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Critical behavior of the six-state clock model in two dimensions

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We have examined the critical properties of the $q=6$ clock (vector Potts) model in two dimensions through Monte Carlo simulations. The model was investigated on $L \times L$ square lattices of size $L=4$ to $L=72$ with periodic boundary conditions. We found an intermediate XY-like phase between a low-temperature ordered phase and a high-temperature disordered phase. The phase transitions occur at $k_B T_1/J=0.68\pm0.02$ and $k_B T_2/J=0.92\pm0.01$ and are of the Kosterlitz-Thouless type. The susceptibility diverges in the intermediate phase and the exponent η varies between 0.100 at T_1 and 0.275 at T_2.

I. INTRODUCTION

The q-state ferromagnetic clock model (also known as the "vector Potts model") is a discrete version of the XY (plane rotator) model and consists of two-dimensional planar spins restricted to q evenly spaced directions. The interaction energy of the spins is proportional to their scalar product. If $\vec{s}_i=(\cos\theta_i,\sin\theta_i)$, where θ_i is the angle the spin makes with an arbitrary axis, the site variable p_i representing the state of the ith spin, is defined through $\theta_i=2\pi p_i/q$, with $p_i=1,2,\ldots,q$. The Hamiltonian may be written as

$$H=-J\sum_{\langle ij\rangle}\cos[2\pi(p_i-p_j)/q] \; . \tag{1}$$

Here, J is the strength of the interaction and the sum is over nearest-neighbor pair ij. ($q=2$ yields the Ising model and in the limit $q\rightarrow\infty$ we get the XY model.)

Theoretical interest in clock models was stimulated after Kosterlitz and Thouless[1] showed that the XY model possessed a novel type of critical behavior with essential singularities and topological ordering. In the Kosterlitz-Thouless theory the correlation length ξ and the susceptibility χ diverge exponentially as $T\rightarrow T_c+$. Below T_c, both quantities are infinite. Though the Mermin-Wagner theorem[2] prohibits conventional ordering in the XY model in two dimensions, Kosterlitz and Thouless showed that a different form of ordering is possible via vortex formation. In this "XY-like" phase, the spin-spin correlation function $G(r)$ decays as a power of the distance r: $G(r)\sim r^{-\eta}$. The phase transition is characterized by the response function of the system (χ) changing drastically due to vortex-pair unbinding.

The theoretical analyses are not exact and have relied chiefly on the close relationship between the clock models and the Villain model[3] (where the partition function is a Gaussian). The first study was by José *et al.*[4] who investigated the planar model with q-fold symmetry-breaking fields h_q. (The perturbative fields were introduced to simulate the crystal fields in real substances and yield the clock model in the limit $h_q\rightarrow\infty$.) Their conclusions are based on the results of a Migdal renormalization scheme as well as a low-temperature expansion for a generalized Villain model. For $q\leq 4$, they found a single power-law transition, but for $q=6$ the theory indicated an intermediate XY-like phase between a low-temperature ordered phase ($T<T_1$) and a high-temperature disordered phase ($T>T_2$). The transitions at T_1 and T_2 were of the Kosterlitz-Thouless type with χ diverging exponentially at the transitions and staying infinite in between. They predicted T_2 to be the critical temperature of the XY model and T_1 was found to vary as $k_B T_1/J=4\pi^2/1.7q^2$. The exponent η was found to vary between $\eta(T_1)=4/q^2$ and $\eta(T_2)=\frac{1}{4}$.

Elitzur *et al.*[5] considered a discrete Villain model with Z_q symmetry. By using duality arguments and a Griffiths inequality for the correlation functions, they established the existence of an intermediate massless (XY-like) phase for q greater than a critical value q_c (which they estimated to be 4). By using a Coulomb gas representation they were also able to recover the results of José *et al.* (which were really valid for small h_q).

Subsequent analytical work on more general forms of Z_q models extended the results given above and revealed a complex phase structure. Thus, Cardy[6] investigated the duality properties of general Z_q models and predicted that for $q\geq 5$ the system would order via a first-order transition, two Kosterlitz-Thouless transitions, or successive Ising, three-state Potts, or Ashkin-Teller transitions. Domany *et al.*[7] studied a general Z_5 model analytically as well as through simulations and concluded that the transition from a disordered to an ordered phase could take place either through an intermediate XY-like phase or a single first-order transition. There have also been conflicting results for q_c. Roomany and Wyld[8] obtained $q_c=5$ by using a finite-lattice method. Rujan *et al.*[9] confirmed the existence of three phases for $q=6$ and 7 but their results were not conclusive for $q=5$.

