Transitions and crossover phenomena in fully frustrated *XY* systems

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We study the two-dimensional fully frustrated *XY* (FF*XY*) model and two related models, a discretization of the Landau-Ginzburg-Wilson Hamiltonian for the critical modes of the FF*XY* 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 $T_{\rm ch} > T_{\rm sp}$ respectively, of the Ising and Kosterlitz-Thouless type. At $T_{\rm ch}$ 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 $\nu_{\rm eff} \approx 0.8$.

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The nature of the phase transitions in frustrated systems is of great interest in statistical physics. The two-dimensional fully frustrated *XY* (FF*XY*) model[1] is defined by the Hamiltonian

$$\mathcal{H}_{\rm FFXY} = -J \sum_{\langle xy \rangle} \cos(\theta_x - \theta_y + A_{xy}), \qquad (1)$$

where the sum is over all nearest-neighbor pairs of a square or triangular lattice, and A_{xy} satisfy the constraint $\Sigma A_{xy} = \pi$ around any plaquette. It is experimentally relevant for Josephson-junction arrays in a magnetic field.[2] The angle variable θ_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 FF*XY* 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 Π we define the chirality

$$C_n \equiv \sum_{\langle xy \rangle \in \Pi} \sin(\theta_x - \theta_y + A_{xy}), \qquad (2)$$

where n is the dual-lattice site at the center of Π. On the square lattice the staggered magnetization $M_C \equiv \Sigma_n (-1)^{n_1+n_2} C_n / V$ defines an order parameter, which competes with the spin modes to determine the phase diagram of the FF*XY* model. The critical behavior has been much investigated during the last few decades (see, e.g., Refs. 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, and coupled *XY* models.

In spite of all this work, the phase diagram and critical behavior of the FF*XY* 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 FF*XY* 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: 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 FF*XY* model (implemented by alternating vertical lines with ferromagnetic and antiferromagnetic couplings) and two related lattice models. The first one is a ϕ^4 model defined by the Hamiltonian

$$\mathcal{H}_\phi = -J \sum_{\langle xy \rangle, i} \phi_{i,x} \cdot \phi_{i,y} + \sum_{x,i} [\phi_{i,x}^2 + U(\phi_{i,x}^2 - 1)^2] + 2(U+D) \sum_x \phi_{1,x}^2 \phi_{2,x}^2, \qquad (3)$$

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 $\mathcal{H}_\phi$ is expected to describe the critical modes of the FF*XY* model. It corresponds to a straightforward lattice discretization of the Landau-Ginzburg-Wilson theory ob-

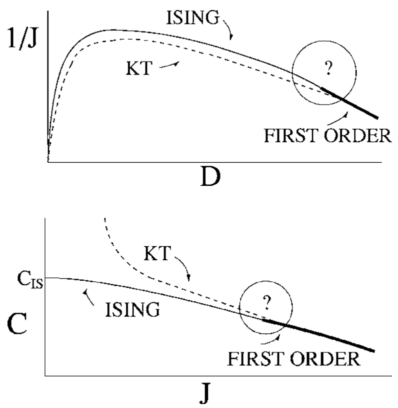

FIG. 1. Sketches of the phase diagrams of the ϕ^4 model for $U=1$ (above) and of the IsXY model (below). The behavior in the circled region where the transition lines meet is unclear.

tained 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 analog of the $\mathbb{Z}_2$ chiral symmetry of the FFXY model. The chiral order parameter is

$$C_x = \phi_{1,x}^2 - \phi_{2,x}^2. \tag{4}$$

When $D=0$, the 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]

$$\mathcal{H}_{\mathrm{Is}XY} = -\sum_{\langle xy \rangle} \left[\frac{J}{2}(1+\sigma_x\sigma_y) s_x \cdot s_y + C\sigma_x\sigma_y \right], \tag{5}$$

where $\sigma_x = \pm 1$, and the two-component spins s_x satisfy $s_x \cdot s_x = 1$. Here s_x and σ_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 $L=O(10^3)$. We used mixtures of Metropolis and overrelaxation updating algorithms, as proposed in Ref. 23. Here 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 ϕ^4 and IsXY models for extended ranges of the parameters $D>0$ and C. No evidence of unique continuous transitions is 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 ϕ^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. Furthermore, we consider the staggered chirality correlation function $G_c(x)$. In the ϕ^4 model the spin and chiral correlation functions are defined by $G_s(x) \equiv \langle \Sigma_i \phi_{i,0} \cdot \phi_{i,x} \rangle$ and $G_c(x) = \langle C_0 C_x \rangle_c$. In the Is$XY$ 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 χ_s and χ_c, and second-moment correlation lengths ξ_s and ξ_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 Υ.

