

# Static and Dynamic Critical Phenomena of the Two-Dimensional $q$ -State Potts Model

K. Binder<sup>1</sup>

Received January 8, 1980

---

The  $q$ -state Potts model on the square lattice is studied by Monte Carlo simulation for  $q = 3, 4, 5, 6$ . Very good agreement is obtained with exact results of Kihara *et al.* and Baxter for energy and free energy at the critical point. Critical exponent estimates for  $q = 3$  are  $\alpha \approx 0.4$ ,  $\beta \approx 0.1$ ,  $\gamma \approx 1.45$ , in rough agreement with high-temperature series extrapolation and real space renormalization-group methods. The transition for  $q = 5, 6$  is found to be a very weakly first-order transition, i.e., pronounced "pseudocritical" phenomena occur, specific heat, susceptibility, etc. (nearly) diverge at the first-order transition temperature. Dynamics is associated to the model in the same way as for the kinetic Ising model, and the nonlinear slowing down of the order parameter and of the energy is studied. The dynamic exponent is estimated to be  $\Delta (= z\nu) \approx 1.9$ . Within our accuracy no  $q$  dependence is detected. The relaxation is found to be consistent with dynamic scaling predictions, and dynamic scaling functions associated with the nonlinear relaxation are estimated.

---

**KEY WORDS:** Potts model; first-order transition; second-order transition; Monte Carlo; critical slowing down; critical exponents; dynamic scaling; nonlinear relaxation.

## 1. INTRODUCTION

Recently there has been much interest in the critical behavior of the  $q$ -state Potts model,<sup>(1,2)</sup> whose Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \quad s_i = 1, 2, \dots, q \quad (1)$$

where the summation extends over all nearest neighbor pairs on the lattice. Note that certain physical systems belong to the same universality class as

---

<sup>1</sup> IFF, KFA Jülich, Jülich, West Germany.

this model, such as ordered absorbed monolayers<sup>(3-5)</sup> (for dimensionality  $d = 2$ ) and (in the case  $q = 3$ ,  $d = 3$ ) cubic ferromagnets in a field applied in the [111] direction,<sup>(6,7)</sup> or certain structural transitions.<sup>(8a),2</sup> In addition, this model is a stringent testing ground for approximate theories on phase transitions, because the *order of the transition* depends on both  $q$  and  $d$  in a sensitive way: Landau theory<sup>(9)</sup> (as well as mean-field<sup>(2)</sup> and related<sup>(10)</sup> approximations) predict the transition to be first order for all  $q \geq 3$  irrespective of  $d$ . Renormalization-group  $\epsilon$ -expansions<sup>(11-14)</sup> show that this is correct close enough to the marginal dimensionality  $d^* = 6$ , while it is known exactly<sup>(15)</sup> that the transition is of second order for  $q \leq 4$  and  $d = 2$ . High-temperature series expansions show the transition to be of first order for  $q = 4$ ,  $d = 4$ ,<sup>(16)</sup> but cannot give a clear answer concerning the order of the transition at lower  $q$  and lower  $d$ .<sup>(9,17-22)</sup> The suggestion<sup>(21)</sup> that for  $d = 3$ ,  $q = 3$  a weak first-order transition could be accompanied by critical divergences received some recent support from Monte Carlo work<sup>(23)</sup> (which also suggests that the case  $d = 3$ ,  $q = 4$  is clearly first order), while Monte Carlo renormalization<sup>(24)</sup> suggests for  $q = 3$ ,  $d \geq 3$  the occurrence of a "pseudospinodal singularity"<sup>(25)</sup> of metastable states in the close neighborhood of the transition temperature. While for  $d = 2$  this method<sup>(26)</sup> as well as standard real space renormalization-group approaches<sup>(4,27-33)</sup> yield reasonable exponent estimates for  $q \leq 4$ . Only one recent version<sup>(33)</sup> yielded a change in the order of the transition (from second to first order for  $q > q_c$ , with  $q_c = 4.73$ ). While in the case  $d = 2$ ,  $q = 3$  series expansion estimates for the specific heat exponent ranged from  $\alpha = 0.05$ <sup>(9)</sup> to  $\alpha = 0.42$ <sup>(34)</sup> or  $\alpha = 0.30$ ,<sup>(35)</sup> and the adsorption experiment yielded  $\alpha = 0.36$ ,<sup>(36)</sup> for  $q = 4$  the series estimates range from  $\alpha = 0.45$ <sup>(35)</sup> to  $\alpha = 0.64$ .<sup>(37)</sup> On the other hand, it has been conjectured that  $\alpha(q = 3) = 1/3$  and  $\alpha(q = 4) = 2/3$  hold exactly.<sup>(38)</sup>