Experimental verification of the theories has so far not been possible and we must resort to computer simulations to test the predictions. Tobochnik[10] simulated the model for $q=4$, 5, and 6 using a Monte Carlo renormalization-group method. He concluded that for $q=4$ there was only one transition with a finite value for the exponent ν, but that for $q=5$ and 6 there were two transitions with $\nu=\infty$ (thus indicating the XY-line nature of the intermediate phase[1]). He estimated that for $q=6$ the transitions took place at $k_BT_1/J=0.6$ and $k_BT_2/J=1.3$, with η varying between 0.10 and 0.32 at $k_BT/J=0.6$ and 1.0, respectively.

Our own work involves Monte Carlo simulations on several lattice sizes using a different sampling scheme from that of Tobochnik[10] and making careful finite-size analyses of the data. We have two objectives in studying the $q=6$ model. First, we wish to verify the predictions concerning the nature of the phases and the transitions. This should prove useful when two-dimensional systems with the requisite symmetry are available. (Solids with a fivefold symmetry are not realizable.) Second, we hope our work will yield useful knowledge regarding the simulational treatment of essential singularities in critical phenomena. We reported earlier[11] from preliminary results that although two transitions could be clearly seen in moderately large lattices for $q=6$, we did not find an XY-like intermediate phase. Our subsequent research (described later in this paper) has enabled us to confirm the XY-like phase, obtained estimates for the exponent η, and locate T_1 and T_2 quite precisely.

The rest of the paper is organized as follows. Section II gives a description of the methods used in our analysis. Section III presents our results and comparisons with other work. Section IV presents a summary of our conclusions.

II. METHODS

A. The Monte Carlo method

A standard importance sampling method[12] was used to simulate the behavior of the model on $L\times L$ square lattices with periodic boundary conditions. In a single Monte Carlo step per site (MCS) each site in the lattice is visited in turn to test the spin for "flipping" from a state p_i to a random new state p_i'. The probability of a flip is proportional to the Boltzmann factor $\exp(-\beta\Delta E)$, where β is the inverse temperature and ΔE is the change in internal energy due to the flip. (This is in contrast to Tobochnik's method[10] where only flips with $\Delta p_i=p_i'-p_i=\pm 1$ were allowed. His rationale was that at low temperatures flips of one unit to the right or left will be the most favored so that fewer MCS will be necessary for the system to reach equilibrium. However, it has been our experience that flips with $\Delta p_i>1$ formed a fair fraction of the total number of flips. Thus, for $L=16$ in the range of temperatures studied, the larger flips accounted for 15–40% of the total number.) The thermodynamic variables were obtained by averaging over many MCS after discarding several thousand to allow the system to reach equilibrium.

We performed simulations on lattices of size $L=4$, 8, 12, 16, 20, 32, 48, and 72. For each lattice size we made several runs ranging from 4000 to 40 000 MCS. Each run was made with a different initial configuration or random-number sequence. The number of MCS needed varies with temperature since large runs are needed in the critical region to compensate for the long relaxation times. The number of MCS also varies with lattice size because (especially in the critical region) large lattices have large fluctuations. The total number of MCS kept for each data point was determined from two properties of the simulation. First, we examined the averages to see if they changed appreciably as data from additional runs were added in. In addition, we monitored the "coarse-grained" statistical errors obtained at each stage of the analysis. The data we used for analysis represent averages over 250 000 MCS in the critical region and 8000 to 50 000 MCS outside it.

The order parameter m_L is defined as the absolute value of the magnetization $\overline{m}_L$ given by

$$\overline{m}_L=\left[\sum_i \cos\theta_i, \sum_i \sin\theta_i\right]\Big/ N\ , \tag{2}$$

where N is the number of sites ($N=L^2$). The specific heat C_L and the susceptibility χ_L were computed from the fluctuation results:

$$C_L=N(\langle E_L^2\rangle-\langle E_L\rangle^2)/k_BT^2\ , \tag{3}$$

$$\chi_L=N(\langle m_L^2\rangle-\langle m_L\rangle^2)/k_BT\ , \tag{4}$$

where E is the internal energy per site and k_B is the Boltzmann constant. Equation (4) is valid in the ordered regime. Where it is known that $\langle m_L\rangle=0$ for the infinite lattice, it is more appropriate to define the susceptibility through

$$\chi_L=N\langle m_L^2\rangle/T\ . \tag{5}$$

We also computed the fourth-order cumulant:

$$U_L=1-\langle m_L^4\rangle/3\langle m_L^2\rangle^2\ . \tag{6}$$

This quantity is used in the cumulant method described later in this section.

