we assume the phase transition occurs well below the mean-field critical temperature. Amplitude fluctuations in ψ_1 and ψ_2 are irrelevant so $|\psi_1|^2$ and $|\psi_2|^2$ are well approximated by their mean-field values. A straightforward minimisation shows that for the action of equation (2) the corresponding values are

$$|\psi_{1,2}|^2 = -\frac{r_1 + r_2}{4(u' + v - u'')} \pm \frac{r_1 - r_2}{4(v - u'')}.$$
 (3)

Considering only phase fluctuations we then generalise (2) to a lattice Hamiltonian of the form:

$$H/kT = -\sum_{\langle rr'\rangle} A_{rr'} \cos(\theta_r - \theta_{r'}) - \sum_{\langle rr'\rangle} B_{rr'} \cos(\varphi_r - \varphi_{r'}) - h \sum_r \cos 2(\theta_r - \varphi_r)$$

with
$$A_{rr+\hat{x}} = |\psi_1|^2 e_1$$
, $A_{rr+\hat{y}} = |\psi_1|^2 f_1$, $B_{rr+\hat{x}} = |\psi_2|^2 e_2$ and $B_{rr+\hat{y}} = |\psi_2|^2 f_2$.

In general the couplings in (4) are all different and this Hamiltonian describes coupled anisotropic XY models. They depend, in a rather complicated way, on η but their exact form is of no interest here. In the isotropic case when $A_{rr'} = \alpha$ and $B_{rr'} = \beta$, this model has been analysed in some detail in the plane $\alpha \times \beta$ (Granato and Kosterlitz 1985). The analysis is based on an electrodynamic representation for the partition function given by

$$Z = \left(\prod_{r} \sum_{S(r)}^{\prime}\right) \left(\prod_{R} \sum_{M(R)}^{\prime} \sum_{N(R)}^{\prime}\right) \exp[A(M, N, S)]$$
 (5)

where

$$A(M, N, S) = \pi \alpha \sum_{R,R'} M(R)G(R - R')M(R') + \pi \beta \sum_{R,R'} N(R)G(R - R')N(R')$$

$$+ 2\pi g \sum_{R,R'} M(R)G(R - R')N(R') + 2i \sum_{r} \sum_{R} S(r)\theta(r - R)$$

$$\times (M(R) - N(R)) + \frac{(\alpha + \beta + 2g)}{\pi(\alpha\beta - g^2)} \sum_{r,r'} S(r)G(r - r')S(r').$$
(6)

The primes on the summations of the three integer fields indicate they are subject to the neutrality condition

$$\sum_{R} M(R) = \sum_{R} N(R) = \sum_{r} S(r) = 0.$$

The large-distance behaviour of G(R, R) and $\theta(r)$ is given by

$$G(R - R') = \ln(|R - R'|/a)$$

and $\theta(r) = \tan y/x$. The renormalisation-group analysis leads to the schematic phase diagram shown in figure 2. In the case of anisotropic coupled XY models an electrodynamic representation with effective couplings

$$\alpha_{\text{eff}} = \frac{1}{2}(A_{rr+\hat{x}} + A_{rr+\hat{y}})$$
 and $\beta_{\text{eff}} = \frac{1}{2}(B_{rr+\hat{x}} + B_{rr+\hat{y}})$

is obtained if the anisotropy is sufficiently small. For $\eta=1$ we have isotropic couplings $A_{rr'}=B_{rr'}$ and the fully frustrated XY model has the line of initial points $\alpha=\beta$ shown in figure 2. Thus in this case the phase transition has the peculiar Ising- and XY-like character. For $\eta\simeq 1$ we obtain $\alpha_{\rm eff}-\beta_{\rm eff}\propto 1-\eta$ and a double transition is expected with an Ising transition followed by an XY transition as the temperature is increased.

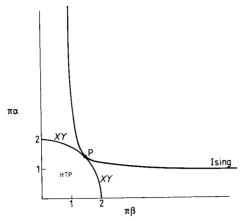


Figure 2. Phase diagram for coupled XY models. The manner in which lines merge at P and the nature of the phase transition at this point has not been conclusively determined. The high-temperature phase is denoted by HTP.

Thus we expect that close to $\eta=1$, the fully frustrated XY model can be represented as coupled XY models with $\alpha \neq \beta$. $A_{rr'}$ and $B_{rr'}$ vary slowly with η for $\eta>1$ in contrast with the region $\eta<1$ and this gives rise to the asymmetry between these two regions in the phase diagram shown in figure 1. One can see that the $\alpha=\beta$ line in the phase diagram given in figure 2 plays the same role as $\eta=1$ in the model (1), for in this case it is known that this model possess a 'gauge' symmetry in addition to the continuous and discrete symmetries mentioned before (Halsey 1985, Yosefin and Domany 1985).

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