Monte Carlo simulation for square planar model with a small fourfold symmetry-breaking field

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Monte Carlo (MC) simulations on the square planar rotator model with small fourfold symmetry-breaking field h_4 points out the existence of a Berezinskii-Kosterlitz-Thouless phase at intermediate temperatures between the low-temperature ferromagnetic phase and the high-temperature paramagnetic phase. This result contrasts with the expectation of a single order-disorer phase transition characterized by nonuniversal critical exponents for any h_4 as suggested by a renormalization group analysis and confirmed by MC simulations for intermediate and large symmetry-breaking fields.

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The phase diagram of the two-dimensional (2D) planar model with symmetry-breaking fields is characterized by a low-temperature ferromagnetic phase and a high-temperature paramagnetic phase. When the order of the symmetry-breaking field h_p is $p \leqslant 4$ only an order-disorder phase transition is expected.[1] For $p=4$ the phase transition is characterized by nonuniversal critical exponents. On the contrary, when $p>4$ a Berezinskii-Kosterlitz-Thouless (BKT) phase[2] is believed to occur between the low-temperature ferromagnetic phase and the high-temperature paramagnetic phase. The phenomenology of the planar rotator model is strongly affected by the presence of symmetry-breaking fields which are always *relevant* at low temperature, destroying the BKT phase. However, the occurrence of a BKT phase at intermediate temperatures is determined by the order p of the symmetry-breaking field. Indeed for $p>4$ two critical temperatures are suggested by a RG analysis on a generalized Villain model believed to be in the same universality class of the planar rotator model with symmetry-breaking fields:[1] one—say, T_1—at which the symmetry-breaking field becomes irrelevant and one—say, T_2—at which the vortices break free. The BKT phase that occurs in the range $0<T<T_2$ for $h_p=0$ (planar rotator model) survives in a restricted range $T_1<T<T_2$ only if $p>4$.

Monte Carlo (MC) simulations were performed on models with $h_p \to \infty$ (p-state clock models).[3,4] For $p=4$ a single phase transition was found with a critical temperature and critical exponents that agree with the Ising exponents as it must since the four-state clock model on a square lattice is equivalent to two decoupled Ising models.[5] For the five-state[3] and six-state[3,4] clock models two successive phase transitions are found: the former corresponding to the ferromagnetic-BKT phase transition, the latter to the BKT-paramagnetic phase transition.

Only recently have MC simulations on the planar model with *finite* symmetry-breaking field h_p been performed[6] on square and triangular lattices with symmetry-breaking fields of fourth and sixth order, respectively. For the fields at which MC simulations were performed ($h_p \geqslant 1$) the results confirmed the RG expectation according to which a BKT phase is found for $p=6$ and a second-order phase transition with nonuniversal critical exponents is found for $p=4$. MC simulations agree with the p-state clock model results of Refs. 3 and 4 in the limit $h_p \to \infty$.

Here we show results of MC simulations on a planar model with *small* fourfold symmetry-breaking fields ($h_4 \lesssim 0.5$) and we find, unexpectedly, that the scenario is very similar to that found in the h_6 case. Indeed a *bubble* of BKT phase occurs also for the fourfold symmetry-breaking field at odds with the RG expectation.[1] The BKT bubble shrinks to a second-order transition line for $h_4 \simeq 0.5$ so that the transition characterized by nonuniversal critical exponents is recovered only for $h_4 \gtrsim 0.5$.

The Hamiltonian of the model reads

$$\mathcal{H}/J = -\sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - h_4 \sum_i \cos(4\theta_i), \tag{1}$$

where the first sum is restricted to couples of nearest neighbors, i and j run over a square lattice, θ_i is the angle the classical two-component unit vector, located on the site i, makes with the x axis, $J>0$ is the ferromagnetic exchange coupling, and $h_4>0$ is the fourth-order symmetry-breaking field.

