Kink-Antikink Unbinding Transition in the Two Dimensional Fully Frustrated XY Model

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We carry out the first numerical simulations to directly confirm the existence of a kink-antikink unbinding transition along Ising-like domain walls in the two dimensional fully frustrated XY model. We comment on the possible implications of kink-antikink unbinding for the bulk phase transition of the model.

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I. INTRODUCTION

The two dimensional (2D) fully frustrated XY model (FFXY)\textsuperscript{10} is one of the most intriguing of “simple” statistical mechanics models. The doubly degenerate checkerboard pattern of vortices in the ground state leads to an Ising-like discrete Z(2) symmetry in addition to the Kosterliz-Thouless-like continuous O(2) symmetry associated with the uniform rotation of all phase angles.\textsuperscript{2} It remains controversial whether there are two distinct phase transitions $T_{KT} < T_I$, with $T_{KT}$ marking the breaking of the O(2) symmetry and $T_I$ marking the breaking of the Z(2) symmetry,\textsuperscript{2} or rather a single transition in which both symmetries are broken simultaneously.\textsuperscript{10}

Recently, Korshunov\textsuperscript{11} presented an argument for a new interfacial transition $T_w$ in the 2D FFXY model, lying well below the bulk transition(s), arising from the unbinding of step excitations of unit height ("kink-antikink pairs") on the domain walls associated with the Z(2) symmetry. Korshunov argued that the kink-antikink unbinding transition leads to a decoupling of phase coherence across domain boundaries, supporting the identification of the FFXY with the coupled XY-Ising model.\textsuperscript{12} Korshunov further argued that this effect necessarily leads to the scenario of two distinct bulk transitions, $T_{KT} < T_I$.

Earlier, Lee and co-workers, first in simulations of the 2D FFXY model with Langevin dynamics,\textsuperscript{10} and then in its dual Coulomb gas (CG) model with Monte Carlo (MC) dynamics,\textsuperscript{11} found evidence for a transition in domain wall morphology in simulations of the ordering kinetics of domain growth following a sudden quench. They interpreted this as a finite temperature roughening transition of the Ising-like domain walls. Jeon et al.\textsuperscript{12} made similar conclusions in simulations of the 2D FFXY with resistively shunted junction dynamics. Korshunov, however, has argued that domain walls should be rough at all temperatures.

In this paper we present the first direct numerical evidence demonstrating the existence of the kink-antikink unbinding transition at a temperature $T_w$ below the bulk transition(s). In agreement with Korshunov’s predictions, we show that phase angles on opposite sides of the domain wall decouple above $T_w$. The numerical value we find for $T_w$ is comparable to that of the morphological transition found by Lee et al.,\textsuperscript{11} however we explicitly demonstrate that domain walls are rough at temperatures well below $T_w$. This indicates that the transition seen by Lee and co-workers is really kink-antikink unbinding, rather than roughening.

II. THE MODEL

A. The fully frustrated XY model

We study the 2D FFXY model on a square lattice, given by the Hamiltonian:\textsuperscript{10}
\begin{equation}
\mathcal{H}[\theta(r_i)] = \sum_{i,\mu} V(\theta(r_i + \hat{\mu}) - \theta(r_i) - A_\mu(r_i)) \ . \tag{1}
\end{equation}

Here $\theta(r_i)$ is the thermally fluctuating phase angle of the planar XY spin on site $r_i = x_i, y_i$ ($x_i, y_i$ integers) of a $L_x \times L_y$ periodic square lattice, $\hat{\mu} = \hat{x}, \hat{y}$ label the bond directions of the lattice, and $A_\mu(r_i)$ is the quenched gauge field on the bond leaving site $r_i$ in direction $\mu$ (with $A_{-\mu}(r_i + \hat{\mu}) \equiv -A_\mu(r_i)$). For full frustration, the $A_\mu(r_i)$ are constrained so that their directed sum going counterclockwise around any plaquette $P$ of the lattice is fixed (modulus $2\pi$) to,
\begin{equation}
\sum_P A_\mu(r_i) = \pi \ . \tag{2}
\end{equation}

To implement the constraint of Eq. (2), we use the specific gauge choice,
\begin{equation}
A_x(r_i) = 0, \quad A_y(r_i) = (-1)^{x_i}(\pi/2) \ . \tag{3}
\end{equation}

