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LETTER TO THE EDITOR

Monte Carlo simulation of the fully frustrated XY model

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Abstract. We present results from Monte Carlo simulation of the fully frustrated XY model, or alternatively a Josephson junction array in an external field. Positional disorder of the junctions is allowed for and we find that this disorder splits the XY and Ising phase transitions of the model, as predicted by Granato and Kosterlitz.

The phase transition in the fully frustrated XY model is far from being fully understood. Unlike the simple XY model, where an explicit operator equivalence exists between the model and the quantum field theory it renormalizes onto, at its critical point (Amit *et al* 1980), the location in the space of $O(2)\times Z_2$-invariant quantum field theories which describes the combined XY and Ising transitions of the fully frustrated XY model is not known. In this letter we present results from our Monte Carlo simulation of the fully frustrated XY model and speculate as to the nature of the effective critical theory.

The Hamiltonian (neglecting kinetic terms) of the frustrated XY model is

$$H=-J\sum_{(i,j)}\cos(\theta_i-\theta_j-A_{ij}). \tag{1}$$

Here we follow the conventions of Granato and Kosterlitz (1989), to whom the reader is referred for a fuller discussion. This Hamiltonian describes an array of Josephson junctions, or alternatively a grainy superconductor, under the identification of θ_i with the phase of the grain i. The link integrals A_{ij} arise from the application of an external field, $A_{ij}=(2\pi/\phi_0)\int_i^j \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{l}$, where the flux quantum $\phi_0=hc/2e$. We consider the sites i to have the topology of a square lattice, though they may be randomly displaced from the perfect lattice with a Gaussian probability distribution of width Δ. We restrict ourselves to the fully frustrated case, where the average number of flux quanta per unit area is $\frac{1}{2}$.

Our Monte Carlo procedure follows recent studies of the pure XY model (Gupta *et al* 1988, Wolff 1989). We use a large lattice, 128^2 sites, and study the correlation length and susceptibility in the high-temperature phase, then fit to appropriate scaling forms to withdraw critical exponents. A more detailed exposition of this method and its possible pitfalls may be found in the review by Baillie (1990). The specific algorithm we have used is hybrid Monte Carlo (Duane *et al* 1987), which consists of including kinetic terms in the Hamiltonian (1), then generating trial configurations by integrating Hamilton's equations for a number of timesteps, followed by a global accept–reject.

Previous simulations of this model include those of Teitel and Jayaprakash (1983a, b), Choi *et al* (1987), Thijssen and Knops (1988) and Scheinine (1989). We

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define our order parameters following the paper by Scheinine. Specifically, the XY susceptibility is defined as a sum over sublattices as in equations (3.6a, b) of Scheinine

$$\chi^{XY} = (1/4) \sum_{j=1}^{4} \chi^{(j)}$$

$$\chi^{(j)} = (\beta/2N)\left[\left\langle\left(\sum_{i=1}^{N/4} \cos\theta_i^{(j)}\right)^2 + \left(\sum_{i=1}^{N/4} \sin\theta_i^{(j)}\right)^2\right\rangle - \left(\left\langle\sum_{i=1}^{N/4} \cos\theta_i^{(j)}\right\rangle^2 + \left\langle\sum_{i=1}^{N/4} \sin\theta_i^{(j)}\right\rangle^2\right)\right] \tag{2}$$

and the local Ising order parameter $s_\square$ as in equation (3.8) of Scheinine

$$s_\square = \sum_\square \sin(\theta_i - \theta_j - A_{ij}). \tag{3}$$

From this local Ising order parameter we may calculate a susceptibility and correlation function (from which we extract the correlation length, as explained in Baillie (1990) in the usual way, by fitting the correlation function to a hyperbolic cosine). However, for the XY correlation function we use the definition of Fradkin *et al* (1978)

$$\Gamma_{ij} = \langle\cos(\theta_i - \theta_j - A_{ij})\rangle. \tag{4}$$

This function is gauge invariant, but depends on the path connecting the sites i and j. We choose $j = i + n\mu$, $n = 0, 1, \ldots$, where μ is a lattice unit vector, and we average Γ over the two lattice directions.

