Domain Walls and Phase Transitions in the Frustrated Two-Dimensional *XY* Model

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We compare the critical properties of the two-dimensional (2D) *XY* model in a transverse magnetic field with filling factors $f = 1/3$ and $2/5$. To obtain a comparison with recent experiments, we investigate the effect of weak quenched bond disorder for $f = 2/5$. A finite-size scaling analysis of extensive Monte Carlo simulations strongly suggests that the critical exponents of the phase transition for $f = 1/3$, and for $f = 2/5$ with disorder, are those of the pure 2D Ising model. Studying the possible domain walls in the system provides some explanations for our results. [S0031-9007(97)03625-9]

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The frustrated *XY* model provides a convenient framework for studying a variety of fascinating phenomena displayed by numerous physical systems. One experimental realization of this model is in two-dimensional arrays of Josephson junctions and superconducting wire networks [1–3]. A perpendicular magnetic field induces a finite density of circulating supercurrents, or vortices, within the array. The interplay of two length scales—the mean separation of vortices and the period of the underlying physical array—gives rise to a wide variety of interesting physical phenomena. Many of these effects show up as variations in the properties of the finite-temperature superconducting phase transitions at different fields. Recent and ongoing experiments have measured the critical exponents in superconducting arrays [3], opening the opportunity to do careful comparison of theory and experiment. In this Letter we examine the critical properties of the 2D *XY* model for two different values of the magnetic field in the densely frustrated regime ($f \gg 0$) and in the presence of disorder.

The Hamiltonian of the frustrated *XY* model is

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j - A_{ij}), \tag{1}$$

where θ_j is the phase on site j of a square $L \times L$ lattice and $A_{ij} = (2\pi/\phi_0) \int_i^j \mathbf{A} \cdot d\mathbf{l}$ is the integral of the vector potential from site i to site j with ϕ_0 being the flux quantum. The directed sum of the A_{ij} around an elementary plaquette $\sum A_{ij} = 2\pi f$, where f, measured in units of ϕ_0, is the magnetic flux penetrating each plaquette due to the uniformly applied field. We focus here on the cases $f = p/q$ with $p/q = 1/3$ and $2/5$.

A unit cell of the ground state fluxoid pattern for these f is shown in Fig. 1(a) [4]. The pattern consists of diagonal stripes composed of a single line of vortices for $f = \frac{1}{3}$ and a double line of vortices for $f = \frac{2}{5}$. (A vortex is a plaquette with unit fluxoid occupation, i.e., the phase gains 2π when going around the plaquette.) The stripes shown in Fig. 1(a) can sit on q sublattices, which we associate with members of the Z_q group. They can also go along either diagonal, and we associate these two options with members of the Z_2 group. A common speculation for commensurate-incommensurate transitions and the frustrated *XY* model is that the transition should be in the universality class of the q-state (or $2q$-state) Pott's model. We find that this is not the case because domain walls between the different states vary considerably in both energetic and entropic factors.

Table I lists the energy per unit length σ for straight domain walls between the various ground states at zero temperature. We also numerically calculated the energy of domain walls that are not straight. Closed domains, such as those seen in the simulations, of linear dimension L from 10 to 60 unit cells in a system of size 120×120 have energies that scale linearly in L to very high accuracy (Unusual patterns of vortices could have energies which scale with a higher power of L, but these were not observed in the Monte Carlo simulations.) Examining two domain walls as a function of their distance apart shows only short range forces between them, and the closed domains constructed from the lowest energy walls are neutral and have no net dipole moment [5]. This strongly indicates that we can treat the energy of these domains as being linear in L. Another type of excitation is vacancy-interstitial pairs. Such pairs have logarithmic interactions and can undergo a Kosterlitz-Thouless (KT) transition [6]. We first focus on domain wall excitations.

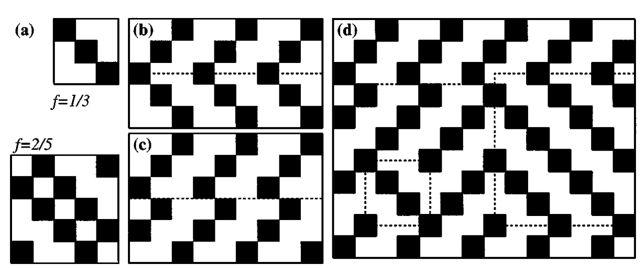

FIG. 1. Fluxoid pattern for (a) unit cells of $f = \frac{1}{3}$ and $f = \frac{2}{5}$, and domain walls for $f = \frac{1}{3}$ for the (b) herringbone wall, (c) shift-by-one wall, and (d) shift-by-one wall branching into two herringbone walls (a vortex is shown as a dark square).

