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Phase Transitions in Coupled XY-Ising Systems

Phase Transitions in Coupled *XY*-Ising Systems

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We study the critical behavior of fully frustrated *XY* and Josephson-junction systems by means of a coupled *XY*-Ising model. From Monte Carlo and transfer-matrix calculations, we find separate *XY* and Ising and first-order transitions, depending on the parameters. In addition, a line of continuous transitions is found, with simultaneous loss of *XY* and Ising order and novel critical behavior. This result is supported by Monte Carlo simulations of frustrated *XY* models on square and triangular lattices.

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Models containing both continuous U(1) and discrete Z_2 symmetry can give rise to interesting and unusual critical behavior. In general, one expects one of three scenarios: Transitions of the Ising and *XY* types occur at different temperatures or at the same temperature in a decoupled fashion, or else, in the case of strongly coupled excitations, a single transition in a different universality class. The nature of this single transition is one of the most important issues but is also less amenable to numerical or analytical approaches. A prototype of this system is a fully frustrated (FF) *XY* model on a triangular or a square lattice. This system has attracted great attention in recent years,[1-15] as it can be physically realized as a Josephson-junction array of large capacitance in a perpendicular magnetic field corresponding to a half-flux quantum per plaquette. The model is defined by the Hamiltonian

$$H/kT = -\sum_{ij} J_{ij}\cos(\theta_i-\theta_j)\ , \qquad (1)$$

where $J_{ij}=\pm J$ ($J>0$) for i,j nearest neighbors subject to the constraint that the gauge-invariant product of J_{ij} around a plaquette is negative. For the square lattice, this can be accomplished by ferromagnetic horizontal rows and alternating ferromagnetic and antiferromagnetic columns and for the triangular lattice by isotropic antiferromagnetic couplings. This leads one to frustration and a double degeneracy in addition to the degeneracy due to the continuous symmetry.

From renormalization-group ideas and universality, it is quite natural to expect that the critical behavior of the FF *XY* model, arising from the interplay between *XY* and Ising-like excitations, could be described by a coupled *XY*-Ising model. In fact, a Ginzburg-Landau free energy of the FF *XY* models[4,6-8] and renormalization-group analysis leads one to consider a coupled *XY*-Ising model of the form[8,15]

$$\frac{H}{kT} = -\sum_{\langle ij\rangle}[(A+B\sigma_i\sigma_j)\cos(\theta_i-\theta_j)+C\sigma_i\sigma_j]\ , \qquad (2)$$

where A, B, and C are effective couplings depending on the initial values of the parameters in the Ginzburg-Landau free energy.[16] As a consequence, the square and triangular FF *XY* models[17] can be considered to be at different initial points in the parameter space of the same model of Eq. (2). The isotropic FF *XY* models correspond to $A=B$, but a generalized version of the FF *XY* model on a square lattice,[9] where the antiferromagnetic couplings have different magnitudes compared to the ferromagnetic ones, corresponds to $A\neq B$.[7] An early study of this model[8] revealed a bifurcation point close to $C=0$ in the subspace $A=B$. For larger positive C there is a double transition with an *XY* followed by an Ising as temperature is increased, while if $C<0$ there is a single transition with simultaneous loss of *XY* and Ising order. An identical topology of the phase diagram has also been found in a generalized Coulomb-gas representation of the FF *XY* model containing fractional charges.[10] An important feature of the phase structure when $A=B$ is that Ising disorder induces *XY* disorder. In the model of Eq. (2) this can be seen as arising from the special coupling between the variables since a domain wall in the Ising variables leaves the *XY* spins uncoupled as $1+\sigma_i\sigma_j=0$ at a wall. Although physically different, this is similar to the mechanism for a single transition in the FF *XY* model.[3] The role played by the fractional corner charges in that model, which, when the walls melt, trigger an unbinding of integer charges destroying *XY* order, is played here by the domain wall itself. Our claim is that, in spite of the apparent discrepancies between the FF *XY* models[1,2] of Eq. (1) and the Coulomb-gas representation[10,11] of frustrated junction arrays, both can be accommodated in the $A=B$ subspace of Eq. (2). Changing the temperature in either corresponds to different paths through the same phase diagram. In experiments, positional disorder can lead to a double transition if there is a single one in the ideal system. These transitions, however, will be in different universality classes, as this kind of disorder acts as a random bond for the Ising and random dipoles for integer charges in the Coulomb-gas representation.[18]