We have performed MC simulations on lattices of size $L \times L$ with periodic boundary conditions, where $L=16$, 24, 32, 48, and 64. The most part of the data points are obtained by an average of 8 independent runs of $10^5 - 10^6$ MC steps taking a configuration every 10 MC steps and disregarding 1000 MC steps for equilibration. The data points are obtained by raising the temperature by $\Delta T = 0.01$ (in units of J/k_B) and assuming as starting configuration the last configuration of the previous temperature. In our simulation we evaluate the specific heat

$$C_L = [\langle \mathcal{H}_L^2 \rangle - \langle \mathcal{H}_L \rangle^2]/(L^2 k_B T^2), \tag{2}$$

the order parameter

$$m_L = (1/L^2)\langle |\boldsymbol{M}_L| \rangle, \tag{3}$$

where

$$\boldsymbol{M}_L = \left(\sum_{i=1}^{L^2} \cos\,\theta_i, \sum_{i=1}^{L^2} \sin\,\theta_i \right), \qquad (4)$$

the susceptibility

$$\chi_L = [\langle \boldsymbol{M}_L^2 \rangle - \langle |\boldsymbol{M}_L| \rangle^2]/(L^2 k_B T), \qquad (5)$$

and the fourth-order cumulant[7]

$$U_L = 1 - \langle \boldsymbol{M}_L^4 \rangle / [3\langle \boldsymbol{M}_L^2 \rangle^2]. \qquad (6)$$

As discussed in Ref. 6 the analysis of $U_{L'}$ as a function of U_L allows us to distinguish between a continuous and a BKT phase transition and one can obtain the critical exponent ν by means of the relationship

$$(\partial U_{L'}/\partial U_L)_{T=T_c} = (L'/L)^{1/\nu}, \qquad (7)$$

where $1/\nu$ is finite for continuous phase transitions and zero for a BKT transition.

In Fig. 1 we give the susceptibility versus temperature for several lattice sizes for $h_4=0.01$, 0.05, 0.1, 0.2, 0.5 and for $h_4 \to \infty$. Notice the similarity of the figures with $h_4<0.5$ with Fig. 8 of Ref. 6 where the size scaling of the susceptibility for the sixfold symmetry-breaking field $h_6=1$ is shown. In that case the existence of a BKT phase was supported by both analytic renormalization group (RG) calculations and MC simulations. The size dependence of the susceptibility observed for $h_4<0.5$ is a strong indication of the occurrence of the BKT phase also in this case. The shoulder in the susceptibility for $h_4<0.5$ increases as L increases and it is expected to diverge for $L\to\infty$ so that a *finite* range of temperature with divergent susceptibility, typical of the BKT phase, is expected in the thermodynamic limit. Note that the size-dependent shoulder appears at lower temperature as h_4 decreases.

For vanishing h_4 the specific heat shows a size-independent peak around $T\simeq 1$, in agreement with the pure planar rotator model. As h_4 goes from 0.05 to 0.5 a size-independent shoulder develops in the specific heat moving from $T\simeq 0.5$ to $T\simeq 1$ and it merges into the BKT peak at $h_4\simeq 0.5$. For $h_4>0.5$ the peak of the specific heat becomes size dependent as shown in Fig. 1 of Ref. 6 for $h_4=1$ and $h_4=2$, eventually leading to a logarithmic divergence for $h_4\to\infty$ (four-state clock model). We recall that a two-peak structure of the specific heat was found for a sixfold anisotropy h_6 where the presence of the BKT phase is assured for any h_6. Obviously, the two-peak structure is expected to meet the one-peak structure of the pure planar model for vanishing symmetry-breaking fields, so that it is not surprising that for $h_4<0.5$ only a vague recollection of the two-peak structure is found.

The order parameter for $0.01<h_4<0.5$ shows three different behaviors: it is size independent at low temperature (ferromagnetic phase) and shows a different size dependence at intermediate (BKT phase) or high temperature (paramagnetic phase). This behavior is similar to that found for a sixfold anisotropy as shown in Fig. 7 of Ref. 6 where the occurrence of the BKT phase is confirmed by both MC simulations and RG analysis. For $h_4>0.5$ the typical behavior of a continuous order-disorder phase transition is recovered until the 2D Ising model behavior is reached in the limit $h_4\to\infty$.