Figures 1 and 2 present our results for no positional disorder, $\Delta = 0$. We have fitted this data to the scaling forms

$$\begin{aligned} \xi^{\text{ising}} &= A(T - T_c^{\text{I}})^{-\nu^{\text{I}}} \\ \chi^{\text{Ising}} &= B(T - T_c^{\text{I}})^{-\gamma^{\text{I}}} \\ \xi^{XY} &= C \exp[D(T - T_c^{XY})^{-\nu^{XY}}] \\ \chi^{XY} &= E \exp[F(T - T_c^{XY})^{-\gamma^{XY}}] \end{aligned} \tag{5}$$

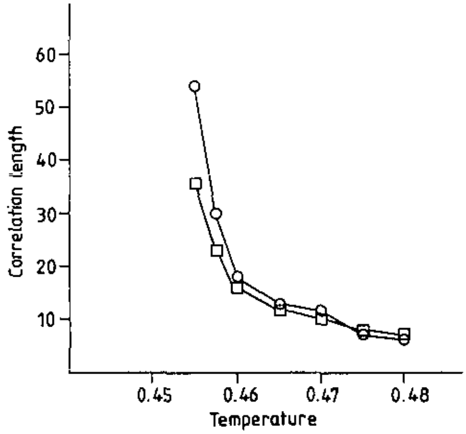

Figure 1. Ising (○) and XY (□) correlation lengths against temperature for a system with no positional disorder. Standard deviations are less than the symbol size, and the lines are merely to guide the eye.

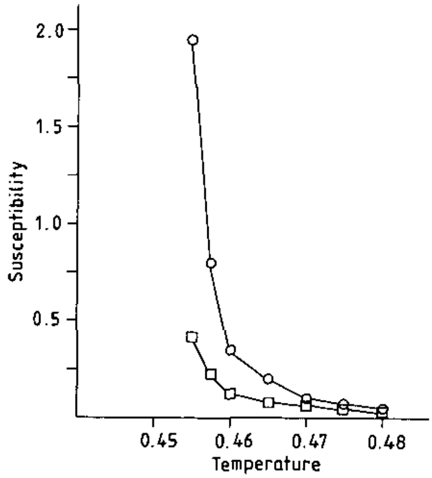

Figure 2. Ising (○) and XY (□) susceptibilities against temperature for a system with no positional disorder. Standard deviations are less than the symbol size, and the lines are merely to guide the eye.

where A, B, C, D, E and F are non-universal constants, and we have, at first, restricted the exponents to their theoretical values $\nu^{\mathrm{I}}=1$, $\gamma^{\mathrm{I}}=\frac{7}{4}$, $\nu^{XY}=\frac{1}{2}$, $\gamma^{XY}=\frac{1}{2}$. This fit gives an estimate of the respective Ising and XY critical temperatures that are equal to within errors: $T_{\mathrm{c}}^{XY}=0.4512\ (16)$, $T_{\mathrm{c}}^{\mathrm{I}}=0.4491\ (20)$. We thus suspect that the effective critical theory at this point may include arbitrary $\mathrm{O}(2)\times Z_2$-invariant operators. A clue to the nature of this effective theory comes from the actual value of the XY critical temperature. Our results, together with the results of Gupta *et al* (1988) and Wolff (1989) for the pure XY model, imply that for the simple square lattice, the fully frustrated XY model has a critical temperature very close to exactly half that of the pure XY model. In transforming these XY models into sine-Gordon models (by way of the Coulomb gas description, see Fradkin *et al* (1978)), the Villain approximation (which is surprisingly good here, see Janke and Kleinert (1986)) implies that the critical temperature of the corresponding sine-Gordon model changes from $\beta^2=8\pi$ in the pure case to $\beta^2=4\pi$ in the fully frustrated case. At this coupling, the generic renormalizable $\mathrm{O}(2)\times Z_2$-invariant quantum field theory is the supersymmetric sine-Gordon (SUSY SG) model (Goldschmidt 1986a, b), described by the Lagrange density

$$\mathscr{L}=\tfrac{1}{2}(\partial\phi)^2+\tfrac{1}{2}\bar{\psi}i\partial\!\!\!/\psi+\frac{1}{2}\frac{\mu_0^2}{a^2\beta_0^2}\cos^2\beta_0\phi-\frac{\mu_0}{a}\bar{\psi}\psi\cos\beta_0\phi. \tag{6}$$

The suggestion that this theory might have something to do with the fully frustrated XY model was first made by Foda (1988). Attempts to substantiate our hand-waving connection between this and the fully frustrated XY model, by constructing an explicit operator equivalence between the models, as between the SUSY SG model and an anisotropic Ashkin–Teller model (Goldschmidt 1986b), are presently under investigation.