The interaction potential $V(\phi)$ is periodic on $[0, 2\pi)$, with a single quadratic minimum at $\phi = 0$. We will take for $V(\phi)$ the commonly used Villain function,\textsuperscript{13}
\begin{equation}
V(\phi) = -T \ln \left[ \sum_{m=-\infty}^{\infty} e^{-J(\phi-2\pi m)^2/2T} \right] \ . \tag{4}
\end{equation}
The boundary conditions for the phase angles are, in the most general case,
\[
\theta(r_i + L \cdot \hat{\mu}) - \theta(r_i) = \Delta_\mu, \tag{5}
\]
where $\Delta_\mu \in [0, 2\pi)$ is the total twist applied across the system in direction $\hat{\mu}$. $\Delta_\mu = 0$ corresponds to periodic boundary conditions. Alternatively, if one makes the change of variables, $\theta'(r_i) \equiv \theta(r_i) - r_i \cdot d$, with $d_\mu \equiv \Delta_\mu/L$, then the system has periodic boundary conditions in the $\theta'(r_i)$ and the applied twist appears as an additive constant to the gauge field, $A_\mu(r_i) \rightarrow A_\mu(r_i) + \Delta_\mu/L$.

To study the behavior of the Ising-like domain walls we consider systems with sizes $L_x = L$, $L_y = L + 1$, with $L$ even. The odd length $L_y$ forces into the ground state checkerboard pattern of vortices a single straight domain wall running the length of the system in the $\hat{x}$ direction. This is illustrated in Fig. 1, where a (+) signifies a vortex in the phase angles $\theta(r_i)$, and a (−) signifies the absence of a vortex.

Phase coherence in the FFXY model is most conveniently studied by considering the dependence of the total free energy $F$ on the total twist $\Delta_\mu$ applied across the system (see Eq. (3)). In a phase coherent ordered state, we expect $F(\Delta_\mu)$ to vary with the twist $\Delta_\mu$; in a phase incoherent disordered state, we expect $F(\Delta_\mu)$ to be independent of $\Delta_\mu$, in the thermodynamic limit of $L \rightarrow \infty$. The dependence of the free energy on $\Delta_\mu$ is readily obtained by using fluctuating twist boundary conditions, in which one treats the applied twist $\Delta_\mu$ as a thermally fluctuating degree of freedom. If $Z$ is the partition function for this ensemble, then the probability $P(\Delta_\mu)$ of finding a state with a particular twist $\Delta_\mu$ is given by,
\[
P(\Delta_\mu) = \frac{e^{-F(\Delta_\mu)/T}}{Z}, \tag{6}
\]
and so the free energy with respect to a reference twist $\Delta_{\mu 0}$ is,
\[
F(\Delta_\mu) - F(\Delta_{\mu 0}) = -T \ln \left[ P(\Delta_\mu)/P(\Delta_{\mu 0}) \right]. \tag{7}
\]

The probability $P(\Delta_\mu)$ is directly measured within our fluctuating twist Monte Carlo simulation. We choose the reference twist $\Delta_{\mu 0}$ to be the value of the twist that minimizes the free energy $F(\Delta_\mu)$. For the gauge choice of Eq. (3), it is straightforward to see that the minimizing twist in the $\hat{x}$ direction is at $\Delta_{\mu 0} = 0$. In our simulations we keep a fixed twist $\Delta_\mu = 0$, and consider only the dependence of the free energy on the varying twist $\Delta_\mu$, transverse to the Ising-like domain wall that is introduced in our $L \times (L + 1)$ systems (see Fig. 1). In Fig. 2 we show sample results from our simulations for $F(\Delta_\mu) - F(0)$ vs. $\Delta_\mu$ at two different values of $T < T_\mu$, for a system of size $L = 128$. We see that $F(\Delta_\mu)$ has two equal minima at $\Delta_\mu = 0$ and $\pi$ (i.e. periodic and antiperiodic boundary conditions). One of these minima corresponds to states where the domain wall sits at even values of the height $y$, while the other corresponds to states where the domain wall sits at odd values of the height $y$. Below the kink-antikink unbinding transition $T_\mu$, the system is in a state of broken translational symmetry; due to the free energy barrier between the two minima, states in which the domain wall is at an even height cannot be reached from states in which the domain wall is at an odd height. As noted by Korshunov, this broken symmetry is restored when phase coherence transverse to the wall is lost, i.e. when $F(\Delta_\mu)$ becomes independent of $\Delta_\mu$, and so the free energy barrier between $\Delta_\mu = 0$ and $\Delta_\mu = \pi$ vanishes. Alternatively viewed, when the domain wall changes its height by an odd number, the system acquires an average twist of $\pi$ in the $\hat{y}$ direction. Thus, restoring the symmetry of domain wall translations leads to phase angle fluctuations that destroy phase coherence transverse to the direction of the wall.

