Transitions and crossover phenomena in fully frustrated XY systems

Martin Hasenbusch, Andrea Pelissetto, and Ettore Vicari

1 Dip. Fisica dell’Università di Pisa and INFN, Largo Pontecorvo 2, I-56127 Pisa, Italy
2 Dip. Fisica dell’Università di Roma “La Sapienza” and INFN, P.le Moro 2, I-00185 Roma, Italy
(March 23, 2022)

Abstract

We study the two-dimensional fully frustrated XY (FFXY) model and two related models, a discretization of the Landau-Ginzburg-Wilson Hamiltonian for the critical modes of the FFXY model and a coupled Ising-XY model, by means of Monte Carlo simulations on square lattices $L^2$, $L \lesssim 10^3$. We show that their phase diagram is characterized by two very close chiral and spin transitions, at $T_{ch} > T_{sp}$ respectively, of the Ising and Kosterlitz-Thouless type. At $T_{ch}$ the Ising regime sets in only after a preasymptotic regime, which appears universal to some extent. The approach is nonmonotonic for most observables, with a wide region controlled by an effective exponent $\nu_{eff} \approx 0.8$.

PACS Numbers: 74.81.Fa, 64.60.-i, 64.60.Fr, 75.10.Hk
The nature of the phase transitions in frustrated systems is of great interest in statistical physics. The two-dimensional fully frustrated XY (FFXY) model [1] is defined by the Hamiltonian

$$\mathcal{H}_{\text{FFXY}} = -J \sum_{\langle xy \rangle} \cos(\theta_x - \theta_y + A_{xy}),$$

(1)

where the sum is over all nearest-neighbor pairs of a square or triangular lattice, and $A_{xy}$ satisfy the constraint $\sum A_{xy} = \pi$ around any plaquette. It is experimentally relevant for Josephson-junction arrays in a magnetic field [2]. The angle variable $\theta_x$ corresponds to the phase of the superconducting order parameter on each superconducting grain, and $A_{xy}$ is the vector potential of a perpendicular magnetic field corresponding to half a flux quantum per plaquette.

The ground state of the FFXY model presents an enlarged $O(2) \otimes \mathbb{Z}_2$ degeneracy. The additional $\mathbb{Z}_2$ degeneracy is related to the breaking of the chiral symmetry [1]. For each plaquette $\Pi$ we define the chirality

$$C_n \equiv \sum_{\langle xy \rangle \in \Pi} \sin(\theta_x - \theta_y + A_{xy}),$$

(2)

where $n$ is the dual-lattice site at the center of $\Pi$. On the square lattice the staggered magnetization $M_C \equiv \sum_n (-1)^{n_1 + n_2} C_n / V$ defines an order parameter, which competes with the spin modes to determine the phase diagram of the FFXY model. The critical behavior has been much investigated during the last few decades (see, e.g., [3–21]) using Monte Carlo (MC) simulations, real-space renormalization-group (RG) techniques, field-theoretical methods, etc. Moreover, several related models have also been considered: for instance the fractional-charge Coulomb gas, coupled Ising-XY models, coupled XY models.

In spite of all this work, the phase diagram and critical behavior of the FFXY model are still rather controversial. Most recent MC simulations favor the existence of two very close transitions [7,8,10,12,13,15,16,19]. The most likely interpretation is that the higher-temperature transition is characterized by the onset of chiral long-range order, while spins remain disordered. The lower-temperature transition is associated with the breaking of the continuous symmetry and is followed by a low-temperature phase in which spin quasi-long-range order coexists with chiral long-range order. The chiral transition is expected to be in the Ising universality class, due to the scalar nature of the chiral order parameter. The second one should be a Kosterlitz-Thouless (KT) transition. This scenario is also supported by arguments based on a kink-antikink unbinding picture [17,21]. The Ising nature of the chiral transition has not been satisfactorily supported by numerical simulations so far. Most MC simulations [4–9,11,12,14,15,19,20] have found that the behavior of the chiral modes—both in the FFXY and in related models—is not consistent with an Ising transition. For example, most finite-size scaling (FSS) analyses have obtained $\nu \approx 0.8$, instead of the Ising value $\nu = 1$. There are several possible explanations. One possibility is that, even if the chiral order parameter is a scalar, the chiral transition belongs to a universality class that is not the Ising one. After all, the estimate $\nu \approx 0.8$ appears to be somewhat universal, the same value being obtained in several different models. A second one is that the Ising regime sets in only on large lattices [10]: the observed behavior is only an intermediate crossover. A
third possibility is that the apparent two transitions are a finite-size effect. On the contrary, spin and chirality order at the same temperature. In this case the critical spin and chiral modes couple at criticality and give rise to a qualitatively new critical behavior, in which chiral modes do not behave as spins in the Ising model.

