# Nonuniversal critical behavior and first-order transitions in a coupled XY-Ising model

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We study, by a Migdal-Kadanoff approximation and Monte Carlo simulations, the phase diagram of a two-dimensional coupled XY-Ising model. This model can describe phase transitions in different systems with underlying continuous and  $Z_2$  symmetries. Depending on the parameters, we find separate XY, Ising and first-order transitions. Also, a line of continuous transitions is found with simultaneous loss of XY and Ising order and varying critical exponents. The fully frustrated XY and Josephson-junction systems can be considered to lie along different paths in the model which can result in nonuniversal behavior if the transition is a single one.

### I. INTRODUCTION

Statistical mechanical models with continuous U(1)and discrete  $\mathbb{Z}_2$  symmetry have attracted much attention in recent years as they can display phase transitions, which can be found in various physical systems of experi-mental interest.<sup>1-19</sup> In general, as the temperature or some other parameter is varied, two successive transitions can occur and, in the case of strongly coupled excitations, a single transition may also take place. The nature of the single transition is one of the most important issues, but, not surprisingly, it also presents some particular difficulties in either numerical or analytical approaches. In numerical studies by Monte Carlo methods, for example, one has to be able to detect very weak firstorder transitions, and in the renormalization-group approach, the region of interest lies outside the range of validity of the recursion relations. A simple model displaying most of these features consists of coupled XY and Ising models of the form  $^{6-10}$ 

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} \left[ (A + B\sigma_i \sigma_j) \cos(\theta_i - \theta_j) + C\sigma_i \sigma_j \right], \quad (1.1)$$

where  $\sigma = \pm 1$  and  $\theta = [0, 2\pi]$ . Besides being of interest in its own right as a particular model with a very rich critical behavior in the parameter space A, B, C, this model is also relevant for the critical behavior of fully frustrated XY (FFXY) models. The latter model can be physically realized as a square or triangular array of Josephson junctions of large capacitance in a perpendicular magnetic field corresponding to a half-flux quantum per plaquette.<sup>2</sup> These physically distinct models, however, turn out to have the same lowest-order Ginzburg-Landau expansion, differing only by irrelevant operators. From the universality hypothesis one may expect them to be in the same universality class, although the particular mechanism driving the phase transition in each case is completely different. Isotropic arrays are described by the model of Eq. (1.1) in the special plane A = B, and an anisotropic square array in which every other column of the lattice has a coupling differing from the others by a constant factor can be described by the more general case  $A \neq B$ <sup>7,9</sup> The model in Eq. (1.1) can also be related to other interesting systems, as, for example, to a Josephson-junction ladder with a half-flux quantum per plaquette undergoing a zero-temperature superconductor insulator transition,<sup>18</sup> to two-dimensional helical XY models<sup>1</sup> and, in a Gaussian approximation, to the antiferromagnetic restricted solid-on-solid model.<sup>19</sup>

We will be concerned in this work with the critical behavior of the coupled XY-Ising model of Eq. (1.1), defined on a square lattice, in the particular subspace A = B,

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} \left[ A \left( 1 + \sigma_i \sigma_j \right) \cos(\theta_i - \theta_j) + C \sigma_i \sigma_j \right], \quad (1.2)$$

which is relevant for the isotropic FFXY models. We will argue that the square and triangular FFXY models can be considered to lie along different initial points (A, C) in the parameter space of the same coupled XY-Ising model (1.2). A previous study of this model<sup>10</sup> revealed a bifurcation point occurring at  $C = C^*$ , where  $C^* \approx 0$ . For  $C > C^*$ , there is a double transition with an XY followed by an Ising transition as temperature in increased. For  $C < C^*$  a single transition occurs of an unknown nature. An identical topology of the phase diagram has also been found in a generalized Coulomb-gas representation of the FFXY model containing fractional charges.<sup>14</sup> An important feature of the phase diagram is that there is no phase with Ising disorder and XY order thus indicating that Ising disorder induces also XY disorder in this model. This can be seen by noting that the parameter space A = B has a rather special symmetry: a domain wall in the Ising variables leaves the XY spins uncoupled, since  $1 + \sigma_i \sigma_i = 0$  in this case. This is similar, although physically different, to the proposed mechanism for a singlephase transition in the FFXY model.<sup>5,11</sup> According to this, the corners of the Ising domain walls act like fractional vortices (or charges in the Coulomb-gas representation), which are estimated to be unbound at the melting of the domain walls thus triggering an unbinding of integer vortices destroying the XY order. The role played by the unbound corner charges in the fully frustrated XYmodel is played in the model of Eq. (1.2) by the domain wall itself. Other scenarios are also possible by allowing

independent parameters for the unbinding of corner and integer charges as well as the melting of the domain walls in a generalized FFXY model. However, in the original model these are related in such a way that the most likely scenario is either a double transition with an XY followed by Ising transition as temperature increases or a single transition in agreement with that expected from the model in Eq. (1.2). Note, however, that in the case of the anisotropic frustrated XY model,<sup>13</sup> which corresponds to  $A \neq B$ , a double transition is expected to occur in an order determined by the value of C. For  $C < C^*$ , this double transition is expected to be in reverse order, and it can be shown that the signature of the Ising transition appears as a logarithmic singularity in the helicity modulus.<sup>9</sup> On the other hand, for  $C > C^*$ , both scenarios are possible. These distinct behaviors of the two cases have given rise to some misleading interpretation in the literature. In Fig. 1 we indicate possible schematic phase diagrams in the A, B plane for  $C > C^*$  and  $C < C^*$  illustrating the various possible sequences of transitions. The details of how the transition lines join in each case will require further investigation. Here we concentrate in the critical behavior along the A = B line.



FIG. 1. Possible phase diagrams of the coupled XY-Ising model of Eq. (1.1) in the A, B plane showing disordered, fully ordered, and partial ordered (XY or Ising) phases.