In this work we report the results of a detailed study by Monte Carlo (MC) simulations of the critical behavior of the coupled XY-Ising model in Eq. (2) along the line of single transitions. We have also performed MC simulations of the original FF XY models of Eq. (1) to compare the critical exponents. The phase diagram obtained by MC simulation is indicated in Fig. 1. We monitor only the Ising variables and find a segment of continuous non-Ising phase transitions starting at P which eventually becomes first order for $C \ll 0$ at a tricritical point T. The results suggest a nonuniversal behavior as the exponents associated with the Ising order parameter vary systematically along the line PT. In addition, an evaluation of the central charge c using a Monte Carlo transfer matrix[19] gives a rather surprising result: c is found to vary from $c \approx 1.5$ near P to $c \approx 2$ near T. For the FF XY model on a square and a triangular lattice, using the same methods to evaluate the critical exponents, we find these exponents to be in fair agreement with the corresponding ones obtained for the coupled XY-Ising model near P. The central charge of the FF XY model evaluated recently by Thijssen and Knops,[13] $c = 1.66(4)$, is consistent with the corresponding result for the coupled XY-Ising model near the bifurcation point.

The simulations were performed employing the standard Metropolis algorithm using small system sizes L to achieve good statistics. Critical exponents and the location of first-order transitions were obtained from long simulations, typically of 5×10^6 MC steps, by means of the histogram method[20] and the finite-size scaling analysis of Lee and Kosterlitz (LK).[21] We also compared our results with those derived by applying the cumulant method[22] and found fair agreement.

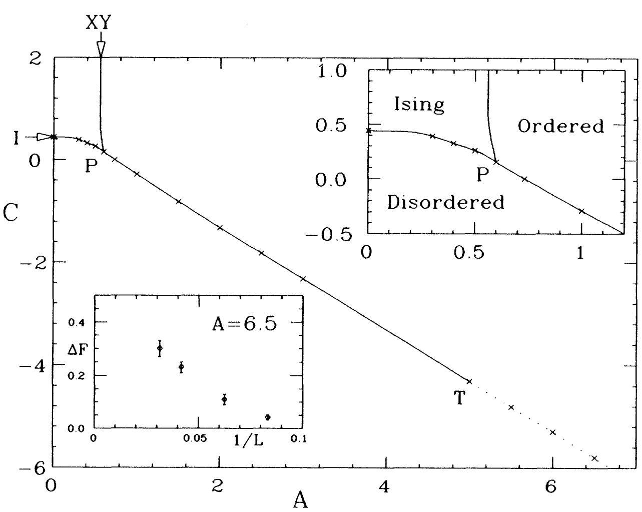

FIG. 1. Phase diagram obtained from MC simulations. Lines through the data points (×) are guides to the eyes. Solid and dotted lines indicate continuous and first-order transitions. Arrows indicate the known critical couplings for the Ising and XY models. Inset on left: Finite-size scaling of free-energy barrier ΔF_E at a first-order point.

The LK method is particularly suited to studying temperature and field-driven first-order transitions by a finite-size scaling analysis of the barriers between different phases at the transition. At a temperature-driven first-order transition, the free-energy barrier ΔF_E between ordered and disordered states is obtained from the energy histogram $N(E;A,C,L)$ as the height of the peak in $-\ln N(E)$. At a first-order transition ΔF_E is a monotonically increasing function of L and we show the results for $A = 6.5$ in an inset of Fig. 1. As we move along the transition line towards P, this peak becomes lower and disappears at T. We identify this as a tricritical point but this may overestimate the range of continuous transitions since the absence of a peak in systems of limited size does not exclude a very weak first-order transition.