B. Finite-size scaling

We have relied on the methods of finite-size scaling[13] to draw our conclusions. As is customary, we argue that the only relevant variable that "rounds off" the divergences in a finite system is the ratio of the lattice size to the correlation length L/ξ. In the Kosterlitz-Thouless theory, ξ and χ behave as

$$\xi\sim\exp(at^{-0.5})\ , \tag{7}$$

$$\chi\sim\xi^{2-\eta}\ , \tag{8}$$

where a is a constant, $t=(T-T_c)/T_c$, and T_c is the critical temperature of the XY model. Since $m\sim(T_c-T)^\beta$ and $\xi\sim(T_c-T)^{-\nu}$ in second-order transitions, it is easy to show that

$$m\sim\xi^{-\eta/2}\ . \tag{9}$$

Here we have used the relation $\beta/\nu=(d-2+\eta)/2$, where d is the lattice dimensionality.[14] (One of the implications of the essential singularities in the Kosterlitz-Thouless theory is that η is the only exponent in zero field. The exponent relations, however, still hold, provided that the exponents are suitably defined.[1]) The singular part of the free energy is considered to be a generalized homogeneous function of L and ξ. χ_L and m_L (which are derivatives of the free energy) are assumed to have the functional forms

$$m_L = L^{-b} Y_1(\xi/L) , \tag{10}$$

$$\chi_L = L^c Y_2(\xi/L) , \tag{11}$$

where b and c are constants and Y_1 and Y_2 are unknown functions. Since we must regain (8) and (9) in the infinite-lattice limit, we obtain

$$b = \eta/2 , \tag{12}$$

$$c = 2 - \eta . \tag{13}$$

Using Eqs. (12) and (13) in Eqs. (10) and (11), we see that at a critical point

$$m_L \propto L^{-\eta/2} \tag{14}$$

or, equivalently,

$$\chi_L \propto L^{2-\eta} , \tag{15}$$

since Y_1 and Y_2 approach constant values. If the intermediate phase is indeed a line of critical points with η varying continuously with temperature, we should find Eqs. (14) and (15) to hold true for all $T_1 \le T \le T_2$.

We may express Eqs. (10) and (11) as

$$m_L L^b = Y_1(L^{-1}\exp(at^{-0.5})), \quad T < T_1 , \tag{16}$$

$$\chi_L L^{-c} = Y_2(L^{-1}\exp(at^{-0.5})), \quad T > T_2 . \tag{17}$$

Here, $t=(T_1-T)/T_1$ for $T<T_1$ and $t=(T-T_2)/T_2$ for $T>T_2$. From the above we derive the important inference that when the parameters a, b, c, T_1, and T_2 are chosen correctly, the data for all the lattice sizes should lie on two curves (which correspond to the universal functions Y_1 and Y_2). This provides an accurate way of obtaining estimates for the critical exponents and the transition temperatures. The above variation of finite-size scaling was used successfully in Monte Carlo studies of the Ising model with competing interactions on a triangular lattice.[15]

C. The cumulant method

We used the fourth-order cumulant U_L defined in Eq. (6), in a finite-size analysis of the type originally suggested by Binder.[16] Binder used the Monte Carlo method to study the probability distribution function $P_L(m_L)$ of the Ising model on lattices of various sizes. These distributions were found to be Gaussian centered about the mean magnetization $\langle m_L \rangle$. In a manner analogous to usual finite-size scaling, he assumed that $P_L(m_L)$ was a generalized homogeneous function of ξ and L. The analysis then led to predictions regarding the behavior of the cumulants of the distribution function. He showed that $U_L \propto L^{-d}$ for $T>T_c$ and $U_L \sim (2-4\langle m_L \rangle^{-2} L^{-d} k_B T \chi_L)/3$ for $T<T_c$. (Here, d is the lattice dimensionality and T_c is the critical temperature of the Ising model.) In the limit $L\to\infty$, $U_L \to \frac{2}{3}$ for $T<T_c$ and 0 for $T>T_c$. At T_c, U_L approaches a universal constant U^* which is independent of L. Therefore, plots of the cumulants for different lattice sizes L and L' at various temperatures should yield estimates of U^* (where $U_L = U_{L'}$) and T_c. If $b=L'/L$ (>1), the slope of the $U_{L'}$ vs U_L plots yields estimates for the exponent ν (Ref. 16):