TABLE I. Comparison of the estimates of η obtained from χ_s, and from R_s and Υ using the relations valid in the XY model, such as Eq. (6), in the low-temperature phase.

Model	J	η	η from R_s	η from Υ
FFXY	2.4	0.1480(5)	0.1479(4)	0.14779(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)
Is$XY, C=0$	1.52	0.1817(7)	0.1821(4)	0.18190(13)

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 η (computed by using $\chi_s \sim L^{2-\eta}$), $R_s \equiv \xi_s/L$, and Υ 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]

$$\Upsilon(\eta) = \frac{1}{2\pi\eta} - \frac{\sum_{n=-\infty}^{\infty} n^2 \exp(-\pi n^2/\eta)}{\eta^2 \sum_{n=-\infty}^{\infty} \exp(-\pi n^2/\eta)} \tag{6}$$

for $0 < \eta \leqslant 1/4$. 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 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 Ref. 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 $R_c = R_{\mathrm{Is}}$, where $R_{\mathrm{Is}} = 0.905048\cdots$ is the corresponding Ising value.[29] Note that such a choice does not represent a bias in favor of an Ising transition. If the transition is unique, also the spin correlation length ξ_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 $T_{\mathrm{ch}} > T_{\mathrm{sp}}$, ξ_s remains finite, so that $R_s \sim 1/L$ for $L \to \infty$. Results for R_s are shown in Fig. 2. They

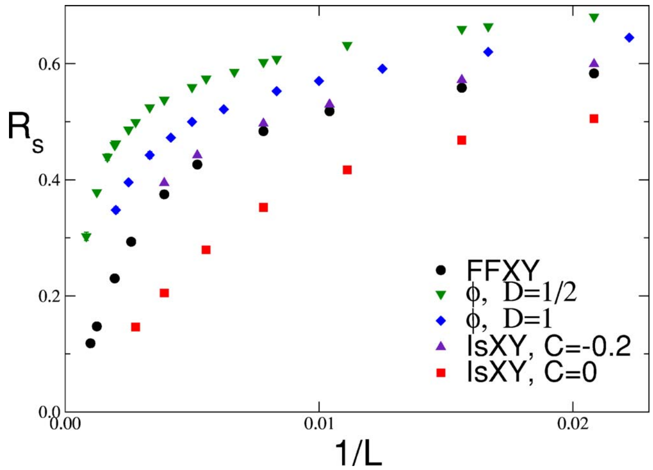

FIG. 2. (Color online) $R_s \equiv \xi_s/L$ at fixed $R_c \equiv \xi_c/L$ vs $1/L$.

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, $\xi_s^{(c)} \approx 380$ for the ϕ^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.

If spin and chiral modes decouple, the chiral transition is expected to belong to the Ising universality class. The best evidence for that is provided by the finite-size behavior at fixed $R_c = R_{\rm Is}$ of the chiral Binder cumulant B_c. In the case of an Ising transition, since $R_c = R_{\rm Is}$, the asymptotic behavior of B_c is expected to be[29,30]

$$B_c = B_{\rm Is} + aL^{-7/4}, \tag{7}$$

where[29] $B_{\rm Is} = 1.167923(5)$ and the leading correction is due to the analytic background. As shown in Fig. 3, B_c clearly approaches the Ising value as L increases; moreover, the predicted convergence rate is also well verified by the data. Note that the Ising asymptotic behavior—the regime in which we observe the approach to the Ising value with the predicted rate of convergence—is observed only for $L \gtrsim 2\xi_s^{(c)}$ with a scaling-correction coefficient in Eq. (7) given by $a \approx 0.14(\xi_s^{(c)})^{7/4}$ (thus $\Delta B_c \equiv B_c - B_{\rm Is} \lesssim 0.01$ only when $L \gtrsim 4\xi_s^{(c)}$). The Ising nature of the chiral transition is further supported by the analysis of the critical exponents. For any invariant quantity S, such as R_c and B_c, we define an effective exponent $\nu_{\rm eff}(L)$ as