In this work we study in some detail the critical behavior of the model of Eq. (1.2) along the line of single transitions. Using a Migdal-Kadanoff renormalization-group approximation,<sup>20,21</sup> we obtain the global phase diagram, and by generalizing the model into a lattice-gas model including the presence of vacancies<sup>22</sup> we are able to locate first-order transitions using a prefacing transformation<sup>23</sup> to generate an initial density of vacancies. From extensive Monte Carlo (MC) simulations we find a segment of continuous phase transitions starting at the bifurcation point, which eventually becomes first order for large negative C. To determine the location of first-order transitions and critical exponents along this line, we make use of a recently developed numerical method.<sup>24</sup> We also use Binder's MC renormalization-group method<sup>25</sup> for an independent evaluation of the critical exponents. From the numerical study we find, on the segment of continuous phase transition, nonuniversal critical behavior as critical exponents associated with the Ising order parameter vary systematically as a function of A and C. Starting at the bifurcation point, the Ising correlation length exponent decreases from the pure Ising value v=1 to  $v \approx 0.85(3)$ and, as one moves away from this point, remains almost constant initially but decreases more rapidly for large deviations. At the same time,  $2\beta/\nu$  starts with a value  $2\beta/\nu \approx 0.24(3)$  consistent with the pure Ising model but increases systematically further from the bifurcation point. It is sufficient to study the Ising variables, since, if  $\nu \neq 1$ , the transition cannot be a decoupled Ising XY or one branch of a double transition and must be single. Moreover, the interpretation of helicity modulus data in a model of this nature is not obvious. In addition to the critical exponents, this line can also be characterized by its central charge. Calculations employing a MC transfer matrix<sup>26</sup> give a rather surprising result. The central charge appears to increase continuously along this line from  $c \approx 1.5$  close to the bifurcation point to c = 2 near the tricritical point.<sup>27</sup> Some of the results presented in this paper have been summarized in Ref. 27.

These results have direct implication for FFXY models, which, being in the same universality class, should have critical exponents different from the pure Ising ones if the transition is found to be a single one. We also expect slightly different exponents for the square and triangular cases, since they lie along close but distinct line of initial points. According to these new results, the critical behavior of the FFXY model is nonuniversal. In a recent Monte Carlo simulation of the FFXY model on a triangular and square lattice,<sup>28</sup> employing the same numerical methods, we found  $v \approx 0.83(4)$  and 0.85(3) for the triangular and square lattice, respectively. They agree with each other within the estimated uncertainties but differ significantly from the pure Ising exponents and agree reasonably well with the exponents of the coupled XY-Ising model near the bifurcation point. Recently, Thijssen and Knops<sup>17</sup> have determined the central charge c for the FFXY model using a Monte Carlo transfer matrix and found c = 1.66(4) consistent with the corresponding value for the coupled XY-Ising model near the bifurcation point.

The paper is organized as follows. In Sec. II we

present the phase diagram obtained from a Migdal-Kadanoff type of approximate recursion relation including vacancies. In Sec. III a finite-size-scaling analysis of Monte Carlo data is used to study the first-order segment of the single transition and obtain the critical exponents on the rest of the line. In Sec. IV we make contact with the FFXY model, which initially motivated this work, and hope to clarify some confusion in the literature. Finally, Sec. V is devoted to the conclusions and final remarks.

# **II. PHASE DIAGRAM**

In this section we use a Migdal-Kadanoff real-space renormalization-group approximation<sup>20,21</sup> to obtain a qualitative global phase diagram of the coupled XY-Ising model defined in Eq. (1.2). For the standard XY model it does not reproduce a true line of fixed points at low temperatuers, although it gives an indication of it in the form of a line of almost fixed points. This apparent fixed line can often be used to identify the XY-like ordered phases in more complicated models, and we shall use this procedure in our case.

To locate the first-order transitions within the Migdal-Kadanoff approximation we generalize the procedure of Nienhuis *et al.*,<sup>22</sup> which reproduces the known first-order transition of the *q*-state Potts model when q > 4. The procedure consists of enlarging the parameter space of the original model by including vacancies, which can give rise to first-order behavior. A prefacing transformation<sup>23</sup> is then used to generate an initial density of vacancies and locate the first-order transitions in the coupled *XY*-Ising model. The details are described in the Appendix.

The phase diagram obtained from the Migdal-Kadanoff approximation is indicated in Fig. 2. There are four different phases: (a) a disordered (high-temperature phase); (b) an intermediate Ising-ordered and XY-



FIG. 2. Phase diagram obtained from a Migdal-Kadanoff approximation for the model of Eq. (1.2). The segment TF is a first-order line when vacancies are allowed in the renormalization-group procedure.

disordered phase, (c) a fully ordered phase (low temperature), and (d) an antiferromagnetic Ising-ordered and XY-disordered phase. The segment TF along the line of single transitions PF is a first-order line when vacancies are allowed in the renormalization-group procedure. The bifurcation point P cannot be located with precision because the ordered XY phase is not a true line of fixed points within this approximation. It seems, however, to lie close to the line of initial points C = 0, but we find no special symmetry along this line, which could suggest the location of P. Moreover, a mean-field analysis of this model gives the position of this multicritical point occurring at C > 0.

#### **III. MONTE CARLO SIMULATIONS**

In this section we turn to a detailed numerical study of the critical behavior near the bifurcation point P of Fig. 2 in the region of single transitions. Here we are faced with a typical problem in MC simulations, which arises when studying an unknown model: one needs to identify the order of the transitions in an unambiguous way. There are many methods available to distinguish numerically between continuous and first-order transitions. They usually depend on observation of hysteresis near the transition or finite-size scaling of the form  $L^{-d}$ , where L is the size of the system in units of the lattice spacing and d the dimensionality. However, hysteresis is difficult to detect in an anambiguous way and finite-size scaling  $L^{-d}$  will set in only for large system sizes  $L > \xi$ , where  $\xi$  is the correlation length. Recently, a new technique has been developed,<sup>24</sup> which suffers less from these deficiencies, and we shall then apply it to our problem. Once the location of the first-order transitions is identified, we will turn



FIG. 3. Phase diagram obtained by Monte Carlo simulations. The lines through the data are guides to the eyes. Continuous and first-order transitions are indicated by solid and dotted lines, respectively.

to a careful determination of the critical exponents along the rest of the line, assuming that the transition is continuous. When possible we will also compare with the results of applying Binder's method of MC renormalization group.<sup>25</sup> In Fig. 3 we show a portion of the phase diagram obtained by Monte Carlo simulations. We find a segment of continuous transitions along the phase boundary separating the fully ordered phase from the fully disordered phase, starting at the bifurcation point, which eventually turns into a line of first-order transitions for large A and roughly constant A + C in qualitative agreement with the analysis of Sec. II. But, more surprisingly, the numerical evaluation of the critical exponents shows that they vary continuously.

#### A. Monte Carlo method

The MC simulations were performed using the standard Metropolis algorithm with the combined variables  $(\sigma_i, \theta_i)$  being updated once in each sequential sweep through the lattice. We have chosen small system sizes to perform long runs in order to achieve good statistics and used periodic boundary conditions on square lattices  $L \times L$  for 10 < L < 32 with a vectorized version of the program code. Most of the data on critical exponents and the location of first-order transition, were obtained from single extensive simulations, typically of  $5 \times 10^6$ Monte Carlo steps (MCS), after discarding  $(1-2) \times 10^5$ MCS for equilibration. The histogram method<sup>29</sup> was used to extrapolate to nearby parameters in the phase diagram. Preliminary simulations with fewer MCS were also used to approximately locate the transition lines.