TABLE I. Domain wall energies.

Domain wall type	Energy per unit length $f = 1/3$	$f = 2/5$
Herringbone	$0.056\,737\,424J$	$0.086\,117\,262J$
Shift-by-one	$0.114\,199\,976J$	$0.158\,899\,286J$
Shift-by-two	$0.166\,666\,666J$	$0.166\,122\,315J$
Shift-by-three	...	$0.147\,648\,594J$
Shift-by-four	...	$0.198\,688\,789J$

The fluxoid pattern for the two lowest energy walls at $f = \frac{1}{3}$ is shown in Fig. 1. The figure shows how a shift wall can be viewed as two adjacent, or *bound*, herringbone walls. For $f = \frac{1}{3}$ the energy of two herringbone walls is less than that of a single shift wall, and, hence, the shift walls are unstable and break up into herringbone walls. As a result, we confine our discussion of the $f = \frac{1}{3}$ case to the herringbone walls, as other walls should not be present at large length scales. The energy cost for dividing an $L \times L$ lattice into two domains separated by a solid-on-solid (SOS) wall stretching from one side of the system to the other is

$$\mathcal{H}_{\mathrm{single}}\{z\} = b\sigma L + b\sigma \sum_k |z_k - z_{k-1}|. \qquad (2)$$

The height variables z_k take on integer values ($b = 3$ is the shortest length segment). The partition function can be evaluated to give the interfacial free energy per column [7] $\mathcal{F} = T \ln[e^{b\sigma/T} \tanh(\frac{b\sigma}{2T})]$. The zero crossing of $\mathcal{F}$ gives an estimate of the critical temperature. Plugging in the values for the $f = \frac{1}{3}$ herringbone wall gives $T_c = 0.19J$, in remarkable agreement with the value $T_c = 0.22J$ found in the Monte Carlo simulations described below. Being similar to Ising walls, herringbone walls cannot branch into other herringbone walls; thus the set of possible domain wall configurations is similar to those in an Ising model. We label the fraction of the system in state (s, j) as $m_{s,j}$, where $s = \pm 1$ denotes the member of Z_2, and $j = 1, 2, 3$ denotes the member of Z_3. Below the transition, one state (s, i) spans the system. On this state sit fluctuating domains, bounded by herringbone walls, of each of the states $(-s, 1), (-s, 2)$, and $(-s, 3)$ in equal numbers; therefore the Z_3 symmetry is broken for the (s, j) states, but not for the $(-s, j)$ states. As the transition is approached from below, the domains occupied by the $(-s, j)$ states grow, with smaller domains of the (s, j) states within them. At the transition, the Z_2 symmetry between the $\pm s$ states is restored, and, as a result, the Z_3 symmetry for the (s, j) states is also restored.

The Monte Carlo simulations used a heat bath algorithm with system sizes of $20 \le L \le 96$. We computed between 10^7 and 3×10^7 Monte Carlo steps (complete lattice updates) with most of the data taken close to T_c. Data from different temperatures was combined and analyzed using histogram techniques [8].

If the largest fraction of the system is in state (s, i), then we have three Ising order parameters, $M_j = (m_{s,i} - m_{-s,j})/(m_{s,i} + m_{-s,j})$, $j = 1-3$. On average, these M_j are the same so we just take the average as M. To calculate the $m_{\sigma,i}$, we examine the Fourier transform of the vortex density $\rho_{k\pm}$ at the reciprocal lattice vectors $\mathbf{k}_\pm = \frac{\pi}{3}(1, \pm 1)$ of the ground state vortex lattices. Starting from the definition of the Fourier transform, and using the vortex states given above, one finds $\rho_{k\pm}/\rho_g = m_{\pm 1,1} + m_{\pm 1,2}e^{i2\pi/3} + m_{\pm 1,3}e^{-i2\pi/3}$, where ρ_g is the modulus in the ground state. In practice, $\rho_{k\pm}$ is reduced by small short-lived regions which don't quite match any of the six states. Since this effect is the same for all states, it cancels when calculating M. Using $\rho_{k\pm}$, in addition to $\sum_j m_{\pm 1,j}$, calculated from the direct vortex lattice as in [9], we can find the $m_{\sigma,j}$.