It is well known that in the BKT phase the finite-size scaling of the order parameter is $m_L \simeq L^{-\eta/2}$ where η is a function of the temperature. For sixfold symmetry-breaking fields[1,6] η increases from $\eta\simeq 0.10$ at T_1 to $\eta\simeq 0.25$ at T_2. In Fig. 2 the log-log plot of the order parameter versus lattice size for several temperatures with $h_4=0$, 0.01, 0.05, 0.1, 0.2, and 0.5 shows curves with upward concavity (ferromagnetic phase), straight lines (BKT phase), and curves with downward concavity (paramagnetic phase). We have located the temperature region where the BKT phase occurs, fitting data points with a straight line and looking at the error on its slope η. The error is minimum for true straight lines (less than 0.1%). Following this criterion we determine T_1 and T_2 within 1%–2%. This temperature region $(T_1<T<T_2)$ shrinks going from $h_4=0$, where $T_1=0$ and $T_2=T_{BKT}\simeq 0.9$, to $h_4=0.5$, where $T_1=T_2\simeq 0.95$, pointing out that a second-order phase transition replaces the BKT phase. The critical exponent η at $T=T_2$ is $\eta\simeq 0.25$ for any h_4.

In Fig. 3 we show the fourth-order cumulant U_{64} as function of U_{32}. For $h_4=0.5$ a single crossing of the data points with the straight line $U_{64}=U_{32}$ is clearly seen, in agreement with the occurrence of a continuous phase transition as obtained in Ref. 6 for $h_4\geqslant 1$, whereas for $h_4=0.2$, 0.1, 0.05, 0.01 the data points make a bump at low temperatures and fall on the straight line $U_{64}=U_{32}$ at intermediate temperatures. This behavior is the signature of the existence of the BKT phase as discussed in Ref. 6 for $p=6$. Finally, the paramagnetic phase is pointed out by the shifting of the data points from the straight line. The range of the BKT phase shrinks at increasing h_4 in agreement with the range of temperature where the size dependence of the susceptibility is observed in Fig. 1 and the linear behavior of the order parameter versus size is shown in Fig. 2. The finite-size scaling equations of the magnetization and the susceptibility expected for a BKT phase are given by[4]

$$m_L L^b = f_1(L^{-1} e^{a t^{-1/2}}), \qquad (8)$$

$$\chi_L L^{-c} = f_2(L^{-1} e^{a t^{-1/2}}), \qquad (9)$$

where $b=\eta(T_1)/2$ with $t=(T_1-T)/T_1$ in Eq. (8) and $c=2-\eta(T_2)$ with $t=(T-T_2)/T_2$ in Eq. (9). The critical exponent $\eta(T)$, related to the algebraic decaying of the correlation function, is obtained at T_1 and T_2 from Fig. 2 by the slope of the straight lines $\ln(m_L)$ vs $\ln(L)$. For example, for $h_4=0.1$ one has $T_1=0.85$ with $\eta(T_1)=0.18$ and $T_2=0.91$ with $\eta(T_2)=0.25$. The susceptibility appearing in Eq. (9) is evaluated as[4] $\chi_L=\langle M_L^2\rangle/(L^2 k_B T)$. In Fig. 4 we show the universal behavior of the magnetization for $T_1=0.85$ and of the susceptibility for $T_2=0.91$ with $h_4=0.1$. Note that the choice of T_1, T_2, $\eta(T_1)$, and $\eta(T_2)$, obtained by the finite-size scaling of the order parameter $m_L\simeq L^{-\eta/2}$, is crucial to get the universal curves of Fig. 4.