In our numerical work we will use two convenient measures of the variation of $F(\Delta_\mu)$ with $\Delta_\mu$. The first is the helicity modulus, $\Upsilon_\mu$, which measures the curvature of $F(\Delta_\mu)$ at its minimum,
\[
\Upsilon_\mu(L_x, L_y) = \frac{L_x^2}{L_x L_y} \left. \frac{\partial^2 F}{\partial \Delta_\mu^2} \right|_{\Delta_\mu = 0}\]

FIG. 1: Various configurations of the domain wall in a $L \times (L + 1)$ system: (a) ground state, (b) finite width step of unit height (kink-antikink pair), (c) isolated kink of unit height, (d) isolated kink of height two. A (+) indicates the presence of a vortex in the XY model, or a charge $q_i = 1/2$ in the dual Coulomb gas; a (−) indicates the absence of a vortex in the XY model, or a charge $q_i = -1/2$ in the dual CG. $\hat{x}$ is the horizontal direction, and $\hat{y}$ is the vertical direction.

FIG. 2: Variation of total free energy $F$ with total twist $\Delta_\mu$, applied transverse to the Ising-like domain wall, for two different temperatures in a system of size $L = 128$. The probability $P(\Delta_\mu)$ is directly measured within our fluctuating twist Monte Carlo simulation. We choose the reference twist $\Delta_{\mu 0}$ to be the value of the twist that minimizes the free energy $F(\Delta_\mu)$. For the gauge choice of Eq. (3), it is straightforward to see that the minimizing twist in the $\hat{x}$ direction is at $\Delta_{\mu 0} = 0$. In our simulations we keep a fixed twist $\Delta_\mu = 0$, and consider only the dependence of the free energy on the varying twist $\Delta_\mu$, transverse to the Ising-like domain wall that is introduced in our $L \times (L + 1)$ systems (see Fig. 1). In Fig. 2 we show sample results from our simulations for $F(\Delta_\mu) - F(0)$ vs. $\Delta_\mu$ at two different values of $T < T_\mu$, for a system of size $L = 128$. We see that $F(\Delta_\mu)$ has two equal minima at $\Delta_\mu = 0$ and $\pi$ (i.e. periodic and antiperiodic boundary conditions). One of these minima corresponds to states where the domain wall sits at even values of the height $y$, while the other corresponds to states where the domain wall sits at odd values of the height $y$. Below the kink-antikink unbinding transition $T_\mu$, the system is in a state of broken translational symmetry; due to the free energy barrier between the two minima, states in which the domain wall is at an even height cannot be reached from states in which the domain wall is at an odd height. As noted by Korshunov, this broken symmetry is restored when phase coherence transverse to the wall is lost, i.e. when $F(\Delta_\mu)$ becomes independent of $\Delta_\mu$, and so the free energy barrier between $\Delta_\mu = 0$ and $\Delta_\mu = \pi$ vanishes. Alternatively viewed, when the domain wall changes its height by an odd number, the system acquires an average twist of $\pi$ in the $\hat{y}$ direction. Thus, restoring the symmetry of domain wall translations leads to phase angle fluctuations that destroy phase coherence transverse to the direction of the wall.

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where $\phi_{\mu} \equiv \phi_{\mu}(r_i) \equiv \theta(r_i + \hat{\mu}) - \theta(r_i) - A_{\mu}(r_i)$, $V'$ and $V''$ are the first and second derivatives of the Villain function of Eq. (4), and $(\ldots)_0$ indicates a thermodynamic average in the ensemble with fixed twist $\Delta_{\mu} = 0$. A second measure is,

$$\Delta F = F_{\text{max}} - F_{\text{min}} = F(\pi/2) - F(0) ,$$

where $F_{\text{max}}$ and $F_{\text{min}}$ are the maximum and minimum values of $F(\Delta_y)$, as $\Delta_y$ is varied at fixed $\Delta_x = 0$. Since $\Upsilon(\mu)$ is an intensive quantity, it should approach a value independent of system size as $L \to \infty$. The parameter $\Delta F$ scales as $\Upsilon(\Delta/L)^2 L^{D}$ in $D$ dimensions, and so for $D = 2$ it also becomes independent of system size as $L \to \infty$.