In this paper we consider the square-lattice FFXY model (implemented by alternating vertical lines with ferromagnetic and antiferromagnetic couplings) and two related lattice models. The first one is a $\phi^4$ model defined by the Hamiltonian

$$H_\phi = -J \sum_{(xy),i} \phi_{i,x} \cdot \phi_{i,y} + \sum_{i,x} \left[ \phi_{i,x}^2 + U (\phi_{i,x}^2 - 1)^2 \right] + 2 (U + D) \sum_x \phi_{1,x}^2 \phi_{2,x}^2,$$

where $\phi_{1,x}, \phi_{2,x}$ are real two-component variables defined on the sites $x$ of a square lattice, $\phi_i^2 \equiv \phi_i \cdot \phi_i$, and $J, U, D > 0$. Hamiltonian $H_\phi$ is expected to describe the critical modes of the FFXY model. It corresponds to a straightforward lattice discretization of the Landau-Ginzburg-Wilson theory obtained by applying a Hubbard-Stratonovich transformation to the FFXY model, see, e.g., Ref. [5]. Here we set $U = 1$; all results reported below refer to this case. The symmetry $\phi_1 \leftrightarrow \phi_2$ is the analogue of the $\mathbb{Z}_2$ chiral symmetry of the FFXY model. The chiral order parameter is

$$C_x = \phi_{1,x}^2 - \phi_{2,x}^2.$$

When $D = 0$ model (3) becomes O(4) symmetric; it does not have any transition at finite temperature, but its correlation length diverges exponentially for $J \to \infty$, see, e.g., Ref. [22]. We also consider the coupled Ising-XY (IsXY) model [4]

$$H_{\text{IsXY}} = - \sum_{(xy)} \left[ \frac{J}{2} (1 + \sigma_x \sigma_y) s_x \cdot s_y + C \sigma_x \sigma_y \right],$$

3
where $s_x = \pm 1$, and the two-component spins $s_x$ satisfy $s_x \cdot s_x = 1$. Here $s_x$ and $\sigma_x$ correspond to spin and chiral variables, respectively. Note that, by taking the limit $U \to \infty$ and then $D \to \infty$ in model (3), one recovers the IsXY model for $C = 0$.

We performed MC simulations on $L \times L$ lattices with periodic boundary conditions, and sizes up to $L = O(10^4)$. We used mixtures of Metropolis and overrelaxation updating algorithms, as proposed in Ref. [23]. In this paper we present the main results; details will be reported elsewhere. We find two very close Ising and KT transitions in the FFXY model, and in the $\phi^4$ and IsXY models for extended ranges of the parameters $D > 0$ and $C$. No evidences of unique continuous transitions are found. For sufficiently large $D$ and $-C$, i.e. $D \gtrsim 50$ and $C \lesssim -5$, we find instead a single first-order transition. The phase diagrams of the $\phi^4$ and IsXY models are shown in Fig. 1 [24]. Little is known about the region where the two continuous transition lines turn into a single first-order one. Another interesting feature emerges from our numerical results: the asymptotic critical behavior at the chiral transition is observed only after a peculiar nonmonotonic crossover regime, which appears universal to some extent.

In the FFXY model the square lattice can be divided into four sublattices, so that the four sites of every plaquette belong to different sublattices. The ground state is translation invariant within these sublattices. We define the spin correlation function $G_s(x)$ as the correlation between two spins in the same $L/2 \times L/2$ sublattice. Then we consider the staggered chirality correlation function $G_c(x)$. In the $\phi^4$ model the spin and chiral correlation functions are defined by $G_s(x) \equiv \langle \sum_i \phi_{i,0} \cdot \phi_{i,x} \rangle$ and $G_c(x) = \langle C_0 C_x \rangle_c$. In the IsXY model we have $G_s(x) \equiv \langle s_0 \cdot s_x \rangle$ and $G_c(x) = \langle \sigma_0 \sigma_x \rangle_c$. From $G_s$ and $G_c$ we define the susceptibilities $\chi_s$ and $\chi_c$, and second-moment correlation lengths $\xi_s$ and $\xi_c$. We also consider $R_s \equiv \xi_s/L$, $R_c \equiv \xi_c/L$, the spin and chiral Binder parameters $B_s$ and $B_c$, and the helicity modulus $\Upsilon$.