A comparison with the expectations of Ref. 1 is in order. Indeed a RG analysis of a generalized Villain model which is believed to have the same symmetry properties of the planar rotator model with the symmetry-breaking fields leads to the

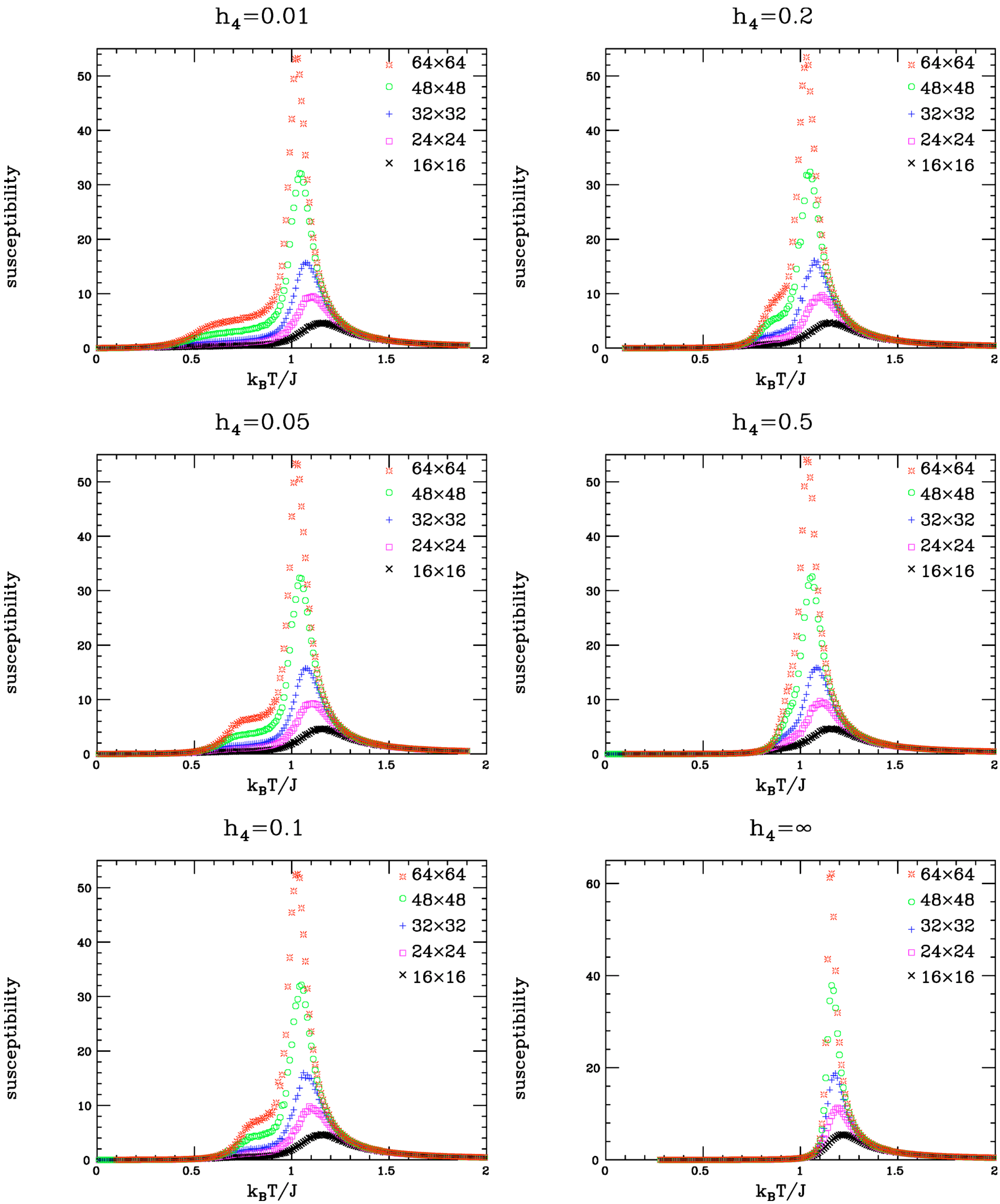

FIG. 1. Susceptibility for $h_4=0.01$, 0.05, 0.1, 0.2, 0.5, ∞ (four-state clock model) for different lattice sizes $L=16$, 24, 32, 48, 64.