$$dU_{bL}/dU_L = b^{1/\nu} . \tag{18}$$

In general, there is a size dependence for the estimates of ν and T_c obtained in this fashion and one must extrapolate against $(\ln b)^{-1}$ to obtain accurate values.

The cumulant method worked very well for the Ising model studied by Binder and has the advantage that it eliminates the need for a simultaneous fit of three parameters used in conventional finite-size scaling. Our chief interest in the method stems from the fact that an intermediate XY-like phase (if it exists) should show up in the cumulant plots as a line of points where $U_L = U_{L'}$ (since $\nu=\infty$ for the XY model). The method was successfully used in simulations of the XY model with a fourth-order anisotropy field h_4 (Ref. 17), where the low-temperature phase of the XY model ($h_4=0$) was clearly manifest as a line of critical points.

III. RESULTS

Figure 1(a) shows the temperature variation of the internal energy for three lattice sizes. Figure 1(b) shows the variation of the internal energy with lattice size for

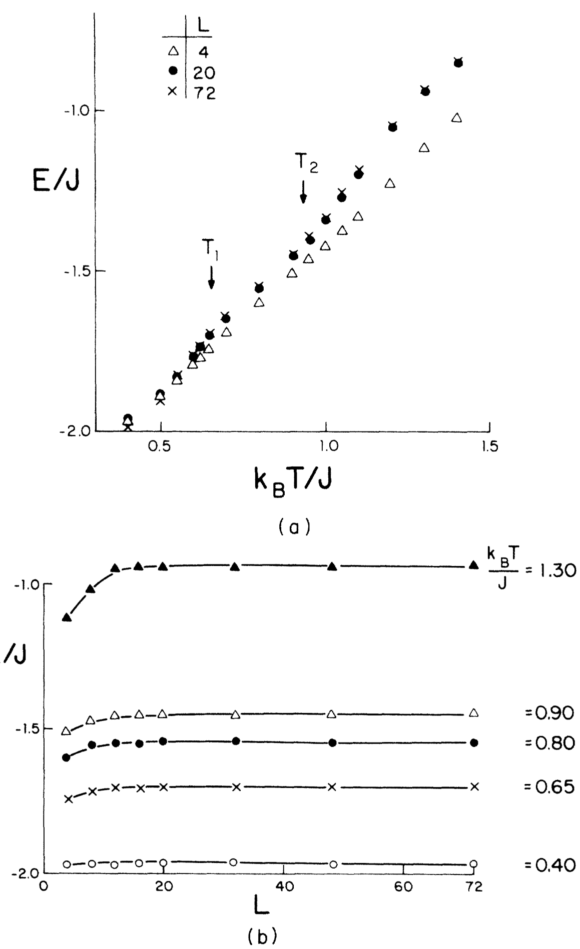


FIG. 1. (a) Variation of internal energy with temperature for three lattice sizes. Results of only the heating runs are shown because the results of the cooling runs are identical. (b) Variation of internal energy with lattice size at different temperatures.

several temperatures. We did not see any interesting features such as hysteresis or finite-size effects for large L.

Figure 2(a) represents the variation of the specific heat with temperature for several lattice sizes. While the two peaks clearly suggest two phase transitions, it should be noted that the peaks are not located at the transition temperatures (as determined from finite-size scaling). They shift only slightly toward T_1 and T_2 as we increase the lattice size. While there is a slight size dependence of the peak heights, we believe that this tendency will disappear for large enough lattices. This may be seen from Fig. 2(b). These results are in general agreement with those obtained by Tobochnik.[10]