$$1/\nu_{\rm eff}(L) = (\ln\ dS/dJ|_{2L} - \ln\ dS/dJ|_L)/\ln 2. \tag{8}$$

Similar to B_c, $\nu_{\rm eff}(L)$ appears to approach the Ising value $\nu = 1$ only for $L \gtrsim \xi_s^{(c)}$, after a nonmonotonic crossover characterized by a plateau at $\nu_{\rm eff}(L) \approx 0.8$. We shall return to this point below.

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

$$\Upsilon = 0.63650817819\cdots + \frac{0.318899454\cdots}{\ln L + c} + \cdots . \tag{9}$$

In most cases, including the FFXY model, the chiral and the spin transitions are very close. If $\delta \equiv J_{\rm sp}/J_{\rm ch} - 1$, $J_{\rm sp}$ and $J_{\rm ch}$ being the location of the two transitions, we find $\delta = 0.0159(2)$ for the FFXY model [$J_{\rm ch} = 2.20632(5)$ and $J_{\rm sp} = 2.2415(5)$], $\delta = 0.0025(2)$ in the ϕ^4 model for $D=1/2$, $\delta = 0.0167(7)$ in the IsXY model with $C=0$.

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 ϕ^4 model with $0 \lesssim D \lesssim 2$, and in the IsXY model for $-0.5 \lesssim C \lesssim 0.2$. Figure 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

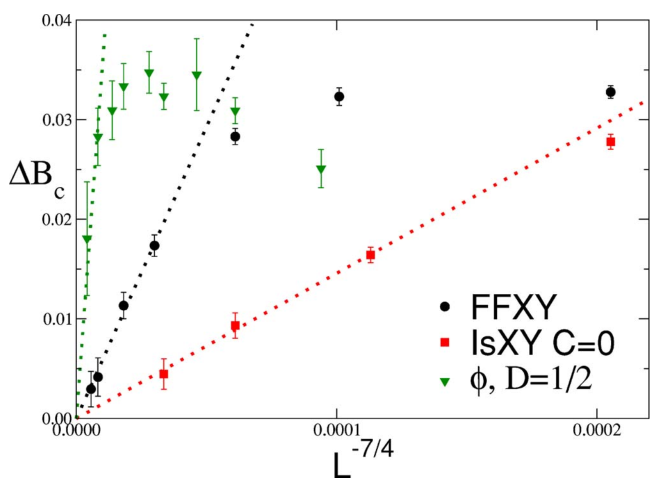

FIG. 3. (Color online) $\Delta B_c \equiv B_c - B_{\rm Is}$ at fixed $R_c \equiv \xi_c/L$ vs $L^{-7/4}$. $B_{\rm Is} = 1.167923(5)$ is the value of the Binder parameter at the critical point in the Ising model (Ref. 29). The dotted lines correspond to linear fits of the data for the largest available lattices.

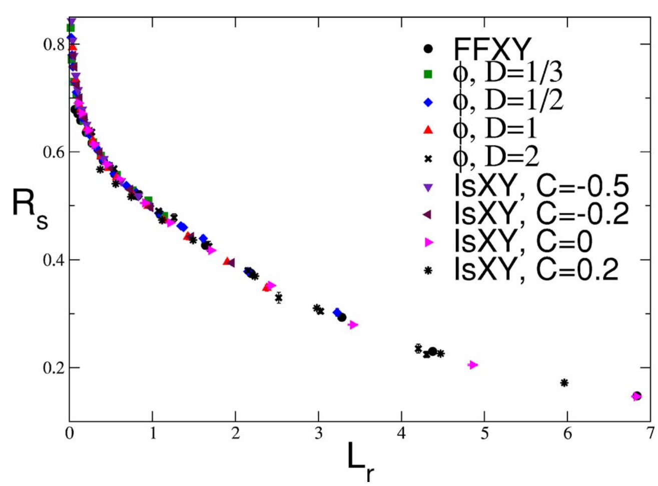

FIG. 4. (Color online) R_s at fixed R_c vs $L_r = L/l$. We set $l = \xi_s^{(c)} \approx 118$ for the FFXY model.