recursion equations given by Eqs. (5.17) of Ref. 1 which are expected to be correct to the the leading order in y_0 (a parameter related to the presence of unbound vortices) and y_p (a parameter related to the symmetry-breaking fields). Note that the Villain model[8] is recovered for $y_0=1$ and $y_p=0$. It is direct to obtain the asymptotic solution ($l\to\infty$) of Eqs. (5.17). Two kinds of solutions are found for $p\leqslant 4$. For initial conditions $T<T_2(h_p)$, $y_0=1$, and $y_p=2h_p$ with $T_2(0)=1.362\,80$ one finds that $T\to 0$, $y_0\to 0$ and $y_p\to\infty$ for $l\to\infty$. This is the signature of the ferromagnetic phase where

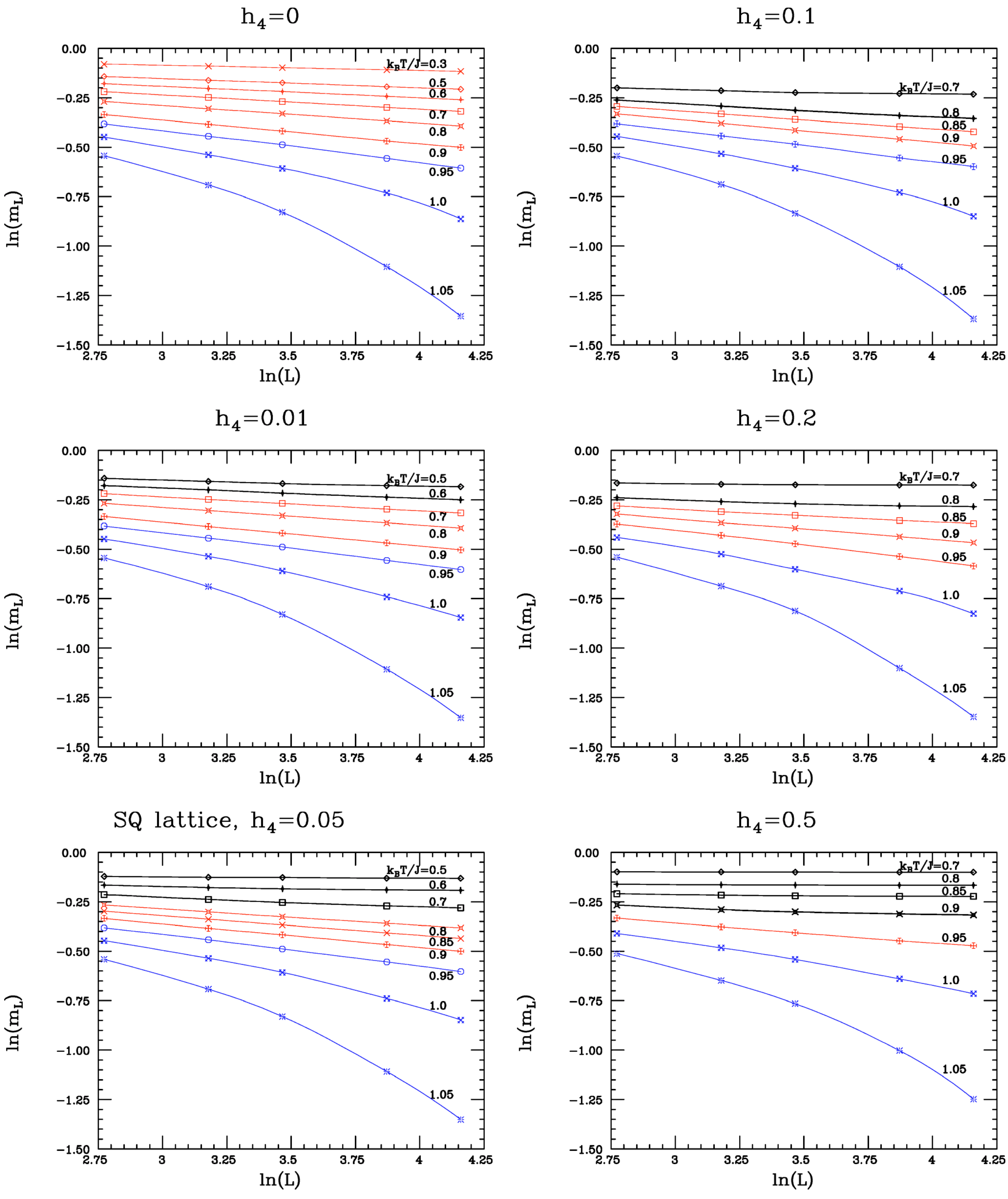

FIG. 2. Log-log plot of the order parameter vs lattice size for several temperatures for $h_4=0$, 0.01, 0.05, 0.1, 0.2, 0.5.