We first show that the low-temperature phase of these models is characterized by the breaking of the $\mathbb{Z}_2$ chiral symmetry and by a spin quasi-long-range order analogous to the one of the standard XY model. Indeed, chiral modes are magnetized and, in the large-$L$ limit, the exponent $\eta$ (computed using $\chi_s \sim L^{2-\eta}$), $R_s \equiv \xi_s/L$, and $\Upsilon$ satisfy the universal relations that hold among the corresponding quantities in the low-temperature phase of the XY model on a $L \times L$ square lattice with periodic boundary conditions. For example [25,26]

$$\Upsilon(\eta) = \frac{1}{2\pi \eta} - \frac{2}{\eta^2} \sum_{n=-\infty}^{\infty} n^2 \exp(-\pi n^2/\eta)$$

for $0 < \eta \leq 1/4$. As shown by the results of Table I, the agreement is very good and provides a conclusive evidence that the low-temperature phase of the FFXY and related models is

| model     | $J$  | $\eta$            | $\eta$ from $R_s$ | $\eta$ from $\Upsilon$ |
|-----------|-----|-------------------|-------------------|------------------------|
| FFXY      | 2.4 | 0.1480(5)         | 0.1479(4)         | 0.1477(11)             |
|           | 2.3 | 0.1750(5)         | 0.1752(4)         | 0.1758(3)              |
|           | 2.26| 0.2023(11)        | 0.2015(7)         | 0.2021(5)              |
| $\phi$, $D = 1/2$ | 1.50 | 0.1341(6)        | 0.1346(4)         | 0.13425(12)            |
|           | 1.48 | 0.1675(16)       | 0.1672(10)        | 0.1670(4)              |
| $\phi$, $D = 99$ | 1.6005 | 0.120(3)        | 0.1214(6)         | 0.1202(5)              |
| IsXY, $C = 0$ | 1.52 | 0.1817(7)        | 0.1821(4)         | 0.18190(13)            |
controlled by the same line of Gaussian fixed points that is relevant for the XY model.

To determine the number of transitions, we perform a FSS analysis using the method proposed in Ref. [27], see also [28]. Instead of computing the various quantities at fixed Hamiltonian parameters, we compute them at a fixed value of a chiral—this guarantees that we are observing the chiral transition—RG invariant quantity; in our specific case we choose $R_c \equiv \xi_c / L$. This method has the advantage of not requiring a precise estimate of the critical temperature. We fix $R_c = R_{Is}$ where $R_{Is} = 0.905048...$ is the corresponding Ising value [29].

Note that such a choice does not represent a bias in favor of an Ising transition. $R_c$ can be fixed to any value $R_{c, \text{fix}}$; the conclusions are independent of $R_{c, \text{fix}}$. If the transition is unique, also the spin correlation length $\xi_s$ diverges, and thus $R_s \equiv \xi_s / L$ at fixed $R_c$ is expected to converge to a nonzero value. If there are two transitions and $T_{ch} > T_{sp}$, $\xi_s$ remains finite, so that $R_s \sim 1/L$ for $L \to \infty$. Results for $R_s$ are shown in Fig. 2. They appear to decrease with increasing $L$, without showing any hint at a convergence to a nonzero value. This shows that the spin correlation length $\xi_s^{(c)}$ at the chiral transition is finite, though quite large. For example, for $L \to \infty$ we have $\xi_s^{(c)} = 118(1)$ for the FFXY model, $\xi_s^{(c)} \gtrsim 400$ for the $\phi^4$ model with $D = 1/2$, $\xi_s^{(c)} = 52.7(4)$ for the IsXY model at $C = 0$. Additional evidence is provided by the helicity modulus. At the chiral transition, it appears to vanish in the large-$L$ limit, consistently with the fact that spin variables are disordered.