#### **B.** First-order transitions

In order to locate the first-order transitions in the phase diagram we made use of a recently developed method based on the scaling behavior of the free-energy barrier between ordered and disordered states.<sup>24</sup> First we obtain the histogram of the energy distribution

$$N(E;\beta,L) = \aleph Z^{-1}(\beta,L)\Omega(E,L)e^{-\beta e} = e^{-A_E(\beta,L)}, \quad (3.1)$$

Ζ where number of MCS, X is the  $=\sum_{E} \Omega(E,L) \exp(-\beta E)$  the partition function, and  $\Omega(E,L)$  the degeneracy of the energy E. At a first-order transition N develops a characteristic double-peak structure in the vicinity of  $T_c$ . This arises because of the bulk free-energy barrier  $\Delta F_E(L)$  between ordered and disordered states. This free-energy barrier at  $T_c$  can be obtained from the histogram of energy distribution [Eq. (3.1)] as

$$\Delta F_E(L) = A_{E_m}(\beta, L, \aleph) - A_{E_1}(\beta, L, \aleph) , \qquad (3.2)$$

where  $E_1(L)$  is the energy corresponding to one of the equal depth minima of  $A_E$  and  $E_m(L)$  is the position of



FIG. 4. Typical plot of  $\Delta F_E$  obtained from  $A(E;\beta,L,N)$  as a function of energy.

the maximum. Note that  $\Delta F_E(L)$  is independent of  $\aleph$ . For a first-order transition it grows slowly at a rate controlled by the critical point for  $L \ll \xi$  and as  $L^{d-1}$  for  $L \gg \xi$ . If  $\Delta F_E(L)$  as measured from simulations of the energy distribution is found to increases with L, then according to this method the transition is unambiguously first order. A typical diagram of  $\Delta F_E$  obtained from the histogram is shown in Fig. 4. The histogram at the pseudotransition point is found by adjusting the parameters in the Hamiltonian until the two peaks are at the same height.

To construct the energy histograms we rewrite the Hamiltonian (1.2) as

$$-\beta H = AE_{XY} + CE_I , \qquad (3.3)$$

where

$$E_{XY} = \sum_{\langle ij \rangle} (1 + \sigma_i \sigma_j) \cos(\theta_i - \theta_j) ,$$
  

$$E_I = \sum_{\langle ij \rangle} \sigma_i \sigma_j .$$
(3.4)

The histogram at nearby couplings A',C' can be obtained directly from the data at A,C. From Eqs. (3.1) and (3.3) and the normalization  $\sum_{E} N(E) = \aleph$ ,

$$N(E_{XY}, E_I; A', C') = \frac{N(E_{XY}, E_I; A, C)e^{-(A'-A)E_{XY}-(C'-C)E_I}}{\aleph^{-1} \sum_{E_{XY}, E_I} N(E_{XY}, E_I; A, C)e^{-(A'-A)E_{XY}-(C'-C)E_I}}$$
(3.5)

This extrapolation is feasible as long as the additional factor  $\approx e^{(\Delta A + \Delta C)L^d}$  in the Boltzman weight is sufficiently small compared to  $\Omega(E)$ . Typically A' - A, C' $-C \approx 10^{-3}$  and  $\Omega(E) \approx 10^4$  in our extrapolations, which clearly satisfy this requirement. To find  $\Delta F_E$ , we construct histograms as a function of  $E_I$ , which is a discrete variable and therefore more convenient for the purpose of storing the data.

In Sec. II we found that for sufficiently large negative C the line of single transitions may become first order (Fig. 2). To locate these transitions we performed Monte Carlo simulations at different values of A = 3.0, 5.0, 6.5,with roughly constant  $A + C \approx 0.7$  at a particular system size L = 16. To locate the transition we extrapolate in C following Ferrenberg and Swendsen.<sup>29</sup> No double-peak structure appears for A = 3.0 and 5.0, but for A = 5.0 a shoulder in the histogram can be noticed, as indicated in Fig. 5. However, when adjusting C to obtain the histogram at the transition no double peak appears for the Lvalues used in our simulations. We note that this behavior is very similar to that observed in the q = 4 Potts model in two dimensions, which is known to separate second-order transitions  $(q \leq 4)$  from first-order transitions (q > 4). So this behavior suggests we are in the neighborhood of a tricritical point. Indeed, finite-size scaling of  $\Delta F_E$  at A = 6.5 shows a monotonic increase with the system size L as indicated in Fig. 6, which is a definite signal of a first-order transition. We also checked that the histograms in terms of  $E_I$  and  $E_{XY}$ , both show a double peak structure separately as they should at a discontinuous phase transition. Note that this transition is between the fully ordered phase and the disordered phase. In Fig. 7 we show the staggered magnetization histogram at the transition. A sharp single peak at zero appears indicating that this transition lies outside the antiferromagnetic ordered phase as indicated in Fig. 2.

It is not possible to locate the tricritical point with any precision. The method can unambiguously determine that a transition is first order from the monotonic increase in  $\Delta F_E$  with increasing L. However, the absence of a peak in  $\Delta F_E$  for the available system sizes does not



FIG. 5. Energy histogram at A = 5.0 as a function of C near the transition point.



FIG. 6. Finite-size behavior of  $\Delta F_E$  for A = 6.5 indicating a first-order transition.

preclude a very weak first-order transition, since a peak may develop for yet larger sizes. Thus, the absence of a peak does not guarantee that the transition is continuous. From these simulations, our best guess for the location of the tricritical point is  $A \approx 5$ ,  $C \approx -4.3$ . However, the estimates of the critical exponents for A < 5 under the assumption that the transition is continuous show some strange behavior, which leads us to suspect that the tricritical point may be as low as  $A \approx 3$ . Also, a preliminary study of the central charge by MC transfer matrix method,<sup>27</sup> which approaches the tricritical point from A < 3 suggests that this latter value may be a better estimate.