In view of all these efforts, it seems interesting to apply Monte Carlo methods<sup>(39)</sup> to this model also for  $d = 2$ : first we can check whether this method is able to correctly distinguish the order of the transitions and accurately estimate the magnitudes of first-order jumps. This question is nontrivial, since using too short observation times, one will observe an apparent hysteresis even for second-order transitions, due to critical slowing down.<sup>(40)</sup> We suspect the hysteresis reported for  $q = 3$ ,  $d = 3$  in Ref. 24 may be exaggerated due to this effect, since other studies employing longer observation times found no hysteresis but slow, smooth relaxation instead.<sup>(23)</sup> Furthermore, one can check whether the Monte Carlo data are consistent with the exponent predictions mentioned above. One obtains data also on thermodynamic functions away from the critical point, which

<sup>2</sup> See Ref. 8b for a discussion of the relevance of the Potts model for liquid mixtures.

could be used to check corresponding real space methods [which so far have been applied to the Ising case ( $q = 2$ ) only,<sup>(41)</sup> however]. Since the Monte Carlo method has a stochastic dynamics intrinsically built in,<sup>(39)</sup> one can at the same time study the critical dynamics of the model in much the same way as was done for the kinetic Ising model for  $d = 3$ <sup>(42)</sup> and  $d = 2$ .<sup>(43)</sup> Hence we first (Section 2) discuss static properties and compare them to the various theoretical predictions mentioned above, and then study dynamic properties (Section 3), for which a real space renormalization-group treatment is underway.<sup>(44)</sup> Our emphasis will be on nonlinear relaxation, which has found most interest recently (see, e.g., Refs. 43 and 45–50). Section 4 contains our conclusions.

## 2. STATIC PROPERTIES

We have applied standard Monte Carlo methods,<sup>(39)</sup> studying finite square lattices with periodic boundary conditions, using lattice sizes  $N$  from  $N = 16 \times 16$  up to  $N = 200 \times 200$  to detect finite-size effects, and observation times of up to  $10^4$  Monte Carlo steps (MCS)/site. As initial condition we typically used an ordered state  $\{s_i = 1\}$  and then let the system relax toward equilibrium, recording energy per site  $U(t) = \mathcal{H}/N$  and order parameter  $M(t)$ ,

$$M(t) = [qN_1(t)/N - 1]/(q - 1) \quad (2)$$

where  $N_\mu(t)$  is the number of sites  $i$  with  $s_i = \mu$  at time  $t$  of the simulation. Averaging of both energy and order parameter was begun only when both quantities had safely reached equilibrium, and “susceptibilities”  $\chi_1, \chi_2$  as well as the specific heat  $C$  were calculated from the fluctuation formulas

$$\begin{aligned} k_B T \chi_1 &= [\langle N_1^2(t) \rangle - \langle N_1(t) \rangle^2]/N \\ k_B T \chi_2 &= \sum_{\mu=2}^q [\langle N_\mu(t) \rangle - \langle N_\mu(t) \rangle^2]/[N(q - 1)] \\ (k_B T/J)^2 C &= N[\langle U^2(t) \rangle - \langle U(t) \rangle^2] \end{aligned} \quad (3)$$

Note that in the disordered regime above  $T_c$  we have  $\chi_1 = \chi_2$ , of course.

Neither for  $q = 5$  nor for  $q = 6$  did we succeed in observing any clear indication of the hysteresis associated with metastable states that one expects to occur at first-order transitions, and have indeed been observed in Monte Carlo studies of the field-induced first-order transition of Ising models below  $T_c$ .<sup>(51)</sup> One rather observes monotonic relaxation toward equilibrium which becomes very slow near  $T_c$  (Fig. 1), and the behavior is very similar to that for  $q = 3$  or  $q = 4$  (Fig. 2). If we would follow the standard behavior of recording hysteresis loops with the Monte Carlo