B. The Coulomb gas

Although our simulations are carried out in the XY variables $\theta(r_i)$, it is helpful to consider the situation from the viewpoint of the dual CG model of logarithmically interacting half integer charges. For the case of a fixed total twist $\Delta_{\mu}$, the XY Hamiltonian of Eq. (1) maps onto,

$$\mathcal{H}_{\text{CG}} = \mathcal{H}_0 + \mathcal{H}_1 .$$

$\mathcal{H}_0$ is the logarithmic interaction of the charges,

$$\mathcal{H}_0 = \frac{1}{2} (2\pi J) \sum_{i,j} q_i G(r_i - r_j) q_j ,$$

where $q_i = \pm 1/2$ are the half integer charges, neutrality is imposed, $\sum_i q_i = 0$, and $G(r)$ is the 2D periodic lattice Coulomb potential with $G(r) \sim -\ln |r|$ for large $1 \ll |r| \ll L/2$. $\mathcal{H}_1$ arises from the fixed twist boundary condition and is given by

$$\mathcal{H}_1 = V_x \left( \Delta_x - A_x^0 + \frac{2\pi p_y}{L_y} \right) + V_y \left( \Delta_y - A_y^0 + \frac{2\pi p_x}{L_x} \right) ,$$

where $V_x$ and $V_y$ are Villain functions as in Eq. (5), but with couplings $J_x = J(L_y/L_x)$ and $J_y = J(L_x/L_y)$ respectively, $p$ is the total dipole moment,

$$p = \sum_i q_i r_i ,$$

and $A_x^0 = \sum_x A_x(x, y = 0)$, $A_y^0 = \sum_y A_y(x = 0, y)$. For the gauge choice of Eq. (13) we have,

$$A_x^0 = 0, \quad A_y^0 = (L + 1)\pi/2 .$$

For the ground state as illustrated in Fig. 1a, one has $p_x = 0$, and so again it is easy to see from Eq. (12) that the total ground state energy is minimized when $\Delta_x = 0$. However, for this ground state one has $p_x = L/4$, hence the ground state energy is minimized when $\Delta_y = (L + 1)\pi/2 - \pi/2 = L\pi/2$. If the location of the domain wall was shifted by one unit in height, then the ground state would have $p_x = -L/4$, and the energy would be minimized when $\Delta_y = (L + 1)\pi/2 + \pi/2 = L\pi/2 + \pi$. For $L$ even, as we have required, these two values, modulus $2\pi$, are just equal to $0$ and $\pi$.

The helicity modulus $\Upsilon_y/J$ maps onto the inverse dielectric function $\varepsilon_x^{-1}$ of the CG. As noted by Koshunov, in order for the domain wall to move a unit lattice spacing in height, it must first form a unit step of finite width $\ell$; $\ell$ must be even to preserve charge neutrality (see Fig. 1b). We denote the left hand edge of the step as the $\text{kink}$, and the right hand edge as the $\text{antikink}$. As the kink and antikink separate out to infinity, the domain wall moves one unit in height. As shown by Halsey, a corner in a domain wall carries with it a net charge of $\pm 1/4$. The kink, consisting of two successive corners with equal $+1/4$ charge, carries a net charge of $q_{\text{kink}} = +1/2$; the antikink carries a net charge of $q_{\text{antikink}} = -1/2$. At low temperatures, the logarithmic attraction between the kink and antikink charges keeps them bound with a largest separation $\ell_{\text{max}}(T)$. At higher temperatures, entropy wins out over energy, and there is a kink-antikink unbinding transition at $T_w$, where $\ell_{\text{max}}(T_w) \to \infty$. Above $T_w$, the kink-antikink unbinding leads to diverging dipole fluctuations in the $\hat{x}$ direction, driving $\varepsilon_x^{-1}$ (and hence $\Upsilon_y$) to zero.

The problem of logarithmically interacting charges in one dimension (1D) has been treated by Bulgadaev. Koshunov has applied these results to the unbinding transition of the kink-antikink pair along the one dimensional Ising-like domain wall. To include the screening effect of charge excitations in the bulk of the system on either side of the Ising-like domain wall, we take as the coupling between kink-antikink pairs separated at large distance to be the helicity modulus of the FFXY for an arbitrary $L \times L$ system, $\Upsilon(L, L)$, in the limit of large enough $L$. Applying Bulgadaev’s exact result for the unbinding transition temperature, we conclude,

$$\frac{2\pi \Upsilon(L, L) q_{\text{kink}}^2}{T_w} = 2, \quad \text{or} \quad T_w = \frac{\pi}{4} \Upsilon(L, L) .$$