# C. Critical exponents

We now turn to the determination of the critical exponents along the segment PT of assumed continuous transitions in Fig. 3. In principle, there are at least two kinds of critical exponents to be determined, since we



FIG. 7. Staggered magnetization histogram at the same values of A, C of Fig. 6.

have Ising and XY type variables. However, here we will be concerned only with the evaluation of the first kind. The reason is that these can be obtained quite accurately by studying the finite-size scaling of the bulk free-energy barrier between states with discrete symmetry. This free energy,  $\Delta F_m(L)$ , is defined in a similar way as in Eq. (3.2) by constructing the histogram as a function of the magnetization  $m = (1/L^d) \sum_i \sigma_i$ . At the critical point,  $\Delta F_m(L)$  becomes a constant for large L. For  $T < T_c$ ,  $\Delta F_m(L)$  increases with L as  $L^{1/\nu}$  for  $L \ll \xi$  and for  $T > T_c$  approaches zero. This change of behavior near  $T_c$  can be used to determine the critical parameters with good precision. However, the exponent itself can be obtained quite easily from the slope of a log-log plot of  $(\partial \Delta F_m / \partial C)$  as a function of L, which yields  $1/\nu$  from a one parameter fit without requiring a precise determination of  $T_c$ . The exponent  $2\beta/\nu$  can be obtained from the scaling of the location of one the peaks in the histogram, which should scale as  $L^{-\beta/\nu}$  at the critical point. This, however, will depend on a precise location of the critical point and hence will be subject to larger uncertainty. In Fig. 8 we show some of the exponents obtained by the method described above at a point along the line of single transitions and also on the Ising transition line.

It is interesting to note that  $\Delta F_m(L)$  reaches a maximum in the form of a cusp, at a particular value of A as indicated in Fig. 9. It is quite natural to assume this is the location of the bifurcation point in the phase diagram. In fact, its location coincides with the point where  $1/\nu$  sharply increases from its value along the Ising transition line to a significantly larger value along the boundary between fully ordered and fully disordered phases. At present we do not know how to analyze the behavior of  $\Delta F_m(L)$  near the maximum but we expect that it

should provide some information about the critical exponents associated with the bifurcation point itself.

In Fig. 10 we show the variation of the exponents with A near the bifurcation point. It is quite clear from this figure that the exponents deviate significantly from the pure Ising values  $(v=1, 2\beta/v=\frac{1}{4})$  and seems to vary systematically with the parameters A and C indicating a nonuniversal critical behavior.

We have also obtained independent estimates of the critical exponents using Binder's phenomenological renormalization group of Monte Carlo data.<sup>25</sup> There are two versions of this method. In one of them, the finite system is divided into blocks, while in the other a set of independent blocks each with periodic boundary conditions is considered. We found that the first version gives rise to large errors and inconsistency of the data so we choose to work with the second version, which has the additional advantage that it can be easily combined with the histogram method, which gives much better results. The method makes use of the size-dependent moments  $\langle m^2 \rangle_L, \langle m^4 \rangle_L$  of the order-parameter probability distribution. The central quantity to calculate is the fourth-order reduced cumulant  $U_L$  defined as

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3 \langle m^2 \rangle L} . \tag{3.6}$$

It can be shown that  $U_L \rightarrow \frac{2}{3}$  for  $T > T_c$  and  $U_L \rightarrow 0$  for  $T < T_c$ . Also  $U_L \rightarrow U^*$ , where  $0 < U^* < \frac{2}{3}$  at  $T = T_c$ . The critical exponents  $2\beta/\nu$  and  $1/\nu$  can be determined by comparing moments and cumulants for two different lattice sizes L and L'=bL. At  $T = T_c$ ,  $U_L = U_{L'} = U^*$ , and it results in



FIG. 8. Data used in the determination of the critical exponents from the finite-size scaling of  $\Delta F_m$ . The curve indicated by + has been reduced by 100 in order to use the same ordinate axis.



FIG. 9.  $\Delta F_m$  at the phase boundary between Ising-ordered and disordered phases plotted as a function of A.

$$\frac{2\beta}{\nu} = \frac{1}{\ln b} \ln(\langle m^2 \rangle_{bL} / \langle m^2 \rangle_L)_{T_c} ,$$

$$\frac{1}{\nu} = \frac{1}{\ln b} \ln \left[ \frac{\partial U_{bL}}{\partial U_L} \right]_{U^*} .$$
(3.7)

The exponents for the infinite system are obtained by extrapolating the values obtained from Eqs. (3.7) to  $\ln b \rightarrow \infty$ , which sometime can be quite ambiguous. Also the final exponents require a rather precise determination of  $T_c$ . Typical results of these calculations are indicated in Fig. 11, where we also compare with the values obtained from the previous method based on the finite size scaling of  $\Delta F_m(L)$ . We observe an overall qualitative agreement.



FIG. 10. Variation of the critical exponents v and  $2\beta/v$  with A. The vertical arrow indicates the location of maximum in  $\Delta F_m$  from Fig. 9, and the horizontal ones indicate the exact Ising exponents.

Additional information on the critical behavior along this line is provided by the central charge c. From conformal invariance, this quantity is related to the finitesize amplitude of the singular part of the free energy in a  $L \times \infty$  strip.<sup>30</sup> For periodic boundary conditions in the L direction, the free energy per site behaves assymptotically as  $f(L)=f(\infty)+\pi c/6L^2$ . Numerical calculations using a MC transfer matrix<sup>26</sup> to evaluate the free energy in the strip geometry gives a value of c varying between 1.5 at the bifurcation point to approximately 2 where the line of first-order transitions start.<sup>27</sup> This range of values is much larger than would be expected  $(c = \frac{3}{2})$  if the critical



FIG. 11. Same critical exponents as in Fig. 8 obtained by a finite-size scaling of the cumulants  $U_L$  for L = 10 and L' = bL. The arrows indicate the exponents obtained from Fig. 8.

behavior were a simple superposition of a critical Ising and Gaussian model.<sup>31</sup> As far as we know, it also does not correspond to any known model, but it is not completely inconsistent with a line of continuous varying critical exponents<sup>32</sup> as suggested by the MC calculations. These results for the central charge are rather preliminary and should be interpreted with caution. In particular, the variation of c along the critical line could be an artifact of crossover or finite-size effects. Further investigation is necessary to resolve this issue.

With all these results in hand, the phase diagram of Fig. 3 can now be constructed. By monitoring the Ising magnetization and the free-energy barrier  $\Delta F_m$ , the decoupled Ising transition with v=1 and the single transition PT with  $v\neq 1$  are identified. The first-order section is obtained from  $\Delta F_E$ . The decoupled XY part is not directly simulated, but is obtained by studying the Ising magnetization m in the  $C > C_I$  region and, where m = 1, finding  $A_{XY}$  by equating  $2A_{XY}$  with the standard XY critical value. Then this line is simply continued to the point P, which is identified by the sudden decrease in v from its pure Ising value. We did attempt to identify the XY transition by studying the helicity modulus, but this was subject to just as large uncertainties.

# **IV. FULLY FRUSTRATED XY MODELS**

In this section we will relate the fully frustrated XY model, on both a triangular and square lattice, to the same coupled XY-Ising model. According to this relation, the triangular and square cases are just different points in the same global phase diagram and the results found in the previous sections concerning the nature of the transitions near the bifurcation point should have direct implications for these models.

