Phase diagram of generalized fully frustrated XY model in two dimensions

Petter Minnhagen,¹ Beom Jun Kim,² Sebastian Bernhardsson,¹ and Gerardo Cristofano³

¹Dept. of Physics, Umeå University, 901 87 Umeå, Sweden
²Dept. of Physics, BK21 Physics Research Division and Institute of Basic Science, Sungkyunkwan Univ., Suwon 440-746, Korea
³Dipartimento di Scienze Fisiche, Università di Napoli “Federico II” and INFN, Sezione di Napoli, Via Cintia, Compl. universitario M. Sant’Angelo, 80126 Napoli, Italy

It is shown that the phase diagram of the two-dimensional generalized fully-frustrated XY model on a square lattice contains a crossing of the chirality transition and the Kosterlitz-Thouless (KT) transition, as well as a stable phase characterized by a finite helicity modulus $\Upsilon$ and an unbroken chirality symmetry. The crossing point itself is consistent with a critical point without any jump in $\Upsilon$, with the size ($L$) scaling $\Upsilon \sim L^{-0.63}$ and the critical index $\nu \approx 0.77$. The KT transition line remains continuous beyond the crossing but eventually turns into a first-order line. The results are established using Monte-Carlo simulations of the staggered magnetization, helicity modulus, and the fourth-order helicity modulus.

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I. INTRODUCTION

The phase transitions of the two-dimensional (2D) fully-frustrated XY (FFXY) model on a square lattice has been a subject of controversy. The emerging consensus is that the model, as the temperature is lowered, first undergoes an Ising-like transition associated with the chirality. At a slightly lower temperature it undergoes a universal jump Kosterlitz-Thouless (KT) transition associated with the phase angles. Since the two transitions are extremely close to each other in temperature the question whether there is only one merged transition associated with the phase angles. An argument for two separate transitions with the KT transition always at a lower temperature than the chirality transition was given by Korshunov in Ref. 5 in terms of a kink-antikink instability of the domain walls separating domains with different chirality. The 2D generalized fully frustrated XY (GFFXY) model has the same degrees of freedom and the same symmetries as the FFXY model. The argument by Korshunov is quite general and appears to hinge only on the combined $U(1)$ and $Z_2$ symmetry of the model and the existence of Ising-like domain walls associated with the broken $Z_2$ symmetry. This strongly suggests that also the generalized model with the very same degrees of freedom and symmetry should always have a KT transition at a lower temperature than the chirality transition. As shown here, this is not the case: The two transitions can merge in a single critical point. The reason for this unexpected result is that the symmetry of the model allows for a new phase 2D “quasi” phase-order.

The present paper is organized as follows: In Sec. II we introduce the generalized fully-frustrated XY model. The results of our numerical simulations are presented in Sec. III for the staggered magnetization, in Sec. IV for the helicity modulus, and in Sec. V for the fourth-order modulus, respectively. Finally, Sec. VI is devoted to the summary of the paper.

II. THE GENERALIZED FFXY MODEL

The XY model on a square lattice in the presence of an external magnetic field transversal to the lattice plane is described by the action:

$$H = -\frac{J}{k_B T} \sum_{(ij)} \cos(\phi_{ij} \equiv \theta_i - \theta_j - A_{ij}) ,$$

where $\theta_i$ is the phase variable at the $i$th site, the sum is over nearest neighbors, $J(>0)$ is the coupling constant, $T$ is the temperature, $k_B$ is the Boltzmann constant, and $A_{ij} = (2e/\hbar c) \int^f A \cdot dl$ is the line integral along the bond between adjacent sites $i$ and $j$. We consider the case where the bond variables $A_{ij}$ are fixed, uniformly quenched, out of equilibrium with the site variables and satisfy the condition $\sum_p A_{ij} = 2\pi f$; here the sum is over each set of bonds of an elementary plaquette and $f$ is the strength of frustration. We assume that the local magnetic field in Eq. (1) is equal to the uniform applied field; such an approximation is more valid the smaller is the sample size $L$ compared with the transverse penetration depth $\lambda_\perp$. In the case of full frustration, i.e., $f = 1/2$, of interest to us here, such a model has a continuous $U(1)$ symmetry associated with the rotation of spins and an extra discrete $Z_2$ symmetry, as it has been shown by analyzing the degeneracy of the ground state. Choosing the Landau gauge, such that vector potential vanishes on all horizontal bonds and on alternating vertical bonds, we get a lattice where each plaquette displays one antiferromagnetic and three ferromagnetic bonds. Such a choice corresponds to switching the sign of the interaction.