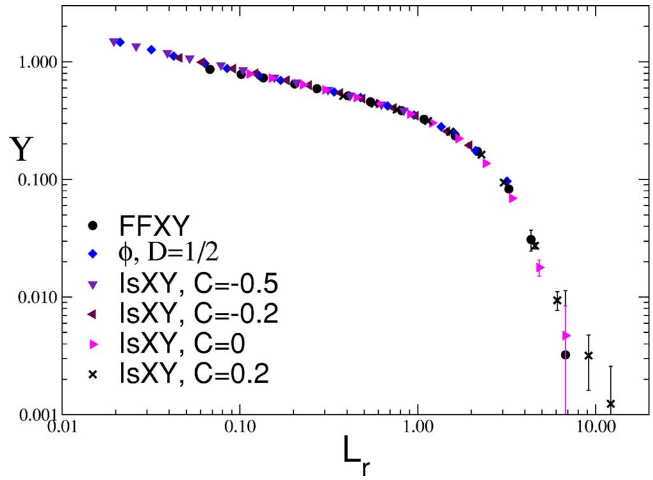

FIG. 5. (Color online) Υ at fixed R_c vs $L_r = L/l$. The rescalings l are the same as in Fig. 4.

chosen judiciously for each different model. The optimal data collapse is obtained for $l/l_{FFXY}=4.5, 3.2, 1.8, 1.0$ for the ϕ^4 model at $D=1/3, 1/2, 1, 2$ and $l/l_{FFXY}=2.6, 1.1, 0.45, 0.089$ for the IsXY model at $C=-0.5, -0.2, 0, 0.2$. Of course, for L large $\xi_s \to \xi_s^{(c)}$ 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 $L/\xi_s^{(c)}$. Using the same length rescalings, a data collapse is also observed for the helicity modulus, see Fig. 5, and the spin and chiral Binder parameters. Figure 6 shows the effective exponent $1/\nu_{\rm eff}$ defined by Eq. (8), 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 $\nu_{\rm eff}$ computed from the chiral variables R_c and B_c (respectively, R_s) is approximately 0.8 (respectively, 0.9). This preasymptotic behavior explains previous estimates $\nu \approx 0.8$ of the chiral exponent, see, e.g., Refs. 4–9, 11, 12, 14, 15, 19, and 20: Simulations with lattices in the range $L \lesssim \xi_s^{(c)}$ would observe $\nu \approx 0.8$ instead of the Ising value. For $L_r \gtrsim 1$, $\nu_{\rm eff}$ obtained from R_c and B_c starts to increase and becomes larger than 1:

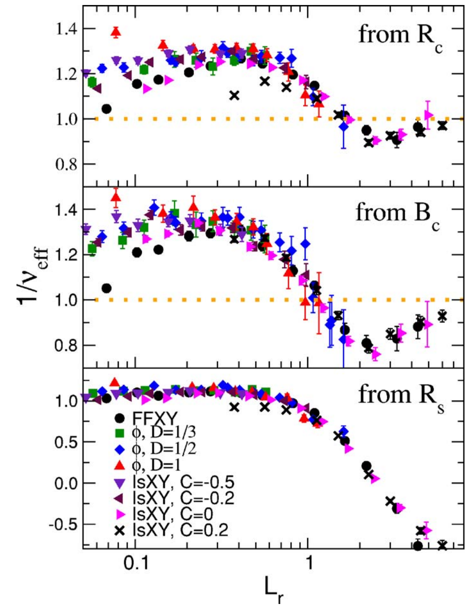

FIG. 6. (Color online) $1/\nu_{\rm eff}$ computed by using R_c, B_c, and R_s vs $L_r = L/l$. The rescalings l are the same as in Fig. 4. For $L_r \to \infty$, $1/\nu_{\rm eff}$ should converge to $1/\nu_{\rm Is}=1$ for R_c and B_c, and -1 for R_s.