One can reproduce this result using a Kosterlitz-Thouless-like argument as follows. In analogy with Lee et al., we consider the total free energy to have a single “free” (i.e. unbound) kink in the domain wall (see Fig. 1f). Fixing the kink at a given position on the domain wall, its free energy (averaging over all other fluctuations) is that of an isolated $+1/2$ vortex in a medium with phase stiffness $\Upsilon(L, L)$; here we use Bulgadaev’s result that kink-antikink pairs in 1D do not lead to a renormalization of the kink-antikink interaction, and so any screening of their interaction is due to charge excitations in the bulk on either side of the domain wall, and so accounted for by the large $L$ value of $\Upsilon$. As $L \to \infty$, the leading contribution to this energy is $E = \pi q_{\text{kink}}^2$ in $L$. 


The entropy of the kink is just that associated with its position along the domain wall, $S = -\ln L$. Combining gives $F_{\text{kin}} = E - TS = (\pi \Upsilon / 4 - T) \ln L$, which as $L \to \infty$ gives the instability temperature for the formation of free kinks as $T_w = \pi \Upsilon / 4$, in agreement with Eq. (15).

III. NUMERICAL RESULTS

A. Helicity modulus

We now present our numerical results. At each temperature, our simulations consist of typically $10^8 - 10^9$ ordinary MC passes through the entire lattice for the largest system sizes. In Figs. 3 and 4 we plot the helicity moduli $\Upsilon_x$ and $\Upsilon_y$ vs. $T$, as computed by Eq. (8) in an ensemble with fixed twists $\Delta_x = \Delta_y = 0$. We show an “ordinary” case (no domain wall at $T = 0$) of size $64 \times 64$, which is large enough that any finite size effects are negligible for the temperatures shown. In comparison, we also show several “anomalous” cases (percolating domain wall at $T = 0$) of sizes $L \times (L + 1)$. For the ordinary case, $\Upsilon_x = \Upsilon_y$ and the bulk transition (where the $\Upsilon_\mu$ jump discontinuously to zero in the thermodynamic limit) is at $T_{KT} \simeq 0.81J$. In comparison, as $L$ increases in the anomalous case, $\Upsilon_x$ (parallel to the domain wall) in Fig. 3 approaches the value of the ordinary case, and so presumably vanishes at the same $T_{KT}$. However the curves of $\Upsilon_y$ (transverse to the domain wall) in Fig. 4 clearly decrease below that of the ordinary case, and presumably vanish in the thermodynamic limit at a lower $T_w$.

The reduction seen in $\Upsilon_y$ for the $L \times (L + 1)$ systems, as compared to the $L \times L$ system, shown in Fig. 4 is due to the kinks at the Ising-like domain wall. To explicitly see this, we can consider the helicity modulus at finite wavevector, $\Upsilon_y(k_x)$, defined as the response to a small sinusoidal perturbation in the vector potential $A_y(r_i)$. If we take,

$$A_y(r_i) \to A_y(r_i) + \sum_{k_x} \delta A_{k_x} e^{ik_x x},$$

then $\Upsilon_y(k_x)$ is defined by,

$$\Upsilon_y(k_x) = \frac{1}{L_x L_y} \frac{\partial^2 F}{\partial \delta A_{k_x} \partial \delta A_{-k_x}} \bigg|_{\delta A_{k_x} = 0}.$$ \hspace{1cm} (17)

In view of the discussion following Eq. (8), equating the application of a uniform twist $\Delta_\mu$ to the addition of a constant to the gauge field $A_\mu$, the helicity modulus $\Upsilon_y$ of Eq. (8) can also be viewed as the zero wavevector helicity $\Upsilon_y(k_x = 0)$. In the CG representation, $\Upsilon_y(k_x)$ becomes the usual formula for the wavevector dependent inverse dielectric function,

$$\Upsilon_y(k_x)/J = 1 - \frac{4\pi^2 J}{T} \frac{\langle q(k_x)q(-k_x) \rangle}{L_x L_y k_x^2},$$ \hspace{1cm} (18)

where $q(k) = \sum_i e^{ik r_i} q_i$ is the Fourier transform of the charge distribution.