The fully frustrated XY model can be defined by the following Hamiltonian

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j) , \qquad (4.1)$$

where  $J_{ij} = \pm J$  subject to the constraint that in each plaquette of the lattice the product of  $J_{ij}$  is negative. For the square lattice, this can be accomplished by ferromagnetic horizontal rows and alternating ferromagnetic and antiferromagnetic columns and for the triangular lattice by isotropic antiferromagnetic couplings. This gives rises to frustration and results in a ground state with continuous U(1) and discrete  $\mathbb{Z}_2$  symmetry. This model can describe Josephson-junction arrays in a magnetic field with half a flux quantum per plaquette by noting that the Josephson coupling between neighbor superconducting grains is of the form  $\cos(\theta_i - \theta_j - A_{ij})$ , where  $A_{ij}$  $=(2\pi/\Phi_0)\int_i^j \mathbf{A} \cdot d\mathbf{l}, \ \theta_i$  is the phase of the superconducting order parameter, and  $\Phi_0$  is a flux quantum. The vector potential **A** must satisfy  $\nabla \times \mathbf{A} = \mathbf{B}$ , the external perpendicular field, which results in the constraint that the directed sum around a plaquette  $\sum A_{ij} = 2\pi f$ , where  $f = \Phi / \Phi_0$  is the number of flux quantum per plaquette. The fully frustrated case corresponds to  $f = \frac{1}{2}$ . Choosing an appropriate gauge,  $A_{ii} = \pi$  (triangular lattice) and

 $A_{ij} = \pi x_i (y_i - y_j)$  (square lattice), where  $(x_i, y_i)$  is the position of a lattice site, one immediately arrives at the model in Eq. (4.1). Real Josephson-junction arrays are more complicated because one has to include disorder, charging effects, and dissipation. In particular, positional disorder can lead to a double transition if there is a single one in the ideal system.<sup>33</sup> Here, however, we will only be concerned with the ideal case.

On the basis of the universality hypothesis, one expects that models with Ginzburg-Landau-Wilson effective Hamiltonians differing only by irrelevant operators are in the same universality class. For the fully frustrated XYmodel in Eq. (4.1), Ginzburg-Landau expansions can be constructed using symmetry analysis or Hubbard-Stratonovich transformations.<sup>6,7,9,34</sup>

Starting from Eq. (4.1) one can apply the Hubbard-Stratonovich transformation in the usual way by introducing an unconstrained auxiliary complex field  $\Psi_i$  coupled linearly to  $\exp(i\theta_i)$ . To fourth order in  $\Psi$  this yields an equivalent Hamiltonian

$$\frac{H}{kT} = \frac{1}{2} \sum_{i,j} \Psi_i^* J_{ij}^{-1} \Psi_j^* - \frac{1}{4} \sum_i |\Psi_i|^2 + u \sum_i |\Psi_i|^4 .$$
(4.2)

A Ginzburg-Landau free energy can now be constructed by introducing Fourier transforms and expanding about the most fluctuating modes. For the triangular lattice, J(q) has two minima at  $\pm Q$  with  $Q = (4\pi/3, 0)$  and for the square lattice, after diagonalizing J(q,q') one finds two minima at (0,0) and  $(0,\pi)$ .<sup>6</sup> In each case, one needs two order parameters,  $\Psi_1$  and  $\Psi_2$ . Retaining these modes only, the quartic term in Eq. (4.2) will couple  $\Psi_1, \Psi_2$  and gives in the continuum limit a free density for the square lattice case on the form

$$F = r_0 (|\Psi_1|^2 + |\Psi_2|^2) + u (|\Psi_1|^2 + |\Psi_2|^2)^2 + v [\operatorname{Re}(\Psi_1^* \Psi_2)^2 - |\Psi_1|^2 \Psi_2|^2], \qquad (4.3)$$

where u, v > 0 and gradient terms have been ignored. Similarly, for the triangular lattice it gives

$$F = r_0 (|\Psi_1|^2 + |\Psi_2|^2) + u (|\Psi_1|^2 + |\Psi_2|^2)^2 + v |\Psi_1|^2 |\Psi_2|^2 , \qquad (4.4)$$

where u, v > 0, and no coupling between phases arises in the quartic term. Note, however, that Eq. (4.4) can be transformed into the same form as Eq. (4.3) by the change of variables  $\Psi_1 \rightarrow \Psi_1 + i\Psi_2$  and  $\Psi_2 \rightarrow i\Psi_1 + \Psi_2$  (see also Ref. 34). So up to fourth order in  $\Psi_1, \Psi_2$  both the square and triangular FFXY models has a free energy precisely of the same form (4.3) but with a different relation between  $r_0$ , u, and v. In both cases we find u, v > 0.

If the free energy (4.3) is extended to general dimensions d and number of components n, an  $\epsilon = 4-d$ renormalization-group analysis<sup>34</sup> reveals the existence of a stable fixed point for some range of n and d. The critical exponents differ from those of the pure O(n) model and suggest a new universality class. We thus expect a rather nontrivial behavior in d = 2 dimensions.

A similar result for the Ginzburg-Landau free energy was obtained by Yosefin and Domany<sup>7</sup> using a symmetry analysis. They also reach the conclusion that both square and triangular cases are described by the same free energy, which however, differ slightly from (4.3) in the last term. They find instead a more general form

$$w |\Psi_1|^2 |\Psi_2|^2 + v \operatorname{Re}(\Psi_1^* \Psi_2)^2$$
, (4.5)

but they assumed w > 0. From a renormalization-group analysis in  $4-\epsilon$  dimensions they concluded that a firstorder transition is expected, since all stable fixed points of the recursion relation were found to reside in the region w < 0. Note, however, that (4.5) reduces to the form found in (4.3) when w = -v, precisely the opposite sign from what was assumed. In this region a stable fixed point is possible, as discussed in Ref. 34. We believe that the free energy in the form given by (4.3) is the appropriate one for the square and triangular FFXY models, since it can be obtained by a Hubbard-Stratnovich transformation, which gives explicitly the coefficients u, w, and vwithout any particular assumption on the sign or magnitude of these quantities. Near d=2 where amplitude fluctuations can be ignored both (4.3) and (4.5) leads to the same result.