the curves of $1/\nu_{\rm eff}$ have a minimum at $L_r \approx 2$ corresponding to $\nu_{\rm eff} \approx 1.1$ for R_c, and $\nu_{\rm eff} \approx 1.2$ for B_c. Then, for $L_r \gtrsim 3$ they apparently converge to the Ising value $\nu = 1$, as already observed for B_c. Thus, very large lattices are needed to fully observe the Ising behavior, and therefore to confirm the two-transition scenario, whenever $\xi_s^{(c)} \gg 1$, as is the case in the square-lattice FFXY model.

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.

[1] J. Villain, J. Phys. C **10**, 1717 (1977); **10**, 4793 (1977).
[2] P. Martinoli and Ch. Leemann, J. Low Temp. Phys. **118**, 699 (2000), and references therein.
[3] S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983).
[4] E. Granato, J. M. Kosterlitz, J. Lee, and M. P. Nightingale, Phys. Rev. Lett. **66**, 1090 (1991).
[5] J. Lee, E. Granato, and J. M. Kosterlitz, Phys. Rev. B **44**, 4819 (1991).
[6] G. Ramirez-Santiago and J. V. José, Phys. Rev. B **49**, 9567 (1994).
[7] J.-R. Lee, Phys. Rev. B **49**, 3317 (1994).
[8] S. Lee and K.-C. Lee, Phys. Rev. B **49**, 15 184 (1994).
[9] Y. M. M. Knops, B. Nienhuis, H. J. F. Knops, and H. W. J. Blöte, Phys. Rev. B **50**, 1061 (1994).
[10] P. Olsson, Phys. Rev. B **55**, 3585 (1997).
[11] M. Benakli and E. Granato, Phys. Rev. B **55**, 8361 (1997).
[12] S. Lee and K.-C. Lee, Phys. Rev. B **57**, 8472 (1998).
[13] L. Capriotti, R. Vaia, A. Cuccoli, and V. Tognetti, Phys. Rev. B **58**, 273 (1998).
[14] E. H. Boubcheur and H. T. Diep, Phys. Rev. B **58**, 5163 (1998).
[15] D. Loison and P. Simon, Phys. Rev. B **61**, 6114 (2000).
[16] G. Franzese, V. Cataudella, S. E. Korshunov, and R. Fazio, Phys. Rev. B **62**, R9287 (2000).
[17] S. E. Korshunov, Phys. Rev. Lett. **88**, 167007 (2002).

[18] P. Calabrese, E. V. Orlov, P. Parruccini, and A. I. Sokolov, Phys. Rev. B **67**, 024413 (2003).
[19] Y. Ozeki and N. Ito, Phys. Rev. B **68**, 054414 (2003).
[20] E. Granato and D. Dominguez, Phys. Rev. B **71**, 094521 (2005).
[21] P. Olsson and S. Teitel, Phys. Rev. B **71**, 104423 (2005).
[22] A. Pelissetto and E. Vicari, Phys. Rep. **368**, 549 (2002).
[23] S. Große Pawig and K. Pinn, Int. J. Mod. Phys. C **9**, 727 (1998).
[24] In the Is*XY* model there is also an antiferromagnetic Ising transition line in the region $C<-C_{\rm Is}$, which starts from the point $C=-C_{\rm Is}$, $J=0$. It is not shown in Fig. 1.
[25] M. Hasenbusch, J. Phys. A **38**, 5869 (2005).
[26] Scaling corrections are expected to be $O(L^{-\zeta})$, with $\zeta=1/\eta-4$ for Υ and $\zeta=\min(2-\eta,1/\eta-4)$ for χ_s and R_s.
[27] M. Hasenbusch, J. Phys. A **32**, 4851 (1999).
[28] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B **63**, 214503 (2001).
[29] J. Salas and A. Sokal, J. Stat. Phys. **98**, 551 (2000).
[30] P. Calabrese, M. Caselle, A. Celi, A. Pelissetto, and E. Vicari, J. Phys. A **33**, 8155 (2000).