The finite-size effects in the behavior of the magnetization are striking. Figure 3(a) shows the temperature variation of the magnetization. It may be seen that there is only a slight undulation in the plots near T_1 and that m_L decreases markedly only beyond T_2. While we expect a finite-size tail for $T > T_1$, the values of m_L are unusually large in the intermediate region. That this is a consequence of the infinite correlation length in the intermediate region can be seen from the variation of m_L with L shown in Fig. 3(b). There we see that the magnetization reaches a nonzero value only for $T < T_1$. We see an intermediate phase characterized by excellent linear behavior. Once the temperature is raised beyond T_2, the deviations from straight-line behavior reappear, indicating that the

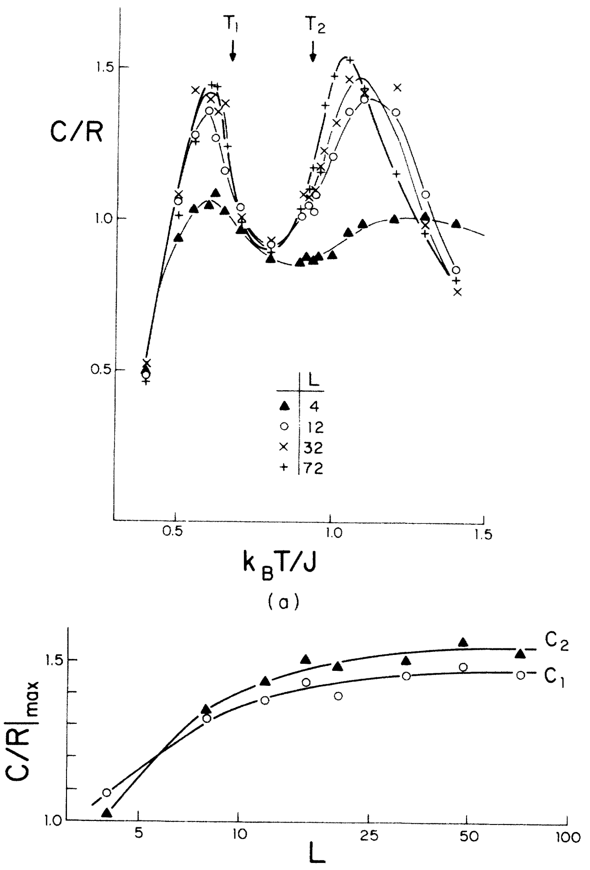


FIG. 2. (a) Variation of specific heat with temperature for various lattice sizes. The bold curve shows the behavior for $L=72$ which we believe is essentially the same as for an infinite lattice. The values of T_1 and T_2 were obtained from the scaling plots in Fig. 4. (b) Variation of the peak values of specific heat with lattice size. C_1 and C_2 represent the specific heat maxima near T_1 and T_2, respectively.