Along the segment TP, we assume that the transition is continuous and, in principle, there are two sets of exponents to be determined since there are both Ising and XY variables. We are able to estimate only those associated with the former to any degree of accuracy and they are obtained from the histogram of Ising magnetization m. The corresponding free-energy barrier ΔF_m between the bulk states $\pm m$ increases as $L^{1/\nu}$ for $L < \xi$ in the ordered state and decreases to zero in the disordered state. This change of behavior can be used to accurately determine the critical values of A and C. More importantly, the exponent ν can be determined from $S = \partial \Delta F_m / \partial C \approx L^{1/\nu}$ without a precise determination of the critical parameters. This is a strength of the LK method as it yields ν from a one-parameter fit[23] in contrast to most earlier MC analyses[1,2] which involve fitting at least two. We identify $\nu \neq 1$ as a single transition since, if the Ising and XY transitions are separate or decoupled, $\nu = 1$ at the Ising transition. We were unable to obtain meaningful results for the helicity modulus near the transition so the line XYP in Fig. 1 is an interpolation from the known position in the phase with $m = 1$. We identify P as the bifurcation point but cannot exclude the possibility of a short segment of single decoupled transition with $\nu = 1$ to the left of P. The exponent $2\beta/\nu$ is obtained from the L dependence of the peak separation in the histogram of m which scales as $L^{-\beta/\nu}$ at criticality, although this is subject to larger uncertainties than ν. Our estimates of the Ising exponents ν and $2\beta/\nu$ are plotted in Fig. 2 along the line PT. It is clear that these differ from the pure Ising values and seem to vary systematically on the transition line indicating nonuniversal behavior. We have also made an independent study using the cumulant method[22] and find consistency.[15]

In order to compare the result for the critical ex-

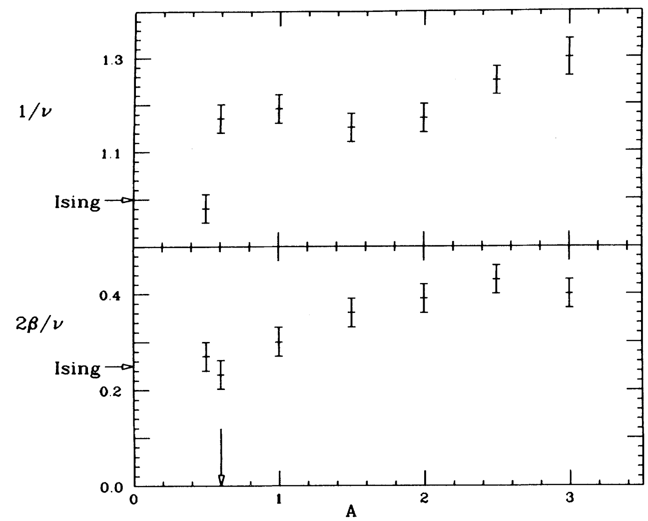

FIG. 2. Critical exponents obtained from a finite-size scaling of ΔF_m on lattices of size $10 \leq L \leq 30$. Horizontal arrows correspond to known results and the vertical arrow indicates the estimated location of the bifurcation point in Fig. 1.