Unlike $\Upsilon_y$ of Eq. (8), which measures the response to a uniform twist applied at the boundaries, $\Upsilon_y(k_x)$ measures the response to a spatially varying twist applied throughout the bulk of the system. For a homogeneous system with periodic boundary conditions, one in general expects $\Upsilon_y = \lim_{k_x \to 0} \Upsilon_y(k_x)$, since the spatially varying twist becomes uniform as $k_x \to 0$, and $\delta A_{k_x} \to \Delta_y / L_y$. For free boundary conditions however, where the phase angle $\theta(x, L_y)$ is not coupled to the phase angle $\theta(x, 0)$, this equality does not hold. For free boundary conditions, the absence of any constraint (such as in Eq. 8) relating $\theta(x, L_y)$ to $\theta(x, 0)$ means that the phase angles are free to untwist any additive constant to the gauge field, $A_y(r_i) \to A_y(r_i) + \Delta_y / L_y$, by choosing $\theta(x, y + 1) - \theta(x, y) = \Delta_y / L_y$; hence if one computes $\Upsilon_y$ by Eq. (8) in a free boundary ensemble, one necessarily has $\Upsilon_y = 0$ at any temperature. For the spatially
varying twist of Eq. (10), however, no such transformation is possible since the perturbing twist is a strictly transverse vector function, while the phase angle differences give a strictly longitudinal vector function. In this case one finds that \( \lim_{k_x \to 0} \Upsilon_y(k_x) \) has the same value, as \( L \to \infty \), that one has for the system with periodic boundary conditions.

We expect a similar effect to be true in our present case. The kink-antikink pairs confined to the one dimensional Ising-like domain wall can be viewed as a relaxation of the boundary condition. They can unwind, or soften the energy of a uniform twist \( \Delta F \) applied at the boundary, but cannot unwind a spatially varying twist \( \delta A \) applied throughout the bulk of the system. We therefore expect that, as \( L \to \infty \), \( \lim_{k_x \to 0} \Upsilon_y(k_x) \) will equal the value of \( \Upsilon_y \) obtained for an ordinary \( L \times L \) system, representing the stiffness of the bulk of the system on either side of the domain wall; \( \Upsilon_y \), however, will be a lower value including effects due to the polarization of the kink-antikink pairs localized to the domain wall.

In Fig. 4 we plot, at several different temperatures around \( T_w \), \( \Upsilon_y(k_x) \) for finite \( k_x \) for \( L \times (L + 1) \) systems with sizes \( L = 64 \) and 128. When we plot the results versus the scaled axis of \( L k_x \), we see that the data for the two different system sizes collapse to essentially a common curve, \( u(L k_x) \), at each temperature. As \( L \to \infty \), such scaling implies that \( \lim_{k_x \to 0} \Upsilon_y(k_x) \) will remain constant as \( L \to \infty \).

To explain the difference between this crossing point at \( \sim 0.60J \) and the above estimate \( T_w \sim 0.71J \), we need to examine the finite size dependence of \( \Upsilon_y(L, L + 1) \) more carefully.

To get the most accurate results, we have found it better to work in the fluctuating twist ensemble and compute the phase coherence parameter \( \Delta F \) of Eq. (9), rather than work with periodic boundary conditions and measure \( \Upsilon_y \). In Fig. 7 we plot our results for \( \Delta F \) versus system size \( 1/L \), for various temperatures \( T \) above and below \( T_w \). We use \( L \times (L + 1) \) systems with \( L \) ranging from 32 up to 512. We note that at low \( T \), the behavior of \( \Delta F \) is non-monotonic; as \( L \) increases, the system first softens with a decreasing \( \Delta F \), but then stiffens again as \( \Delta F \) reaches a minimum and then increases. We denote the system size at this minimum by \( \xi_k \). Since the system becomes stiffer on length scales \( L > \xi_k \), we assume that \( \xi_k \) determines the size of the largest kink-antikink pairs on the domain wall. At higher \( T \), the minimum in \( \Delta F \) disappears, and \( \Delta F \) continues to decrease as \( L \)

This confirms the following conclusion. As \( L \to \infty \) in an \( L \times (L + 1) \) system, the finite wavevector helicity \( \Upsilon_y(k_x) \) is equal to the corresponding helicity modulus of an ordinary \( L \times L \) system for all finite values of \( k_x \); this measures the stiffness of the bulk of the system on either side of the Ising domain wall, and is unaffected by the kinks on the wall. However the zero wavevector response \( \Upsilon_y \) to a uniform twist \( \Delta y \), shown in Fig. 4 is softened, and above \( \Upsilon_y \) reduced to zero, by the polarization of the kinks on the domain wall.