the symmetry-breaking fields are relevant and the unbinding of vortices does not occur. For initial conditions $T > T_2(h_p)$, $y_0 = 1$, and $y_p = 2h_p$ one finds that $T \to \infty$, $y_0 \to \infty$, and $y_p \to 0$ for $l \to \infty$, corresponding to the paramagnetic phase in which the symmetry-breaking fields become irrelevant and the unbinding of vortices occurs. For $p > 4$ a third region appears. Indeed for initial conditions $T_1(h_p) < T < T_2(h_p)$, $y_0 = 1$, and $y_p = 2h_p$ one finds $T \to T_\infty$, $y_0 \to 0$, and $y_p \to 0$ for $l \to \infty$ with $8\pi/p^2 < T_\infty < \pi/2$. This scenario corresponds to the BKT phase since the symmetry-breaking fields are irrelevant and vortices are bound so that the planar rotator model properties are recovered. As one can see the BKT phase is limited be-

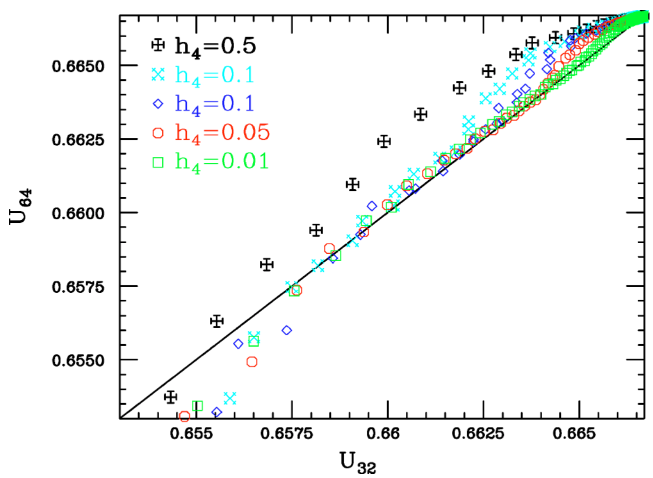

FIG. 3. Fourth-order cumulant U_{64} vs U_{32} for several h_4: $h_4=0.01$ (squares), $h_4=0.05$ (circles), $h_4=0.1$ (diamonds), $h_4=0.2$ (crosses), and $h_4=0.5$ (vertical crosses).

tween T_1 and T_2. For $h_6 \to 0$ the BKT phase is restricted to $0.698\,12 < T < 1.362\,80$. For $p=4$ only one transition is found at $T_2=1.362\,80$ for $h_4=0$ increasing with the symmetry-breaking field—i.e., $T_2=1.403\,46$, $1.448\,26$, $1.491\,60$, and $\pi/2$ for $h_4=0.2$, 0.4, 0.6, and 1, respectively. As one can see from the nature of the differential equations (5.17) of Ref. 1 a *bubble* of BKT phase is prevented by uniqueness of the solution. Indeed the existence of a bubble would imply that the same initial condition for the temperature leads to two different asymptotic solutions $T_\infty = 8\pi/p^2$ and $T_\infty=\pi/2$. On the other hand, MC simulations on the true model indicate the presence of a BKT phase for $h_4 \lesssim 0.5$ extending from 0 to $T_2 \simeq 0.90$ for $h_4 \to 0$. The region shrinks at increasing h_4 until a line is found for $h_4 \gtrsim 0.5$ where the RG scenario is recovered. The MC simulations of the present paper confirm the merits of the generalized Villain model and of the RG analysis performed in Ref. 1 to guess the critical behavior of the planar rotator model with symmetry-breaking fields (true model). However, some peculiarities of the true model seem to escape the generalized Villain model studied in Ref. 1. In particular, the case $p=4$ gives correct results only for intermediate values of the symmetry-breaking field ($h_4 \gtrsim 0.5$). Indeed the critical behavior of the true model seems to be richer than the corresponding generalized Villain model. Another property of the true model escaped the generalized Villain model is the limit of $T_1(h_p)$ for $h_p \to 0$ when $p \geqslant 4$. Indeed Eqs. (5.17) of Ref. 1 give $T_1(h_p) \to T_p \neq 0$ for $h_p \to 0$ (for instance, $T_4=1.362\,80$, $T_5=1.003\,82$, $T_6=0.698\,12$, and $T_8=0.392\,70$) while MC simulations on models with $p=4$ and $p=6$ lead to the conclusion that $T_1(h_p) \to 0$ for $h_p \to 0$.