As a consequence of the large value of $\xi_s^{(c)}$, the eventual Ising regime at the chiral transition may set in only when $L \gg \xi_s^{(c)}$ [10]. This fact is substantially confirmed by our FSS analysis. For instance, if, for any invariant quantity $S$, we define an effective exponent $\nu_{\text{eff}}(L)$ as

$$
1/\nu_{\text{eff}}(L) = (\ln dS/dJ|_{2L} - \ln dS/dJ|_L) / \ln 2,
$$

we find that $\nu_{\text{eff}}(L)$ shows first a plateau at $\nu_{\text{eff}}(L) \approx 0.8$—this is consistent with previous works on small lattices—and only for $L \gtrsim \xi_s^{(c)}$ appears to approach the Ising value. Similar crossover effects are observed in other quantities. For example, the chiral Binder parameter $B_c$ is systematically higher than the Ising value [29] $B_{Is} = 1.167923(5)$. However, as $L$ increases, $B_c$ starts to decrease and, if $L$ is large enough, its behavior is compatible with the
expected one \[30\], $B_c = B_{Is} + aL^{n_{Is}-2} = B_{Is} + aL^{-7/4}$, see, e.g., Fig. 3. This confirms the Ising nature of the chiral transition.

The spin transition, whenever continuous, is expected to be a KT one. We verify that at the KT transition $R_s$ and $\Upsilon$ behave as expected, for example \[25\]

$$\Upsilon = 0.63650817819 + \frac{0.318899454...}{\ln L} + \ldots$$

In most cases, including the FFXY model, the chiral and the spin transitions are very close. If $\delta \equiv (J_{sp} - J_{ch})/J_{ch}$, $J_{sp}$ and $J_{ch}$ being the location of the two transitions, we find $\delta = 0.0159(2)$ for the FFXY model [$J_{ch} = 2.2063(1)$ and $J_{sp} = 2.2415(5)$], $\delta = 0.0025(2)$ in the $\phi^4$ model for $D = 1/2$, $\delta = 0.0167(7)$ in the IsXY model for $C = 0$.

Our FSS analysis definitely shows that the chiral transition, when it is continuous, belongs to the Ising universality class. However, the Ising critical regime is reached only after a crossover region in which effective exponents and RG invariant quantities show a behavior that is surprisingly similar in the FFXY model, in the $\phi^4$ model with $0 \lesssim D \lesssim 2$, and in the IsXY model for $-0.5 \lesssim C \lesssim 0.2$. Fig. 4 shows the FSS curves of $R_s \equiv \xi_s/L$ at fixed $R_c \equiv \xi_c/L$ plotted versus a rescaled lattice size $L_r \equiv L/l$, where $l$ is a rescaling factor that is chosen judiciously for each different model. The optimal data collapse is obtained for $l/l_{FFXY} = 4.6, 3.2, 1.8, 1.1$ for the $\phi^4$ model at $D = 1/3, 1/2, 1, 2$ and $l/l_{FFXY} = 2.6, 1.1, 0.45, 0.09$ for the IsXY model at $C = -0.5, -0.2, 0, 0.2$. Of course, for $L$ large $\xi_s \rightarrow \xi_s^{(c)}$ and therefore, given two different models, $l_1/l_2$ should correspond to the ratio of the corresponding spin correlation lengths at the chiral transition. Thus, the scaling we observe implies that $R_s$ is an approximately universal function of $L/\xi_s^{(c)}$. Fig. 5 shows the effective exponent $1/\nu_{eff}$ defined by Eq. (7), as obtained from $R_c$, $B_c$, and $R_s$, respectively, by using the same rescaling factors $l$ as determined from $R_s$. In all cases we observe an approximate collapse of the data. Note that there is a rather extended region, $L_r \lesssim 1$, i.e. $L \lesssim \xi_s^{(c)}$, in which $\nu_{eff}$ computed from the chiral variables $R_c$ and $B_c$ (resp. $R_s$) is approximately 0.8 (resp. 0.9). This preasymptotic behavior explains previous estimates $\nu \approx 0.8$ of the chiral exponent, see, e.g., \[4-9,11,12,14,15,19,20\]. Actually, the data of $1/\nu_{eff}$ from
FIG. 4. $R_s$ at fixed $R_c$ versus the rescaled lattice size $L_r = L/l$. We set $l = \xi_s^{(c)} \approx 118$ for the FFXY model.