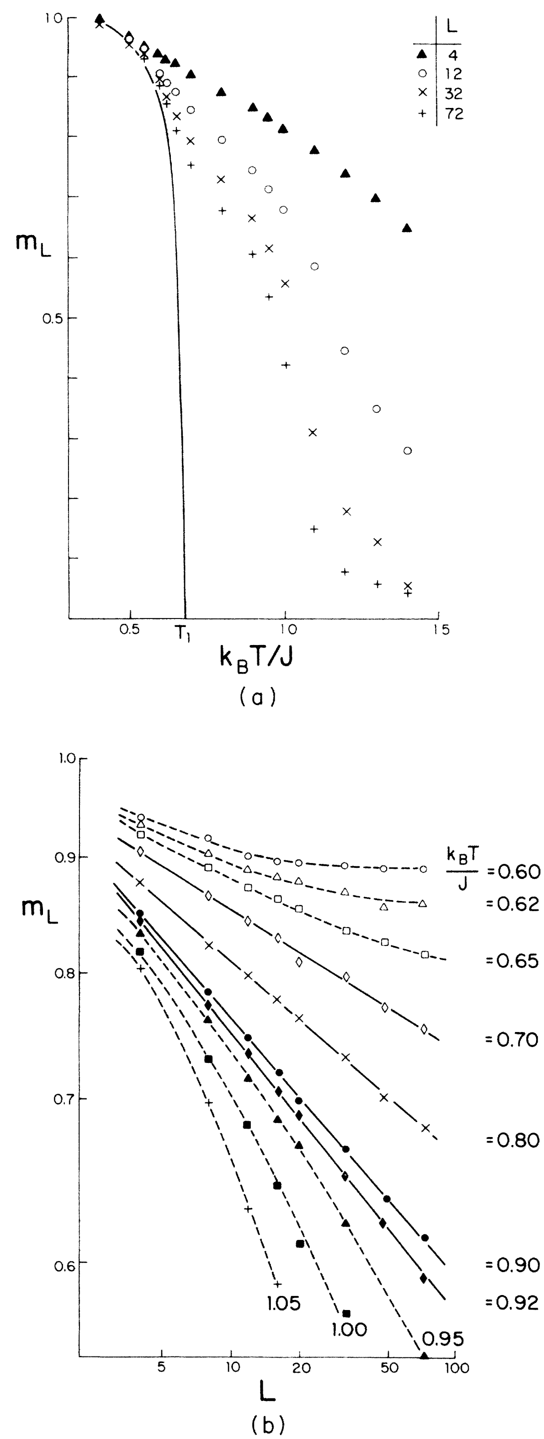
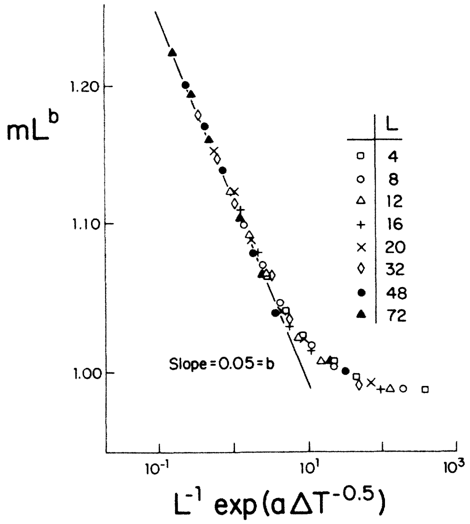
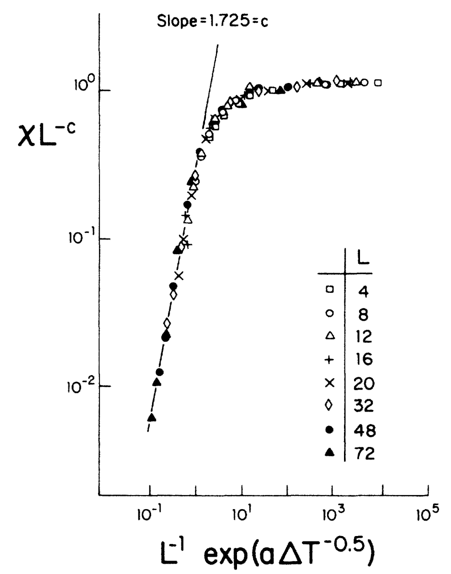


FIG. 3. (a) Temperature variation of the magnetization. The solid curve shows the expected infinite-lattice behavior. (b) Log-log plots of m_L vs L at various temperatures. The dashed curves indicate deviations from straight-line behavior. The solid curves indicate the linear behavior in the intermediate phase.



(a)



(b)

FIG. 4. (a) Finite-size scaling of the low-temperature magnetization data ($T \leq T_1$). [See Eq. (16).] (b) Finite-size scaling of the high-temperature susceptibility data ($T \geq T_2$). [See Eq. (17).]

TABLE I. Variation of the exponent η in the intermediate phase. The values at T_1 and T_2 are obtained from the scaling plots in Fig. 4. The other values are obtained from a least-squares fit to the data in Fig. 3(b).

$k_B T/J$	η
0.68	0.100
0.70	0.128
0.80	0.176
0.90	0.236
0.92	0.275

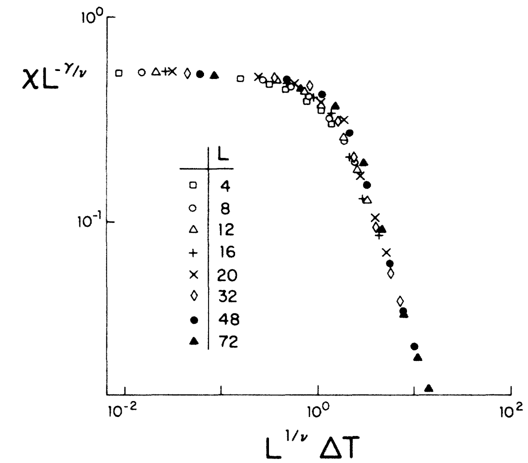


FIG. 5. Scaling of the data in Fig. 4(b) assuming a power-law divergence of the correlation length. [See Eq. (19).]

system is no longer in the critical regime. The values of η are shown in Table I. [η can also be obtained from the divergence of the susceptibility according to Eq. (15) but this does not yield any new information.]