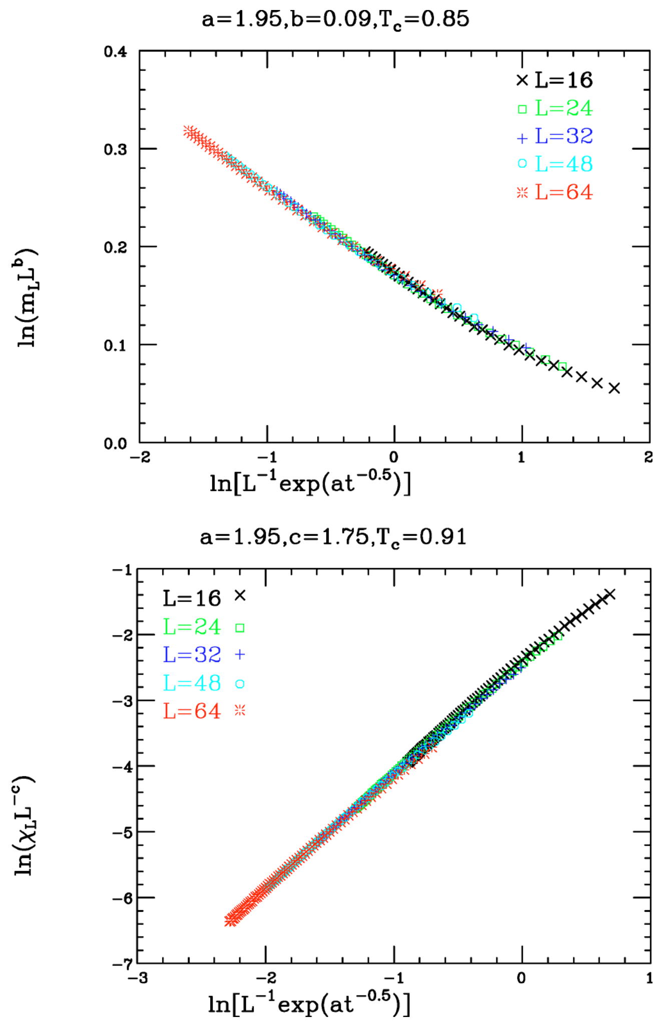

FIG. 4. Finite-size scaling of the magnetization (left) and susceptibility (right) for $h_4=0.1$: $L=16$ (crosses), $L=24$ (squares), $L=32$ (vertical crosses), $L=48$ (circles), and $L=64$ (stars).

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[1] J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).
[2] V. L. Berezinskii, Zh. Eksp. Teor. Fiz. **59**, 907 (1970) [Sov. Phys. JETP **32**, 493 (1971)]; **61**, 1144 (1971) [**34**, 610 (1973)]; J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).
[3] J. Tobochnik, Phys. Rev. B **26**, 6201 (1982); see also *ibid.* **27**, 6972(E) (1983).
[4] M. S. S. Challa and D. P. Landau, Phys. Rev. B **33**, 437 (1986).
[5] M. Suzuki, Prog. Theor. Phys. **13**, 770 (1967).
[6] E. Rastelli, S. Regina, and A. Tassi, Phys. Rev. B **69**, 174407 (2004).
[7] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[8] J. Villain, J. Phys. (Paris) **36**, 581 (1975).