The transition temperature is located using Binder's cumulant [10], $U = 1 - \langle M^4 \rangle / (3\langle M^2 \rangle^2)$, shown in Fig. 2(a). For system sizes large enough to obey finite-size scaling, this quantity is size independent at the critical point. From Fig. 2, we find $T_c = 0.2185(6)J$. T_c can also be determined from the scaling equation for the temperature at the peak of thermodynamic derivatives such as the susceptibility, $T_c(L) = T_c + aL^{-1/\nu}$. We find these other methods give T_c in agreement with that from U.

The exponents for the specific heat α, the order parameter β, the susceptibility γ, and the correlation length ν describe the usual power-law singularities in the infinite system limit. Finite-size scaling [11] at T_c applied to $\partial \ln M / \partial K$ [12] gives $1/\nu = 1.007(25)$, applied to susceptibility χ gives $\gamma/\nu = 1.743(20)$, and applied to M gives $\beta/\nu = 0.142(20)$ [these exponents are determined from the slopes of the lines shown in Figs. 3(a) and 3(b)]. This is in excellent agreement with the Ising values $\nu = 1$, $\gamma = \frac{7}{4}$, and $\beta = \frac{1}{8}$. Figure 2 shows the collapse of the raw data onto the scaling function (inset) for χ.

Two previous examinations of the $f = \frac{1}{3}$ case [13] suggested a continuous transition but did not measure critical exponents. Lee and Lee [9] claim to find separate, closely spaced transitions for the breaking of Z_2 and Z_3. One explanation for their conflicting results comes from the small systems ($L \le 42$) used in their analysis. Below T_c, if the dominant state is (s, i), in small systems you often do not see all three of the $(-s, j)$ states in the system at the same time. This can give the impression

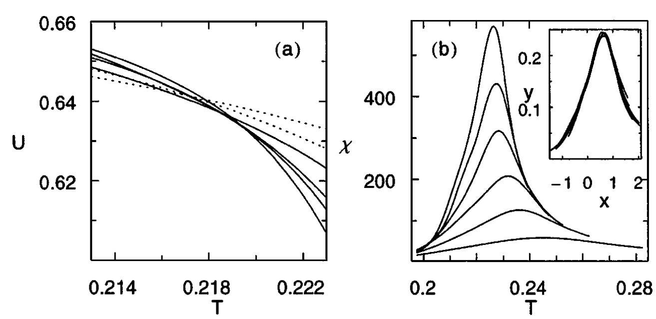

FIG. 2. $f = 1/3$ (a) Binder's cumulant U vs T for $L = 36$ to $L = 84$ (smaller L shown as dotted lines), and (b) χ vs T for $L = 36$ to $L = 84$ and scaling collapse of this data (inset) where $x = (T - T_c)L^{1/\nu}$, $y = \chi L^{-\gamma/\nu}$, $\nu = 1$, and $\gamma = \frac{7}{4}$.

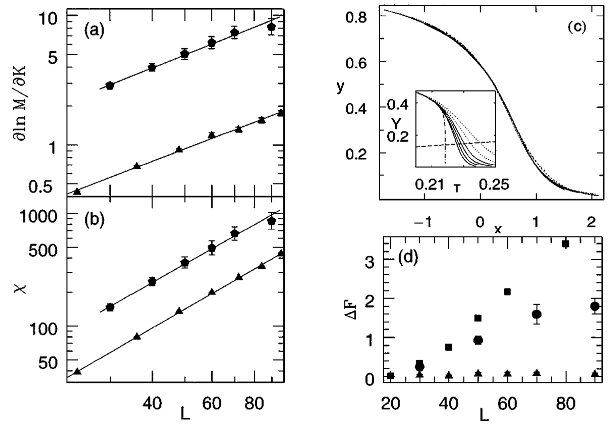

FIG. 3. Finite-size scaling plots for $f = \frac{1}{3}$ (triangles) and $f = \frac{2}{5}, \delta = 0.1$ (pentagons): (a) logarithmic derivative of M vs L, (b) χ vs L. (c) Scaling collapse of Y where $x = (T - T_c)L^{1/\nu}$, $y = YL^{\beta/\nu}$, $\nu = 1$, and $\beta = \frac{1}{8}$. Inset: raw data (solid and dotted), $\frac{2}{\pi}T$ (dashed), and $a|T - T_c|^\beta$ (dot-dashed). (d) Free energy barrier vs system size for $f = \frac{2}{5}$ and $\delta = 0$ (squares), 0.05 (circles), and 0.10 (triangles).

of separate transitions for small L. This impression is enhanced by the presence of a shoulder in the specific heat at intermediate L [9]. For larger L we see this shoulder merge with the main peak, and for $L = 84$ and 96 it is no longer clearly discernible.