The data for all lattice sizes were scaled according to Eqs. (16) and (17). The results are shown in Figs. 4(a) and 4(b). It is evident that the data scale very well with the following values for the parameters:

$$a = 1.54 \pm 0.01, \quad b = 0.050 \pm 0.001, \quad c = 1.725 \pm 0.025 ,$$

$$k_B T_1 / J = 0.68 \pm 0.02, \quad k_B T_2 / J = 0.92 \pm 0.01 .$$

The errors were determined by considering the quality of the fits upon deviating from the best-fit results. We

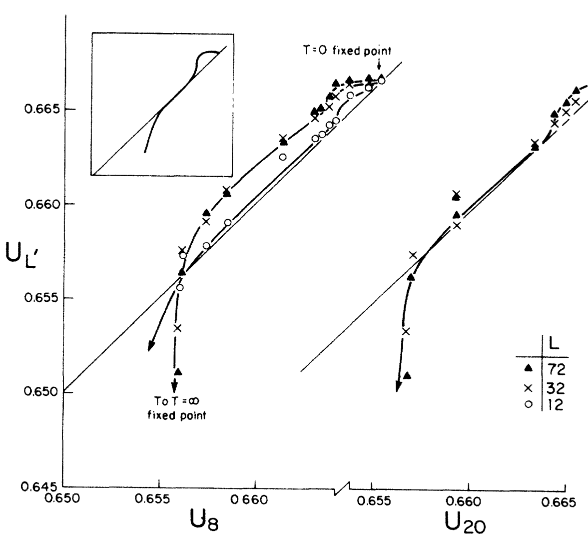


FIG. 6. Examples of the $U_{L'}$ vs U_L plots. The plot on the left is for $L = 8$ and the one on the right is for $L = 20$. Each data point corresponds to a different temperature. Inset shows the expected behavior if the intermediate phase is XY-like. The straight line represents $U_{L'} = U_L$ and its intersection with the plot through the data represents a nontrivial fixed point. The XY-like character of the intermediate phase shows up clearly when L is larger.

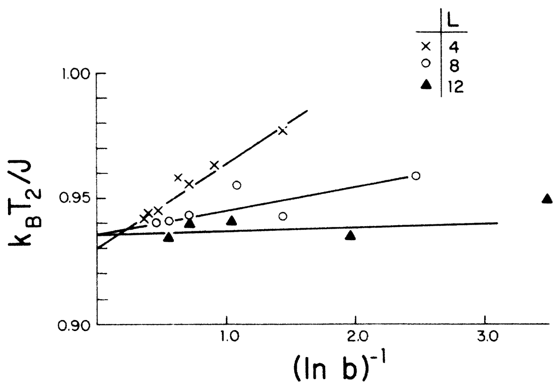


FIG. 7. Extrapolation of the values of T_2 obtained from the $U_{L'}$ vs U_L plots.

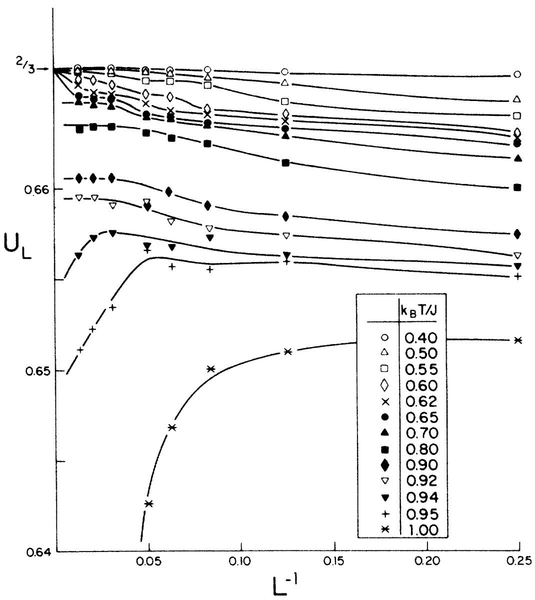


FIG. 8. "Flow diagram" of U_L vs L^{-1} at various temperatures. $U_L = \frac{2}{3}$ represents the trivial fixed point for the ordered phase and $U_L = 0$ is the high-temperature fixed point. The extrapolation for $k_BT/J = 0.65$ is based on the value of T_1 obtained from the scaling plots in Fig. 4.