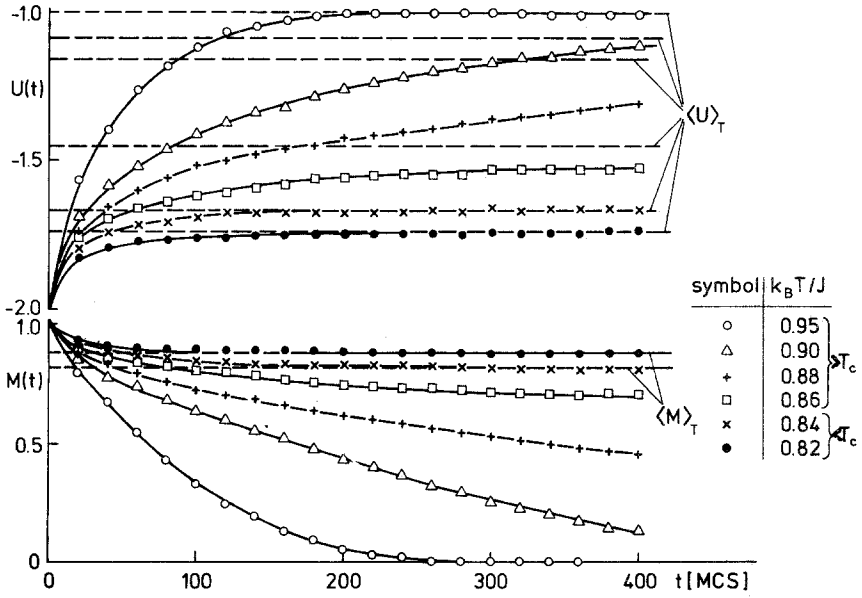


Fig. 1. Energy per site  $U(t)$  [upper part] and order parameter  $M(t)$  [lower part] plotted versus time for  $q = 5$  at various temperatures.

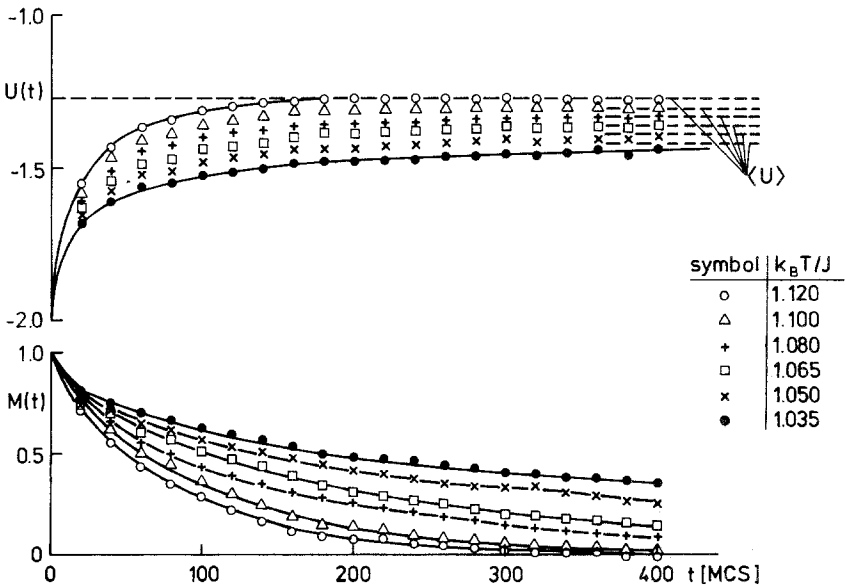


Fig. 2. Energy per site  $U(t)$  [upper part] and order parameter  $M(t)$  [lower part] plotted versus time for  $q = 3$  at various temperatures.

procedure, i.e., taking averages over successive temperatures over the same time interval  $\Delta t$  and using the final state at each temperature  $T$  as starting configuration for the next temperature  $T \pm \delta T$ , we would observe hysteresis for all  $q$ . But this “hysteresis” would strongly depend on the magnitude of  $\Delta t$ , and particularly for a  $\Delta t$  as small as  $\Delta t = 100$  MCS (as used in Ref. 24) and  $k_B \delta T/J = 0.02$  this “hysteresis” would be quite pronounced, as is seen from Fig. 3b. For smaller  $\delta T/\Delta t$  one obtains better results, of course. In Fig. 3a our final estimates for the temperature dependence of the energy is plotted. We have included the exact values of the energy at  $T_c$  from Kihara *et al.*,<sup>(2)</sup>

$$(U_c^- + U_c^+)/2J = -1 - 1/\sqrt{q} \quad (4)$$

where

$$U_c^- = \lim_{T \rightarrow T_c^-} \langle U \rangle \quad \text{and} \quad U_c^+ = \lim_{T \rightarrow T_c^+} \langle U \rangle$$