### B. Finite size dependence

Returning to Fig. 4, we have indicated the kink-antikink unbinding transition temperature \( T_w \), as predicted in Eq. (9), by the intersection of the line \( 4T/\pi J \) with the helicity modulus of the ordinary \( L \times L \) system. This gives an estimate of \( T_w \simeq 0.71J \). This value occurs noticeably above the point where many of the curves \( \Upsilon_y(L, L + 1) \) appear to cross. Such a crossing point, if remaining constant as \( L \) increases, is generally taken as an estimate for the phase transition in a 2D XY system.

Returning to Fig. 5 we plot, at several different temperatures \( T \) for system sizes \( L \times (L + 1) \), with \( L = 64 \) (solid symbols), and \( L = 128 \) (open symbols). The data for the different \( L \) collapse to a common curve at each \( T \).
increases. The temperature that separates the two behaviors is somewhere between $0.68J$ and $0.74J$, in good agreement with the result $T_w \approx 0.71J$ from Fig. 4, based on the theoretical prediction of Eq. (15).

As a further check on our results, we have also directly simulated a 1D neutral system of logarithmically interacting charges $q_k = \pm 1/2$. The 1D interaction potential is taken as the 2D $L \times L$ lattice Coulomb potential, as in Eq. (14), but with height separation fixed at $y = 0$.

We use an interaction coupling constant of $2\pi \Upsilon_y(L, L)$, with $\Upsilon_y(L, L)$ obtained from our simulations of the ordinary $L \times L$ 2D FFXY for $L = 64$, in order to model as closely as possible the interaction between kinks on the domain wall in the true $L \times (L + 1)$ FFXY system. Within this 1D simulation we measure the normalized histogram of the total dipole moment, $P(p_x)$, and use it to construct what would be the free energy $F(\Delta_y)$ of the corresponding $L \times (L + 1)$ 2D FFXY system,

$$F(\Delta_y) = -T \ln \left[ \sum_{p_x} P(p_x) e^{-V_y(\Delta_y - \Delta_y^0 - \frac{2\pi y}{L})}/T \right] + \text{const.}$$

where $V_y$ is the Villain function as in Eq. (12), and “const.” is a constant term independent of $\Delta_y$.

In Fig. 8 we plot the resulting $\Delta F = F(\pi/2) - F(0)$ versus $1/L$ for the same temperatures and sizes $L$ as in Fig. 7. The agreement between Figs. 7 and 8 is not exact, since the coupling between kinks is only equal to $2\pi \Upsilon_y(L, L)$ on large length scales; the true screening of the kink interaction due to charge excitations in the bulk on either side of the domain wall is length scale dependent. Moreover, the domain wall in the 2D FFXY model is not a strictly straight one dimensional line; the roughness of the domain wall (see following section) means that height fluctuations can add to the distance of separation between kinks. Nevertheless, the agreement is qualitatively very good, indicating again that it is the polarization of kink-antikink pairs along the Ising domain wall that is responsible for the decrease in the phase stiffness transverse to the domain wall.

One evident feature of both Figs. 7 and 8 is the very large finite size effect. The asymptotic behavior of $\Delta F$ only sets in at quite large length scales. Equivalently, the correlation length of the kink-antikink pairs, $\xi_k$, grows large well below $T_w \approx 0.71J$. Fitting the data of Fig. 7 to a quadratic in $\ln L$, and determining $\xi_k$ from the minima of these fitted curves, we plot the resulting $\xi_k$ versus $T$ in Fig. 8. The rapidly growing $\xi_k$ means that it is difficult to get a very precise estimate of $T_w$ directly from the data of Fig. 4, without going to prohibitively large system sizes $L \gg 512$. We believe that this is also the reason that Lee et al. report a lower value of $T/J = 2\pi(0.09 \pm 0.01) = 0.57 \pm 0.06$ for the “roughening transition” temperature in their dual 2D Coulomb gas. Lee et al.’s simulations are on a lattice of size $L = 64$. From Fig. 4 we see that $\xi_k \sim 32$ at $T/J \sim 0.58$, hence kinks already look unbound above this temperature for such a small system size. The large values of $\xi_k$ can also be compared to other length scales in the system. The correlation length of the Ising-like order parameter, $\xi_I$, gives the typical size of an Ising-like domain excitation in an ordinary $L \times L$ FFXY model. From Ref. 4 (see Fig. 15) we find that $\xi_I$ is quite small below $T_w \approx 0.71J$; in particular $\xi_I < 2.5$ for $T < 0.77J$. Thus we expect that kink-antikink pairs on the domain wall enclosing a typical thermally excited Ising-like domain are always effectively unbound. The energetics of kink-antikink unbinding will only effect the morphology of domains that are much larger than those due to typical thermal excitations.