The generalized FFXY model is obtained by changing the form of the interaction from $-J \cos \phi$ to $U(\phi)$,

$$U(\phi) = \frac{2J}{p^2} \left[1 - \cos^2 p^2 (\phi/2) \right].$$

This does not alter any symmetry present in the original FFXY model which corresponds to $p = 1$ since $2[1 -$
the helicity modulus $\Upsilon$, which relates to the continuous chirality symmetry, are used to detect phase boundaries. The phase diagram contains all four possible combinations of these two, i.e., $(\Upsilon, m) = (0, 0), (0, \neq 0), (\neq 0, 0), (\neq 0, \neq 0)$. The dashed horizontal line at $p = 1$ corresponds to the usual FFXY model, for which the phase $(\Upsilon \neq 0, m = 0)$ is not realized.

### III. STAGGERED MAGNETIZATION

We first present numerical MC results of the staggered magnetization $m$, defined as:

$$m = \left\langle \frac{1}{L^2} \sum_{l=1}^{L^2} (-1)^{x_l+y_l} s_l \right\rangle,$$

where $\langle \cdots \rangle$ is the ensemble average and the vorticity for the $l$th elementary plaquette at $(x_l, y_l)$ is computed from $s_l \equiv (1/\pi) \sum_{(ij)\in l} \phi_{ij} = \pm 1$ with the sum taken in the anti-clockwise around the given plaquette.

The ground states with the spontaneously broken chirality symmetry correspond to the two possible checker board patterns with alternating positive and negative vorticity. The energy per link in these ground states is given by $U(\pi/4)$ which corresponds to all links contributing the same energy. Since the two ground states with different checker board patterns are separated by an infinite energy barrier in the thermodynamic limit, the phase with the broken chirality symmetry persists at low enough temperatures as long as the pattern, where all links contribute the same energy, indeed corresponds to the ground state. However, this ceases to be true when $p$ becomes larger than $p_c$. In this new region the ground state instead corresponds to a pattern consisting of plaquettes with phase difference 0 on three sides and $\pi$ on the remaining. The energy per link is hence instead $U(\pi)/4$. The critical value $p_c$ is easily computed to be $p_c \approx 1.3479$ from the condition that $U(\pi/4) = U(\pi)/4$. Consequently, the new ground state at $p > p_c$ has no broken chirality symmetry and hence corresponds to $m = 0$.

Figure 2(a) illustrates the vanishing of the staggered magnetization $m$ at $p \approx p_c$ for $T = 0.1$ (the temperature is in units of $J/k_B$ throughout the present work). This horizontal part of the $m$-phase boundary eventually bends down toward smaller $p$ as $T$ is increased. This
part of the m-phase boundary we have traced out by the standard size scaling of Binder’s cumulant $B_m$ for the order parameter $m$ as displayed in Fig. 2(b) for $p = 1$. $T_{ch}$ ≈ 0.452 is obtained, in a good agreement with the earlier value 0.452 in Ref. 4. The complete m-phase line with marked data points are shown in Fig. 4.

IV. HELICITY MODULUS

The quasi 2D phase ordering is measured by the helicity modulus $\Upsilon$ defined as the stiffness in response to the twist $\delta$ of the phase variables across the system: $\Upsilon \equiv (\partial^2 F/\partial \delta^2)_{\beta = 0}$ where $F$ is the free energy. The condition for a KT transition is characterized by the universal jump in the helicity modulus, $\Upsilon(T_{KT})/T_{KT} = 2/(\pi L)$. Thus a KT transition can be located by the crossing point between the line $y = (2/\pi)T$ and the helicity modulus curve $y = \Upsilon(T)$ as illustrated for $p = 1$ in Fig. 3(a).

In practice, a precise determination requires the difficult task of extrapolating to $L = \infty$. Here we use the following method: The values of the $T_{KT}$ at the crossing point with the line $y = (2/\pi)T$ are determined as a function of size $L$. These values are well approximated by a second order polynomial as shown in Fig. 2(b). The extrapolation to $L = \infty$ gives $T_{KT} = 0.447$, which is very close to the value 0.446 obtained in Ref. 4. The close agreement shows that the method gives a good estimate of the KT transition temperature. The data points in Fig. 1 for $p \leq 1.32$ are obtained by this method. One notes that the m-phase line and the KT-line are extremely close for these p-values and only the smaller p-values, like $p = 0.5$, display a clear separation within our accuracy.