$R_c$ and $B_c$ appear to undershoot the Ising value, which is then approached from below. A data collapse is also observed for $B_c$ itself, the helicity modulus, and the effective exponent $\eta_{\text{eff}}$ obtained from $\chi_c$. In conclusion, the crossover to the asymptotic Ising behavior presents interesting features and appears universal to some extent.

The origin of the apparent scaling behavior is not clear. It might reflect the nearby presence of a multicritical point, which could be observed only by performing a further fine tuning of the Hamiltonian parameters, where chiral and spin modes become critical at the same time. The identification of this multicritical point remains an open issue.
REFERENCES

[1] J. Villain, J. Phys. C 10, 1717 (1977); C 10, 4793 (1977).
[2] P. Martinoli, Ch. Leemann, J. Low Temp. Phys. 118, 699 (2000), and references therein.
[3] S. Teitel, C. Jayaprakash, Phys. Rev. B 27, 598 (1983).
[4] E. Granato, J.M. Kosterlitz, J. Lee, M.P. Nightingale, Phys. Rev. Lett. 66, 1090 (1991).
[5] J. Lee, E. Granato, J.M. Kosterlitz, Phys. Rev. B 44, 4819 (1991).
[6] G. Ramirez-Santiago, J.V. José, Phys. Rev. B 49, 9567 (1994).
[7] J.-R. Lee, Phys. Rev. B 49, 3317 (1994).
[8] S. Lee, K.-C. Lee, Phys. Rev. B 49, 15184 (1994).
[9] Y.M.M. Knops, B. Nienhuis, H.J.F. Knops, H.W.J. Blöte, Phys. Rev. B 50, 1061 (1994).
[10] P. Olsson, Phys. Rev. B 55, 3585 (1997).
[11] M. Benakli, E. Granato, Phys. Rev. B 55, 8361 (1997).
[12] S. Lee, K.-C. Lee, Phys. Rev. B 57, 8472 (1998).
[13] L. Capriotti, R. Vaia, A. Cuccoli, V. Tognetti, Phys. Rev. B 58, 273 (1998).
[14] E. Boubcheur, H.T. Diep, Phys. Rev. B 58, 5163 (1998).
[15] D. Loison, P. Simon, Phys. Rev. B 61, 6114 (2000).
[16] G. Franzese, V. Cataudella, S.E. Korshumov, R. Fazio, Phys. Rev. B 62, R9287 (2000).
[17] S.E. Korshumov, Phys. Rev. Lett. 88, 167007 (2002).
[18] P. Calabrese, E.V. Orlov, P. Parruccini, A.I. Sokolov, Phys. Rev. B 67, 024413 (2003).
[19] Y. Ozeki, N. Ito, Phys. Rev. B 68, 054414 (2003).
[20] E. Granato, D. Dominguez, Phys. Rev. B 71, 094521 (2005).
[21] P. Olsson, S. Teitel, Phys. Rev. B 71, 104423 (2005).
[22] A. Pelissetto, E. Vicari, Phys. Rept. 368, 549 (2002).
[23] S. Große Pawig, K. Pinn, Int. J. Mod. Phys. C 9, 727 (1998).
[24] In the IsXY model there is also an antiferromagnetic Ising transition line in the region $C < -C_{Is}$, which starts from the point $C = -C_{Is}, J = 0$. It is not shown in Fig. 1.
[25] M. Hasenbusch, cond-mat/0502556, J. Phys. A in press.
[26] Scaling corrections are expected to be $O(L^{-\zeta})$, with $\zeta = 1/\eta - 4$ for $\Upsilon$ and $\zeta = \min(2 - \eta, 1/\eta - 4)$ for $\chi_s$ and $R_s$.
[27] M. Hasenbusch, J. Phys. A 32, 4851 (1999).
[28] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, E. Vicari, Phys. Rev. B 63, 214503 (2001).
[29] J. Salas, A. Sokal, J. Stat. Phys. 98, 551 (2000).
[30] P. Calabrese, M. Caselle, A. Celi, A. Pelissetto, E. Vicari, J. Phys. A 33, 8155 (2000).
FIG. 5. $1/\nu_{\text{eff}}$ computed by using $R_c$, $B_c$, and $R_s$ vs $L_r = L/l$. For $L_r \to \infty$, $1/\nu_{\text{eff}}$ should converge to $1/\nu_{\text{Is}} = 1$ for $R_c$ and $B_c$, and $-1$ for $R_s$. 