In two dimensions the phase transition occurs well below the mean-field critical temperature and fluctuations in the magnitude of the order parameter are usually irrelevant. So we can approximate these magnitudes by their corresponding mean-field values  $\Psi_{1,2}$  $= -r_0/(4u - 2v)$  obtained by minimizing Eq. (4.3) and consider only phase fluctuations. One then obtains an effective lattice Hamiltonian in the form of two coupled XY models

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} \left[ \alpha \cos(\theta_{1,i} - \theta_{1,j}) + \beta \cos(\theta_{2,i} - \theta_{2,j}) \right]$$
$$-g \sum_{\langle ij \rangle} \cos(\theta_{1i} - \theta_{2i} - \theta_{1j} + \theta_{2j})$$
$$-h \sum_{i} \cos^2(\theta_{1i} - \theta_{2i})$$
(4.6)

with g = 0 and  $\alpha = \beta$  initially. For convenience we define the model on a square lattice.

In Ref. 6 a different conclusion was reached with respect to the triangular case, which was found to be described by two coupled XY models with a coupling term  $\cos 3(\theta_1 - \theta_2)$  instead the one in Eq. (4.6). They arrived at this conclusion by assuming a phase only approximation starting from the free energy in the from (4.4) and noting that coupling between the phases first appears in the sixth-order term. However, since v > 0, the last term in (4.4) favors either  $\Psi_1=0$  or  $\Psi_2=0$ , which invalidates this kind of approximation, since the magnitude of the order parameter must be nonzero. If one instead performs a change of variables, as described above, one obtains (4.3), which is an appropriate starting point. Similar conclusions to ours were also obtained in a slightly different way in Refs. 7, 34, and 35.

Berge et al.<sup>13</sup> have studied by Monte Carlo simulations an anisotropic version of the fully frustrated XY model on a square lattice by introducing antiferromagnetic couplings differing by a factor  $\eta$  from the ferromagnetic ones. Ginzburg-Landau expansions similar to Eq. (4.3) can also be constructed<sup>9</sup> for this case and leads to coupled XY models in Eq. (4.6) with  $\alpha \neq \beta$  when  $\eta \neq 1$ .

The model in Eq. (4.6) has been studied by renormalization-group methods using a Coulomb-gas representation.<sup>8</sup> It was found that g becomes negative and his very relevant under renormalization. Also  $\alpha = \beta$  is only preserved under renormalization if they are initially equal. For  $\alpha \neq \beta$ , a double transition is found with an Ising followed by an XY transition as temperature is increased in agreement with the Monte Carlo simulations.<sup>13</sup> It can also be shown in this case that the signature of the Ising transition appears as a logarithmic singularity in the helicity modulus, which also seems to agree with Monte Carlo simulations.<sup>9</sup> No definitive conclusions, however, could be obtained by these methods in the region of single transitions of interest for the isotropic fully frustrated XY model ( $\eta = 1$ ) because too many parameters become relevant and the renormalization-group approximation breaks down. We can imagine, however, performing a rescaling of the lattice until h is large enough so that we can take the limit  $h \rightarrow \infty$ . In that case  $\theta_{2r} = \theta_{1r} + \pi \tau_r$ , where  $\tau = 0, 1$  and an effective Hamiltonian is obtained in the form of coupled XY-Ising models  $(\sigma_r = 2\tau_r - 1):$ 

$$\frac{H}{kT} = -\sum_{\langle rr' \rangle} [A_{\text{eff}}(1 + \sigma_r \sigma_{r'}) \cos(\theta_r - \theta_{r'}) + C_{\text{eff}} \sigma_r \sigma_{r'}],$$
(4.7)

where  $A_{\text{eff}}$  and  $C_{\text{eff}}$  are effective couplings both depending on the initial values of  $\alpha$  and h and consequently have a different relation for the square and triangular FFXY model. However, the critical behavior of both models can be described using the same effective lattice Hamiltonian. The same result has been obtained by Yosefin and Domany<sup>7</sup> from a Ginzburg-Landau type of expansion obtained from symmetry analysis. They assumed, however, C = 0 for both models.

The precise relation between the renormalized parameters  $A_{\text{eff}}$ ,  $C_{\text{eff}}$  in Eq. (4.7) is difficult to obtain because the limit  $h \rightarrow \infty$  of Eq. (4.6) is outside the range of validity of the renormalization-group approximation. However, from a numerical iteration of the recursion relations<sup>8</sup> we expect that  $|C_{\text{eff}}| \ll A_{\text{eff}}$  but of negative sign. The parameters of the square and triangular cases should lie close to the bifurcation point, and they are likely to be in the region of single transitions in the phase diagram. There is no special symmetry in the model (4.7), which would indicate the position of this bifurcation point so this question can only be answered by performing numerical simulations on the original fully frustrated XY model and detecting either a single or a double transition. The result will also dependent on the form of interaction between the XY spins as this will influence the relative values of the parameters controlling the XY and Ising transition.

A similar situation also occurs in other approaches. In the Coulomb-gas representation of fractional charges,<sup>14</sup> one finds a phase diagram with identical topology as in Fig. 3, where A corresponds to the coefficients K of the logarithmic interacting charges and C to a nearestneighbor Ising coupling J of the antiferromagnetic arrangement of positive and negative charges. The authors assumed that the original model corresponds to J = 0 but the Coulomb-gas representation is obtained from a Villain approximation to the cosine interaction of the original model. The value of J controls the relative position of the XY and Ising-like transitions, and there is no special reason for this relation to remain the same within this approximation. This is possibly the reason why the numerical simulations in the Coulomb-gas representation and in the original phase variables disagree regarding a double or a single transition.<sup>2-4,14,15</sup>

Recently, we have performed Monte Carlo simulations for the FFXY model on a square and triangular lattice.<sup>28</sup> From a finite-size scaling analysis of the data, using the same methods as those described in Sec. III, we obtained v=0.83(4) and 0.85(3), and  $2\beta/v=0.28(4)$  and 0.31(3) for the triangular and square lattices, respectively. They agree with each other within the estimated uncertainties but are significantly different from the pure Ising model, suggesting they lie in the region of single transitions in the phase diagram of the coupled XY-Ising model. These exponents are also consistent with the values obtained from the simulations described in Sec. III. In addition, a recent evaluation<sup>17</sup> of the central charge of FFXY model by a Monte Carlo transfer matrix gives a result c = 1.66(4) within the range of the corresponding result from the coupled XY-Ising model along the line of varying critical exponents.<sup>27</sup> The estimates of  $2\beta/\nu$  of Refs. 17 and 28 agree within numerical uncertainties but not for v. In the latter, v was determined by a very indirect method and found to be consistent with unity. Our Monte Carlo evaluation, which involves a one parameter fit to the data, is definitely inconsistent with v=1.