disagree substantially with Tobochnik's[10] value $k_BT_2/J = 1.3$, while his estimate $k_BT_1/J = 0.6$ differs from ours by about 12%. We note that our value of T_2 is very close to the critical temperature of the plane rotator model (around 0.90) (Ref. 18) and the value of T_c is consistent with that predicted by José *et al.*[4] ($\simeq 0.65$ for $q = 6$). Also, the value for a is in agreement with that given by Kosterlitz[1] ($\simeq 1.5$). However, the exponent values of 0.100 for $\eta(T_1)$ ($= 2b$) and 0.275 for $\eta(T_2)$ ($= 2 - c$) deviate by 10% from the theoretical values.[1,4,5]

We have also attempted to scale the high-temperature susceptibility data assuming a power-law singularity in the correlation length: $\xi \sim (T - T_2)^{-\nu}$. In a manner analogous to that employed in obtaining Eqs. (16) and (17), we can show that

$$\chi_L L^{-\gamma/\nu} = Y_3(L^{1/\nu}\Delta T) , \tag{19}$$

where Y_3 is a universal function. The best results that could be obtained are shown in Fig. 5. We see that while the data scale very well for the extreme values of ΔT, there are *systematic* deviations in the intermediate region. We conclude that scaling indicates exponential singularities unambiguously. As will be seen presently, the cumulant method substantiates this.

The cumulant method was initially not useful in clarifying the nature of the intermediate phase.[11] By extending our simulations to larger lattices and averaging over 250 000 MCS per data point (about 20 hours on the Cyber 750 for a 72×72 lattice), we have obtained a picture consistent with the scaling results. Figure 6 shows typical plots of $U_{L'}$ vs U_L for $L = 8$ and 20 and various values of L'. We draw the attention of the reader to the scale of the plots: the changes in the cumulant as the temperature is varied are minute and can be as low as one part in 6500 for a temperature variation of $k_B\Delta T/J = 0.1$. This is one of the reasons why good quality data were essential. When $L = 8$, we see a "hump" in the intermediate phase when L' is large. We attribute this effect to the finite-lattice size and note that for the cumulant method to yield good results we need $L > \xi$. Thus, this spurious ordered phase has practically disappeared when we examine plots of $U_{L'}$ vs U_{20}. A large value of b ($= L'/L$) is also necessary in order that substantial size effects not be evident in the cumulant. We found that T_2 obtained in this fashion is dependent on the choice of L' and L. In Fig. 7 we present the extrapolation of T_2 vs $(\ln b)^{-1}$ (as in Ref. 16). (The hump obscures the location of T_1 and we are able to make only a rough estimate for the same.) In this fashion, the cumulant method yielded $k_BT_1/J = 0.62$ and $k_BT_2/J = 0.935$. These estimates of the transition temperatures are in general agreement with those obtained from finite-size scaling. However, there is an element of subjectivity in locating a nontrivial temperature in the cumulant method (in the manner of drawing the curves) and we feel that the scaling results are more accurate. Finally, we present in Fig. 8 the behavior of U_L as a function of L at various temperatures. The line of fixed points is clearly manifest in the intermediate phase as the range of temperatures for which U_L becomes independent of L. From the figure it will be readily appreciated that one has to examine rather large lattices in order to extrapolate correctly to the thermodynamic limit. Thus, though the plateau is evident in the smaller lattices even at $k_BT/J = 0.55$, it moves toward $L = \infty$ as we approach T_1 and extends all the way to $L = \infty$ only in the intermediate phase.

IV. SUMMARY

We conclude that the model has two Kosterlitz-Thouless transitions in zero field at $k_BT_1/J = 0.68 \pm 0.02$ and $k_BT_2/J = 0.92 \pm 0.01$. The intermediate phase is XY-like with zero magnetization and infinite susceptibility. The specific heat remains finite at both transitions. The exponent η varies continuously with temperature in the intermediate phase and our estimates for η are close to the theoretical values of José *et al.*[4] The results from the cumulant method are in good agreement with those from finite-size scaling and we conclude that the method works well, but only *provided* the simulations are done on very large lattices.

ACKNOWLEDGMENTS

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