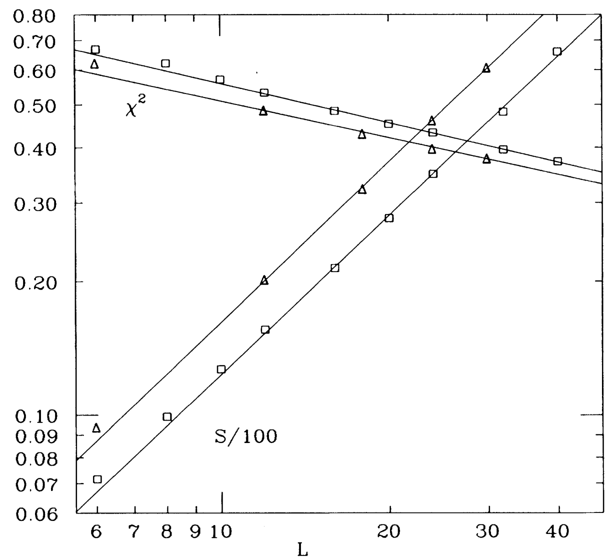

FIG. 3. Finite-size scaling of the peak position χ^2 and $S = \partial \Delta F_\chi / \partial J$ from the histogram of the chirality χ for the square (□) and the triangular (△) FF XY models. Solid lines are least-squares fits to $L > 10$ data.

ponents of the coupled XY-Ising model near the bifurcation point with those of the FF XY model, we used the same methods to evaluate the Ising-like critical exponents for the triangular and the square lattices.[24] Figure 3 shows the result of a finite-size scaling analysis of $S = \partial \Delta F_\chi / \partial J$ for both cases. ΔF_χ was obtained from histograms of the staggered chirality order parameter χ.[2,3] A small curvature is still observed even for the largest system sizes, indicating that correction to scaling is still important. However, if one estimates the exponents from the largest sizes, one obtains $\nu = 0.83(4)$, $2\beta/\nu = 0.28(4)$ (triangular) and $\nu = 0.85(3)$, $2\beta/\nu = 0.31(3)$ (square). Considering the curvature in the data, these can be considered to be upper bounds to the asymptotic result. Even so, they do differ significantly from the pure Ising exponents and seem to be consistent with the values obtained near the bifurcation point in Fig. 1. Note that the correlation lengths probed in the simulations of the FF XY models are much smaller than the ones in the coupled XY-Ising model since the size of the unit cell is larger. Although the exponents for the triangular and the square lattices also seem to agree with each other within the estimated uncertainties, it is perfectly possible that they may eventually differ if simulations are carried out in sufficiently large systems. This nonuniversal behavior of the FF XY model would be in complete agreement with our findings for the coupled XY-Ising models.

Additional information on the nature of the critical behavior on the line PT is provided by the central charge c which, to be consistent with varying exponents,[25] must obey $c \geq 1$. Preliminary investigations, using MC transfer-matrix methods[19] on infinite strips of width up to $L = 16$, yield the very surprising result that c seems to vary continuously from $c \approx 1.5$ at P to $c \approx 2$ at T. This implies that the line PT cannot be described as a superposition of critical XY and Ising lines with $c = 1.5$, as suggested by Foda,[26] but this is a completely new effect. The only models where c is known to vary are models that do not have a symmetric transfer matrix, e.g., the q-state Potts and $O(n)$ models with a continuously varying number of states q and n. Unlike in those models, on the line PT a parameter is changing that does not affect the symmetry. It seems to us that there are three possible explanations: (i) The system is not conformally invariant on the line PT; (ii) the result is an artifact of limited strip widths; and (iii) it is a real and interesting effect. Further investigation is under way.

We note that this variation of c is entirely consistent with the Zamolodchikov c theorem[27] which states that there exists a quantity $c(l)$ such that $dc(l)/dl \leq 0$ along a renormalization-group trajectory and tends to c at a fixed point. The model of Eq. (2) may be obtained by adding a relevant term $h_2 \cos 2(\theta_i - \phi_i)$ to two coupled XY models[7] which implies $c \leq 2$. If, on the other hand, we start from decoupled critical XY and Ising models and add a term $B\sigma_i\sigma_j[1 - \cos(\theta_i - \theta_j)]$, we obtain $c \geq \frac{3}{2}$ since such a term is irrelevant about the decoupled fixed point for B small.[7,28] Since the true model is at $A = B$, this yields the allowed range of $\frac{3}{2} \leq c \leq 2$. We finally note that the value of $c = 1.66$ of Thijssen and Knops[13] for the FF XY model using the same methods is within the allowed range.

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