## **V. CONCLUSIONS**

We have investigated by real-space renormalizationgroup methods and Monte Carlo simulations the phase diagram of a coupled XY-Ising model. This model can describe the critical behavior of various physical systems of theoretical and experimental interest. In particular, the fully frustrated XY model on a square and triangular lattice was analyzed in some detail, and arguments were given showing that these two cases can be considered to lie along different paths in the same coupled XY-Ising model. The same result also applies to Josephsonjunction arrays in a magnetic field with a half flux quantum per plaquette. In either case, changing the temperature will drive the system through a double or a single transition. In the former there will be an XY followed by an Ising transition as temperature is increased, and in the latter a single transition will occur, which can either be continuous or first order depending on the parameters. This line of continuous transitions has varying critical exponents, and so different paths will lead to different critical behavior. This may be the case of the FFXY model on a square and triangular lattice, which have the same symmetries. In fact, a calculation of the critical exponents of FFXY from Monte Carlo simulations,<sup>28</sup> using

the same methods described in this work, gives results very different from the pure Ising model, indicating that they lie in the single transition region, and a nonuniversal behavior is expected.

The line of single transitions, which we have investigated in this work, is expected to be of critical behavior of a new universality class. In addition to varying critical exponents, a calculation of the central charge shows that this quantity appears to vary continuously along this line.<sup>27</sup> Although the results for the central charge are very puzzling and are currently under further investigation,<sup>36</sup> they do seem to support the conclusion that this line is expected to show a rather nontrivial critical behavior, which cannot be described as a superposition of a critical Ising and XY model. The FFXY model on a square lattice, which we expect to undergo a transition corresponding to some point along this line, has already been found to have critical exponents<sup>28</sup> and central charge<sup>17</sup> within the range of the values obtained for the coupled XY-Ising model.

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# APPENDIX

In this Appendix we use a Migdal-Kadanoff renormalization-group approximation to obtain a qualitative global phase diagram of the coupled XY-Ising model defined in Eq. (1.2).

To apply the method we first consider a more general form of Eq. (1.2),

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} \left[ (1 + \sigma_i \sigma_j) V(\theta_i - \theta_j) + C \sigma_i \sigma_j \right], \quad (A1)$$

where  $V(\theta)$  has periodicity  $2\pi$  and initially have the form  $V(\theta) = A \cos\theta$ . Grouping the unit cells of the square lattice into large cells with scale factor *b*, and moving the internal bonds to the perimeter we can integrate out the sites in one dimension obtaining effective interactions between the remaining ones. Using for simplicity b = 2, in terms of  $u(\theta) = \exp[V(\theta) - V(0)]$ ,  $z = \exp[V(0) + C]$ , we obtain renormalized parameters (primed) as

$$(z')^{2} = [z^{4}A_{1}(0) + z^{-4}]/2A_{2},$$
  
$$(u')^{2}(\theta) = [z^{4}A_{1}(\theta) + z^{-4}]/[z^{4}A_{1}(0) + z^{-4}],$$
 (A2)

where

$$A_{1}(\theta) = \int_{0}^{2\pi} \frac{d\phi}{2\pi} u^{4}(\phi) u^{4}(\theta - \phi) ,$$
$$A_{2} = \int_{0}^{2\pi} \frac{d\phi}{2\pi} u^{4}(\phi) .$$

Numerically, it is more convenient to follow the recursion relations for  $u(\theta)$  using its Fourier components u(s). The effective coupling of  $V(\theta)$  can be identified as  $A_{\text{eff}} = \sum_{s} s^2 u(s)$ . For the standard XY model at low temperatures,  $u(\theta)$  relaxes after a few iterations to a Villain potential, with Fourier components  $u(s) \propto \exp(-s^2/2A)$ . For the Villain potential  $A_{\text{eff}} \approx J$  as can be seen by replacing summation by integration. This function is nearly invariant under the renormalization-group transformation when  $A_{\text{eff}} > 2/\pi$ , since the change per iterate is rather small.<sup>37</sup> So will identify the critical  $A_c$  in our case by re-

Eq. (A1). The phase diagram obtained by iterating numerically Eqs. (A2) is indicated in Fig. 2. We find four different phases: (a) a disordered (high-temperature phase where  $C, A_{eff} \rightarrow 0$ , (b) an intermediate Ising-ordered phase where  $C \rightarrow \infty$  but  $A_{\text{eff}} \rightarrow 0$ , (c) an ordered (low-temperature phase where  $C \rightarrow \infty$  and  $A_{\text{eff}} \rightarrow A^*$ , and (d) an antiferromagnetic Ising-ordered phase where  $A \rightarrow 0$ , but  $C \rightarrow \infty$ . In the last phase,  $C \rightarrow \infty$  because, by using the scale factor b=2, the decimation procedure maps the antiferromagnetic ground state into a ferromagnetic one. We have performed the calculation with b = 3, which avoids this problem and get  $C \rightarrow -\infty$  in this phase. However, we found it less time consuming in this case to use a transfer matrix implementation of the decimation procedure.

quiring that after a few iterations  $A'_{\text{eff}} \approx 1/\pi$ , which gives the known result for the XY model in the limit  $C \rightarrow \infty$  in

The line joining point P to F in the phase diagram is not actually a single line within our renormalizationgroup approximation. This comes as no surprise, since **A** is not a true fixed point where the line of almost fixed points at low temperature terminates, as one would expect, in the limit  $C \rightarrow \infty$ . However, within an uncertainty of about 1% they are very close, and so we will hereafter consider it as single line and regard this effect as a shortcoming of the Migdal-Kadanoff approximation. Also for the same reason, we cannot locate point P with precision, although it is close to the line of initial points C=0.

To investigate the first-order transition within our real-space renormalization-group analysis, we generalize the procedure of Nienhuis *et al.*,<sup>22</sup> which reproduces the known first-order transition for the *q*-state Potts model when q > 4. The procedure consists of enlarging the parameter space of the original model by including a local variable  $t_i = 0$  or 1 corresponding to presence or absence of a vacancy state. The Hamiltonian in this lattice-gas version of our coupled XY-Ising model takes the form

$$\frac{H}{kT} = -\sum_{\langle ij \rangle} \left[ (1 + \sigma_i \sigma_j) t_i t_j V(\theta_i - \theta_j) + C t_i t_j \sigma_i \sigma_j + K t_i t_j \right] + \Delta \sum t_i . \quad (A3)$$

The  $C \rightarrow \infty$  of this model has been studied in a different context in Ref. 38.