The helicity modulus Y is the quantity most closely related to experimental measurements [6]. For $f \neq 0$, the scaling of the I-V curves found in experiments is consistent with domain wall activation processes [3]. The theory of Nelson and Kosterlitz for the $f = 0$ case predicts that Y should come down in a characteristic square-root cusp and then jump with a universal value, $2k_B T_{\mathrm{KT}}/\pi$. However, we find an exceptionally good fit [Fig. 3(c)] of our data to $Y = L^{-\beta/\nu}\,\mathcal{M}((T - T_c)L^{1/\nu})$ with $\nu = 1$ and $\beta = \frac{1}{8}$, the scaling form of M. We see two possible interpretations of our result. The first is that Y only receives contributions from the ordered part of the lattice. So comparisons with the $f = 0$ case should examine $Y_m = Y/M$. $Y_m \approx 0.58$ at the transition implies a larger than universal jump. Alternatively, one can say that, although Y is brought down by fluctuations in M, it should still jump when it crosses the universal value, $2k_B T/\pi$. Extrapolating the observed behavior of Y gives $Y_{L\to\infty} = a|T - T_c|^\beta$. This crosses the value of the universal jump at $T_{\mathrm{KT}} - T_c \approx 10^{-6}$. Although we do not see evidence for a jump, a difference in transition temperatures of 10^{-6} would not lead to any observable effects for the system sizes studied here.

While, for $f = \frac{1}{3}$, herringbone walls are the only stable walls, this is not true for $f = \frac{2}{5}$. For $f = \frac{2}{5}$ it is energetically favorable for two herringbone walls to bind and form a shift-by-one or shift-by-three wall. Binding does, however, have an entropic cost. To see if these walls are bound, we consider the following model for two SOS walls:

$$\mathcal{H}_{\mathrm{double}}\{\Delta, z\} = \sum_k \{(2b\sigma + u_\parallel \delta_{z_k,0}) + b\sigma|z_k - z_{k-1}| + (2b\sigma + u_\perp \delta_{z_k,0})\Delta_k + V_r(\{\Delta, z\})\}. \quad (3)$$

z_k is the separation of the walls ($z_k \geq 0$), and Δ_k is the number of vertical steps the two walls take in the same direction in the kth column ($-\infty < \Delta_k < \infty$). $u_\parallel$ and $u_\perp$ are the binding energies parallel and perpendicular to the wall. At this stage we take $V_r = 0$. Summing over Δ_k leaves the partition function in the form of a transfer matrix: $\mathcal{Z} = \sum_{\{z_k\}} \prod_k T_{z_k}^{z_{k-1}}$. A ground state eigenvector $\psi_\mu(z) = e^{-\mu z}$, where $1/\mu$ is the localization length, or a typical distance separating the lines, characterizes the bound state of the two lines. $\mu = 0$ defines the unbinding transition at T_b. One finds $T_b = 0.398J$ for the shift-by-one walls and $T_b = 0.442J$ for the shift-by-three walls. The free energy for these walls crosses zero before they unbind. Hence, at the transition, we expect a branching domain wall structure similar to the $q \geq 5$ Pott's models where a first order phase transition occurs.

In a previous study [14], hysteresis of the internal energy was used as an argument for a first order transition at $f = \frac{2}{5}$. The most direct indication of a first order transition is the presence of a free energy barrier between the ordered and disordered states which diverges as the system size increases [15]. The free energy as a function of energy is obtained using $\mathcal{F}_L(E) = -\ln P_L(E)$ where $P_L(E)$ is the probability distribution for the energy generated by Monte Carlo simulation of an $L \times L$ system. Figure 3(c) shows the growth in this barrier as L increases, giving clear evidence for the first order nature of the transition. Also, according to finite-size scaling, the maximum of C and χ should scale with L^d for first order phase transitions [11]. We find this to be the case and also obtain $T_c = 0.2127(2)J$ [5].