The determination of the KT-line rests on the assumption that the KT-jump has the universal value $2/\pi$. A jump means that the crossing point between the $\Upsilon(T)$ and $b(2/\pi)T$ should give the same $T_{KT}(L = \infty)$ for all $b \leq 1$. Figure 4(c) shows the difference $\Delta T(b,L) = T_{KT}(b,L) - T_{KT}(b/2,L)$ for $b = 1$. Our result is consistent with a universal jump KT transition, since $\Delta T(b = 1,L)$ is consistent with a vanishing for $L = \infty$. On the other hand the jumps size is inconsistent with a double jump since $\Delta T(b = 2,L)$ approaches a finite value. For larger values of $p > p_c$, like $p = 1.5$, the jump is, on the other hand, consistent with a jump larger than the universal jump as illustrated in Fig. 4(d): For this value $\Delta T(b = 2,L)$ is consistent with a vanishing, suggesting that the jump at the KT transition could be larger than the universal KT value. The transition at $p = 1.5$ shows no sign of any first order character from which we conclude that it is continuous. In this case the jump is expected to have the universal value. Our data neither support nor rule out this expectation. Conversely, a continuous KT transition with a nonuniversal jump can neither be ruled out. However, when $p$ is increased further the transition does eventually become first order as can be detected from the double well structure in the energy histogram. For the first order transition the jump should be nonuniversal and larger than the universal jump. In the limit of $p = \infty$ the model reduces to the infinite state Potts model which is known to have a first order transition.

V. FOURTH-ORDER MODULUS

According to the argument given by Korshunov the KT transition always occurs at a lower temperature than the chirality transition. This is consistent with the result we find for p-values below the horizontal line in the phase diagram. In this part of the phase diagram the argument by Korshunov is valid and the chirality transition and the KT transitions are separated with the KT transition always at a lower temperature. On the other hand, when the horizontal phase line meets and crosses the KT line, Korshunov’s argument is no longer valid and one expects a merged character of the transition. The argument by Korshunov fails because it presumes the existence of Ising-like domain walls and such walls do not exist above the horizontal line. In order to monitor the change of character of the transition we study the fourth-
As pictures constitute the characteristics of a KT transition the minimum position towards lower temperature (vertical broken line) with increasing $L$. The size of the minimum extrapolates to a finite value. (a) and (b) show that this typical KT-feature remains intact as $p$ is increased to the vicinity of $p_c$. (c) and (d) show that this KT-feature is dramatically changed in the immediate vicinity of $p_c$, while (e) and (f) show that the KT-feature is recovered for $p$-values above $p_c$.

The shift of the minimum position towards lower temperatures constitutes the characteristics of a KT transition and is well established up to $p = 1.31$ [see Fig. 4(b)]. As $p$ is increased through the crossing region around $p_c \approx 1.3479$ there are dramatic changes but for larger $p$ the typical KT behavior of $\Upsilon_4$ reappears [see Fig. 4(e)]. This is consistent with a crossing where a KT transition disappears and reappears as $p$ is increased. The characteristics close to $p_c \approx 1.3479$ is instead consistent with $\Upsilon_4 = 0$ as $L \to \infty$ [see Fig. 4(c) and (d)].

If $\Upsilon_4 = 0$ then the helicity modulus $\Upsilon$ does not need to have a jump at the transition, which opens up the possibility of a continuous vanishing of $\Upsilon$ and the critical scaling $\Upsilon \sim L^{-\alpha}$. Figure 5(a) shows that such a size scaling is indeed obtained close to $p_c \approx 1.3479$. Furthermore, Fig. 6(b) shows that the standard critical scaling form for a continuous phase transition $\Upsilon = L^{-\alpha}F[L^{1/\nu}(T - T_c)]$ is also valid to very good approximation which suggests that the correlation length $\xi$ diverges as $\xi \sim |T - T_c|^{-\nu}$. The values obtained for the critical indices are $\alpha \approx 0.63$ and $\nu \approx 0.77$.

VI. SUMMARY

The main result of the present work is that in general a model with the same symmetry and degrees of freedom as the 2D fully frustrated XY model can have four stable phases. Only three of these phases are present in
the usual FFXY model. The new phase allowed by symmetry combines unbroken chirality with quasi 2D phase ordering. The existence of this phase also means that the KT and chirality phase lines cross. The crossing point is a critical point at which the helicity modulus obeys scaling and vanishes smoothly without a universal jump.

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