Applying the same Migdal-Kadanoff approximation to this model we obtain in terms of  $u(\theta), z, w = \exp[K + V(0)]$  and  $y = \exp(\Delta)$ , the following recursion relations

$$(z')^{2} = \frac{2w^{-4}y + z^{-4} + z^{4}A_{1}(0)}{2w^{-4}y + 2A_{2}},$$

$$(u')^{2}(\theta) = \frac{2w^{-4}y + z^{-4} + z^{4}A_{1}(\theta)}{2w^{-4}y + z^{-4} + z^{4}A_{1}(0)},$$

$$(A4)$$

$$(w')^{2} = 8(1+y)^{2}(w^{-4}y + A_{2})\frac{2w^{-4}y + z^{-4} + z^{4}A_{1}(0)}{2w^{-4}y + z^{-4} + z^{4}A_{1}(0)},$$

$$(w')^{2} = 8(1+y)^{2}(w^{-4}y + A_{2})\frac{1}{(2w^{-2}y + z^{-2} + z^{2}A_{2})^{4}},$$
  
$$y' = 16y^{2}\frac{w^{-8}(1+y)^{4}}{(2w^{-2}y + z^{-2} + z^{2}A_{2})^{4}}.$$

To obtain the above equations, in the bond moving procedure we chose to distribute the site term  $\Delta t_i$  equally between the adjoining bonds in order to preserve the density of sites after each decimation. This turns out to be important to obtain the correct fixed points at  $K \rightarrow \infty$ , where phase separation can occur.

The first-order line appears in the limit  $K, \Delta, z \rightarrow \infty$ where one finds an almost fixed line when

$$y'(w')^{-2}(z')^{-2} = 4y^4 w^{-8} z^{-8} / [A_1^*(0)]^2$$
 (A5)

To obtain (A5) we have used the Villain form into Eqs. (A4) and replaced summations by integrals. Along the unstable direction we find, for small deviation, an eigenvalue  $\lambda = b^d = 4$ , where d is the dimension of the lattice. This is in accordance with the Nauemberg-Nienhuis<sup>39</sup> criterion for a first-order transition to occur. By numerically iterating Eqs. (A4) we can construct a phase diagram as a function of the vacancy fugacity  $e^{\Delta}$ , and we find a first-order transition beyond a finite value of this fugacity, which decreases as C gets large and negative. This suggests that along the line PF of Fig. 1 a first-order transition can appear.

The original Hamiltonian, however, corresponds to  $\Delta \rightarrow -\infty$  in the lattice-gas version, and this limit is stable under the renormalization-group transformations of Eqs. (A4). This stability, however, is a deficiency of the Migdal-Kadanoff approximation, which leaves invariant the number of states at each site after decimation. In the case studied by Nienhuis et al.<sup>22</sup> a Niemejier-van Leeuwen type of real-space renormalization group<sup>40</sup> was used, which can generate vacancy states after the first step of the renormalization procedure. To correct this deficiency we first apply a prefacing transformation,<sup>23</sup> which allows the generation of vacancy states and then use the resulting Hamiltonian as defining initial parameters from which we continue with the renormalizationgroup transformations given in Eqs. (A4). This type of hybrid approach has also been used by Mizrahi and Domany<sup>41</sup> in a study of the Z(5) model.

Our prefacing transformation consists of dividing the square lattice into cells of four sites each and projecting the configurations of the site variables within a cell into cell variables  $\sigma'$ ,  $\theta'$ , and t. This results in a new restructured Hamiltonian in terms of cell variables with nearest-neighbor couplings A', C' and vacancy fugacity  $e^{\Delta}$ . There is a certain freedom in choosing the projection

operator. We choose the one that generates the minimum number vacancy state, as follows: (a) if the sum of the Ising spins is different from zero, there is no vacancy (t=1), and we then assign a cell Ising spin  $\sigma'=\pm 1$  according to the majority rule and an angle cell variable  $\theta'$  as an average over the coupled sites; (b) to the remaining configurations we assign vacancy state t=0.

This prefacing transformation can be viewed as a first step of a Niemejier-van Leeuwen type of renormalization-group transformation. To evaluate the new coupling parameters we use a cumulant expansion. This consists in dividing the initial Hamiltonian into intracell and intercell parts and developing a cumulant expansion in the intercell couplings. Within a first-order cumulant expansion we obtain

$$A' = 2J(e^{4C}h_1 + 2h_2 + h_3)/(e^{4C}f + 4g)^2,$$
  

$$C' = 2L(e^{4C}f + 2g)^2/(e^{4C}f + 4g)^2,$$
  

$$e^{\Delta} = [4I_0^2(2A) + 2e^{-4C}]/(e^{4C}f + 4g),$$
  
(A6)

where  $I_0$  is the modified Bessel function and

$$h_{1} = \left[ \prod_{i} \int 'd\theta_{i} \right] \exp\{2A \left[ \cos(\theta_{1} - \theta_{2}) + \cos(\theta_{2} - \theta_{3}) + \cos(\theta_{3} - \theta_{4}) + \cos(\theta_{4} - \theta_{1}) \right] \} \cos(\theta_{1} - \theta') ,$$

$$h_{2} = \left[ \prod_{i} \int 'd\theta_{i} \right] \exp\{2A \left[ \cos(\theta_{1} - \theta_{2}) + \cos(\theta_{2} - \theta_{3}) \right] \} \cos(\theta_{1} - \theta') ,$$

$$h_{3} = \left[ \prod_{i} \int 'd\theta_{i} \right] \exp\{2A \left[ \cos(\theta_{1} - \theta_{2}) + \cos(\theta_{2} - \theta_{3}) \right] \} \cos(\theta_{2} - \theta') ,$$

$$f = \left[ \prod_{i} \int 'd\theta_{i} \right] \exp\{2A \left[ \cos(\theta_{1} - \theta_{2}) + \cos(\theta_{2} - \theta_{3}) + \cos(\theta_{3} - \theta_{4}) + \cos(\theta_{4} - \theta_{1}) \right] \} ,$$

$$g = \left[ \prod_{i} \int 'd\theta_{i} \right] \exp\{2A \left[ \cos(\theta_{1} - \theta_{2}) + \cos(\theta_{2} - \theta_{3}) + \cos(\theta_{3} - \theta_{4}) + \cos(\theta_{4} - \theta_{1}) \right] \} .$$
(A7)

The primes to the integrals imply that the integrals are to be carried out under the constraint of  $\theta'$  being the average over the variables  $\theta_i$ . The functions  $h_i$ , f, and g have an implicit dependence on the cell angle  $\theta'$  because of the constraint. We follow Lublin<sup>42</sup> and take an average of these coefficients over the cell angles in order to obtain a  $\theta$ -independent result.

Using Eq. (A6) to obtain initial values of A', C', and

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 $e^{\Delta}$ , we continue with the renormalization-group transformation using Eqs. (A4). We find a tricritical point T along the line C < 0 located at  $A + C \approx 0.49$ ,  $A \approx 1.5$ , where a line of first-order transitions TF starts. The location of this point is only approximate, since it will depend on the choice of the projection operator used in the prefacing transformation.

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