We now consider the effects of disorder on the $f = \frac{2}{5}$ phase transition. Taking the couplings in the Hamiltonian (1) as $J_{ij} = J(1 + \epsilon_{ij})$, the ϵ_{ij} are chosen randomly from a Gaussian distribution with a standard deviation δ. Because of variations of the phase differences across the bonds, a specific realization of random bonds may favor a certain sublattice for the ground state, creating an effective random field. To quantify the effect, we placed the fluxoid configuration of the ground states down on 10 000 separate realizations of the disorder and allowed the continuous degrees of freedom (the phases) to relax and minimize the energy. We find that the changes in energy from the $\delta = 0$ case fit a Gaussian distribution with mean $-0.5\delta^2 L^2$ and standard deviation δL. The difference in energy between states which were degenerate in the clean system is the measure of the random field. This difference centers on zero and has a standard deviation of $0.75\delta L$ for two states related by a shift and $0.57\delta L$ for two states with vortex rows along opposite diagonals. The effect of random fields on discrete degrees of freedom in 2D is marginal [16]. For $D > 2$ there is a critical randomness above which random fields cause the formation of domains in the ground state of size $\sim\xi_{\rm rf}$. Aizenman and Wehr have shown that this critical randomness is zero in 2D [16]. Yet, their result does not preclude the possibility that $\xi_{\rm rf}$ is so large as to be unobservable in a finite-sized sample. Indeed, experiments on superconducting arrays have found apparent phase transitions, including scaling behavior [3], in sample sizes of order 1000×1000. In our simulations with disorder at $\delta \leq 0.1$, all systems had a low temperature state with the order parameter approaching unity. We will, therefore, ignore the effects of random fields for $\delta \leq 0.1$, assuming that $\xi_{\rm rf}$ is larger than the sample size.

At any coexistence point of the clean system, random *bonds* result in different regions of the system experiencing average couplings slightly above or below the critical coupling. As a result, at any given temperature the system will predominantly prefer either the ordered or disordered state wiping out the coexistence region and leaving only a continuous transition [16]. Kardar *et al.* [17] suggested a possible mechanism for this effect. Their renormalization group approximation suggests that the probability of loop formation in the fractal interface of the clean system vanishes marginally at a transition dominated by random bonds. The interface may have some finite width due to a froth of bubbles of different phases, but under renormalization a linear critical interface is obtained and, hence, an Ising transition appears.

The fluxoid configurations from our simulations suggest that, for large enough disorder ($\delta > \delta_f$), the interface is really linear, not just in the renormalized sense. δ_f can be estimated by placing a random potential V_r in Eq. (3). Ignoring the terms involving Δ_k, one obtains the model for wetting in the presence of disorder, solved by Kardar [18] in the continuum limit. He obtained a new length scale due to randomness, $1/\kappa = 2T^3/K\delta^2$, where K is the renormalized stiffness [7]. The unbinding transition is lowered and is now defined by the condition $\mu - \kappa = 0$. When T_b is reduced to the T_c of the clean system any branched domain wall structure is unstable. This is just the last step in a process in which the effective linear interface becomes narrower as disorder increases. In the vicinity of this "final" unbinding, the Ising-type behavior of the system should be visible at any length scale.

We have done a Monte Carlo analysis with bond disorder values of $\delta = 0.05$ and 0.1. Thermodynamic quantities were first calculated for a given realization of the disorder and then averaged over 10 to 15 realizations for $\delta = 0.1$ and 7 realizations for $\delta = 0.05$. Figure 3(c) shows the free energy barrier for $f = \frac{2}{5}$ as a function of system size for $\delta = 0.05$ and 0.1. For $\delta = 0.05$, the barrier first grows with system size and then levels off. At $\delta = 0.1$ the free energy barriers are essentially zero, indicating a continuous transition and that the system sizes are large enough to apply finite-size scaling. Here, we follow the finite-size scaling methods used in [12]. Figure 3 shows the peak values of $\partial \ln M/\partial K$ and χ as a function of L. The slopes of these plots give $1/\nu = 1.05(12)$ and $\gamma/\nu = 1.70(12)$. A similar analysis of $\partial M/\partial K$ gives $(1-\beta)/\nu = 0.94(10)$ [5]. Within errors, these exponents are what one would expect from an Ising model. Experiments at $f = \frac{2}{5}$ [3] also found a continuous transition and measured the critical exponents $\nu = 0.9(5)$ and the dynamic critical exponent $z = 2.0(5)$, consistent with an Ising transition.

In conclusion, we find that the nature and universality class of the phase transitions are quite sensitive to the proximity of the binding transition for the lowest energy domain walls. For $f = 1/3$ the lowest energy walls are never bound and the transition is Ising-like. For $f = 2/5$ domain walls can lower their free energy by binding to each other, resulting in a first order phase transition. Disorder weakens this binding and changes the transition to be continuous and Ising-like. Our results are consistent with the continuous phase transition and critical exponents observed experimentally for $f = 2/5$ [3].

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