Relaxing the constraint that the exponents assume their predicted values, we find $\gamma^{\mathrm{I}}=1.724\ (20)$, $\gamma^{XY}=0.532\ (28)$, $\nu^{\mathrm{I}}=1.009\ (26)$, and $\nu^{XY}=0.678\ (165)$. We also find an estimate of the exponent $\eta=2-F/D=0.257\ (27)$. These values are acceptably close to the theoretical ones, except for the exponent governing the XY correlation length. The χ^2 fit may be caught in a metastable minimum, as discussed by Baillie (1990). Much better statistics are needed.

We have also simulated the model with positional disorder present, at a value of $\Delta = 0.1$. Positional disorder destroys the sublattice structure used in defining the XY susceptibility, so we have located the XY transition temperature by looking at the spin-wave stiffness Υ as defined in equation (3.5) in Scheinine

$$\Upsilon_{xx} = (1/L_x^2)\left\langle \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j - A_{ij})(\hat{e}_x \cdot \hat{e}_{ij})^2 \right\rangle - (\beta/L_x^2)\left[\left\langle \left(\sum_{\langle ij\rangle} \sin(\theta_i - \theta_j - A_{ij})(\hat{e}_x \cdot \hat{e}_{ij})\right)^2 \right\rangle - \left\langle \sum_{\langle ij\rangle} \sin(\theta_i - \theta_j - A_{ij})(\hat{e}_x \cdot \hat{e}_{ij}) \right\rangle^2\right] \tag{7}$$

and plotted in figure 3. Also included in this figure is the prediction of the Kosterlitz–Thouless theory (Nelson and Kosterlitz 1977) that at the transition the spin-wave stiffness should exhibit a universal jump discontinuity of $2/\pi$. As with previous results the jump is slightly larger than the predicted universal value. From this we can roughly estimate $T_c^{XY} \simeq 0.30\,(1)$. The Ising analysis is carried out as for the $\Delta = 0$ case, and we obtain $T_c^{\mathrm{I}} = 0.3515\,(12)$. Thus the splitting of the two transitions, as predicted by Granato and Kosterlitz (1989), but not seen in previous, smaller simulations (Choi *et al* (1987)), is verified.

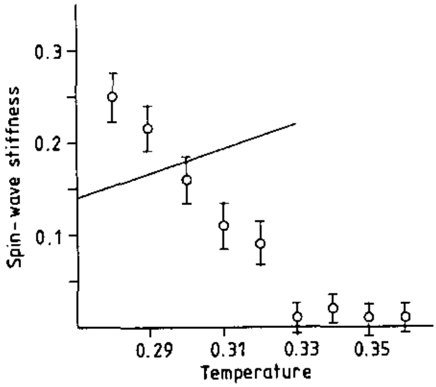

Figure 3. XY spin-wave stiffness against temperature for a system with a positional disorder of $\Delta = 0.1$. The straight line has the slope $2/\pi$, and is explained in the text.

Further work is needed to understand the phase diagram of the fully frustrated XY model, and if simulation is to play a role an effective algorithm which eliminates critical slowing down at the XY–Ising transition is needed. Fourier acceleration is not adequate (Scheinine 1989), but suggests a promising generalization. Fourier acceleration includes a kinetic term in (1), but replaces the mass of the spins by a 'mass tensor' (Bennett 1975), which is independent of the present θ-configuration

$$\tfrac{1}{2} m \sum_i \left(\frac{\partial \theta_i}{\partial t}\right)^2 \rightarrow \tfrac{1}{2} \sum_{(i,j)} \frac{\partial \theta_i}{\partial t} M_{ij} \frac{\partial \theta_j}{\partial t} \tag{8}$$

where $M_{ij} = m\nabla^2_{ij}$ and ∇^2_{ij} is the discrete lattice Laplacian. In fact, an arbitrary θ-dependent orthogonal transformation of this mass tensor is allowed

$$\boldsymbol{M} = \boldsymbol{A}(\theta)\nabla^2\boldsymbol{A}^{\mathrm{T}}(\theta). \tag{9}$$

Ideally, we would like to appeal to mean-field theory and transform ∇^2_{ij} into the stability matrix (Bray and Moore 1982)

$$M_{ij} = -J_{ij}\cos(\theta_i - \theta_j - A_{ij}) + \delta_{ij}\left(\sum_k J_{ik}\cos(\theta_i - \theta_k - A_{ik})\right). \tag{10}$$

Unfortunately, this matrix does not seem to be an orthogonal transformation of the lattice Laplacian. We are at present attempting to find the 'optimal' orthogonal transformation, which should map the eigenvectors of the stability matrix onto the modes of the system in the most effective way.

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