![FIG. 7: $\Delta F$ of Eq. (19) vs. $1/L$ at various temperatures for the 2D FFXY model of size $L \times (L + 1)$.](image)

![FIG. 8: $\Delta F$ of Eq. (19) vs. $1/L$ at various temperatures for as estimated from the dipole histogram of a 1D interacting kink model (see text).](image)
from the data of Fig. 7. To verify this we have explicitly measured the domain wall width squared, \( W^2 \), vs. \( T \), finite energy, and should roughen the domain wall at any finite temperature. To avoid problems with periodic boundary conditions, we always measure the domain wall height as relative to some initial starting position. In Fig. 10 we plot \( W^2 \) vs. \( T/J \) for various temperatures. The linear growth in \( W^2 \) as \( L \) increases indicates that the domain wall is rough for all temperatures shown, including \( T < T_w \). The domain wall diffusion constant, \( dW^2/dL \), shows no observable singularity at \( T_w \approx 0.71J \) (see inset to Fig. 11).

### IV. Discussion

Our numerical results demonstrate the existence of the unbinding transition for kink-antikink pairs along the domain wall of Ising-like excitations in the 2D FFFXY model, and that the behavior of this transition is in good agreement with the theoretical predictions of Korshunov. We show that domain walls are rough at all temperatures, and therefore argue that the “roughening transition” claimed by Lee and co-workers is really the kink-antikink unbinding transition. We show that the effects of kink-antikink pairs are not readily apparent for Ising-like domains such as are typically present due to thermal excitation; because of the large length \( \xi_k \), such effects are important only for much larger domains.

One of Korshunov’s main motivations for investigating the kink-antikink unbinding transition was to argue that such a transition necessarily implies the existence of two separate bulk transitions, \( T_{KT} < T_I \). We now present our own thoughts on this issue. In the original paper by Teitel and Jayaprakash, two possibilities were considered, \( T_{KT} < T_I \) and \( T_{KT} = T_I \). In discussing the first case, Teitel and Jayaprakash presented the following scenario. In terms of the dual CG model, the helicity modulus \( \Upsilon \) gets reduced from its \( T = 0 \) value by fluctuations that produce dipole moments. If Ising domains of typical size \( \xi_I \) carried a total dipole moment proportional to their size, they would drive \( \Upsilon \rightarrow 0 \) continuously due to the diverging \( \xi_I \) as \( T \rightarrow T_I \) from below. However, in addition to these domain excitations, there are also pair excitations. The original Kosterlitz-Thouless instability criteria would imply that pairs unbind once \( \Upsilon \) falls below the critical value \( \Upsilon(T) = 2T/\pi \), which must happen at some \( T_{KT} \) below \( T_I \). However, if one computes domain energies at \( T = 0 \) (and presumably the same holds for domain free energies at low \( T \)), one finds that it is only the domains with vanishing total dipole moment that have energies which scale with the perimeter; i.e. the only domains which are “Ising-like” are those which carry no dipole moment and so cannot give any reduction in \( \Upsilon \! \). Fortunately, once \( T \) increases above \( T_w \), kink-antikink pairs on the boundary of the domain are free to unbind, and the Ising domains can now acquire large dipole moments at no cost in free energy. The scenario of Teitel and Jayaprakash is now restored. This conclusion is in complete agreement with the numerical work of Olsson, who finds two distinct transitions at \( T_{KT} < T_I \), and argues that the non Ising-like critical behavior claimed by some at \( T_I \) is in fact an artifact of finite size effects.

The kink-antikink unbinding transition may also have
implications for the non-equilibrium steady state behavior of the system when the vortices are driven by a uniform force, such as is the case for a fully frustrated Josephson junction array in an applied uniform d.c. current $I$. Since $I$ couples linearly to the total dipole moment of a domain $p$, the force can lead to an instability in domain growth provided the free energy of exciting the domain scales less than linearly with $p$. For $T < T_w$, the binding of kinks to antikinks prevents large dipole moments from building up on domains. The Ising-like domains, whose free energy scales like the domain length $\ell$, are only those domains whose total dipole moment vanishes, and hence these domains remain stable, and the Ising-like order should persist at small drives. For $T > T_w$, kink-antikink pairs can unbind, resulting in domains whose dipole moment may scale at least proportional to their length $\ell$. In this case, when the current exceeds an amount proportional to the Ising domain surface tension, domains will become unstable to growth and the Ising-like order will be destroyed.

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