( $U_c^- \equiv U_c^+$  at second-order transitions, of course). From Baxter’s<sup>(15)</sup> result for the latent heat ( $q > 4$ ,  $\Theta \equiv \text{arcosh} \sqrt{q}/2$ )

$$\frac{U_c^+ - U_c^-}{J} = 2 \left( 1 + \frac{1}{\sqrt{q}} \right) \tanh \frac{\Theta}{2} \prod_{n=1}^{\infty} (\tanh n\Theta)^2 \quad (5)$$

and Eq. (4),  $U_c^+$ ,  $U_c^-$  can be calculated separately, and are included in Fig. 3. It is seen that the jump of the energy for  $q = 5, 6$  is rather small,  $(U_c^+ - U_c^-)/J \cong 0.0529$  for  $q = 5$  and  $(U_c^+ - U_c^-)/J \cong 0.2015$  for  $q = 6$ . Since the energy changes from its low-temperature behavior ( $\langle U \rangle$  close to  $U_0/J = -2$ ) to its high-temperature behavior ( $\langle U \rangle$  close to  $U_\infty/J = -2/q$ ) in a fairly narrow temperature interval, the first-order transition is preceded by strong “precursor effects.” In fact, Fig. 3 would be consistent with a power-law divergence of the specific heat at the first-order transition. For larger  $q$  the jump would be larger [ $(U_c^+ - U_c^-)/J \cong 0.3533$  for  $q = 7$ ,  $(U_c^+ - U_c^-)/J \cong 0.4864$  for  $q = 8$ , etc.], but since  $T_c$  decreases at the same time,<sup>(2)</sup>

$$k_B T_c/J = 1/\ln(1 + \sqrt{q}) \quad (6)$$

the behavior will be qualitatively similar.

A power-law divergence of the specific heat would imply the following behavior of the internal energy:

$$\begin{aligned} \langle U \rangle_{T < T_c} &= U_c^- - A^- (1 - T/T_c)^{1-\alpha_-}, \\ \langle U \rangle_{T > T_c} &= U_c^+ + A^+ (1 - T_c/T)^{1-\alpha_+} \end{aligned} \quad (7)$$

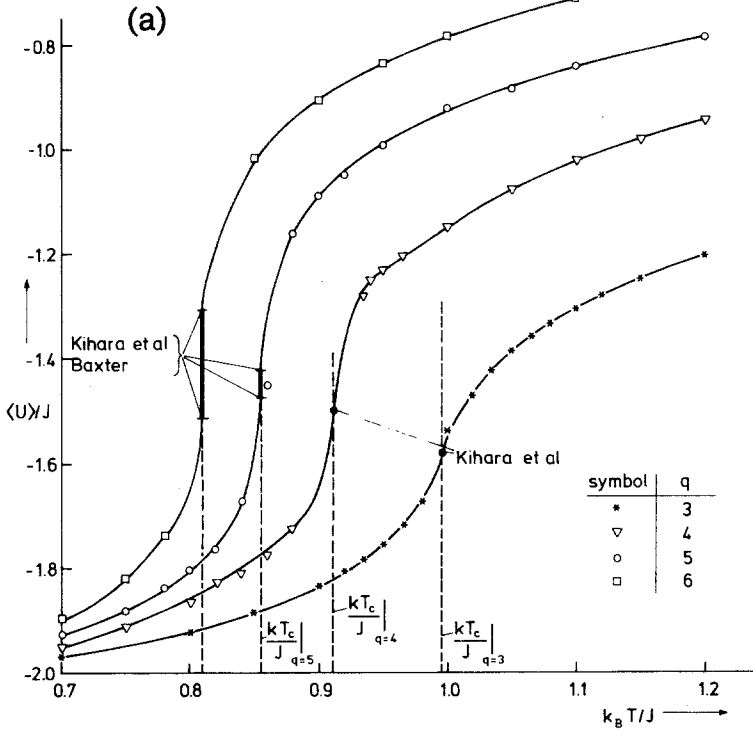


Fig. 3. (a) Equilibrium energy  $U(t)$  plotted versus temperature for  $q = 3, 4, 5, 6$ . Exact critical values are calculated from Kihara *et al.*<sup>(2)</sup> and Baxter.<sup>(15)</sup> (b) Apparent “hysteresis” loop for  $q = 5$  recorded as described in the text.

with exponents  $\alpha_-, \alpha_+ > 0$ . Hence we show energy differences  $(\langle U \rangle - U_c^-) / U_c^-$  and  $(U_c^+ - \langle U \rangle) / U_c^+$  on a log-log plot in Fig. 4. On the other hand, if well-defined metastable states would occur, the energy presumably could be represented in terms of a specific heat diverging at “pseudospinodal temperatures”  $T_c^-, T_c^+$ ,

$$\begin{aligned} \langle U \rangle_{T < T_c} &= (U_c^-)_{\text{sp}} - A^- (1 - T/T_c^+)^{1-\alpha_-} \\ \langle U \rangle_{T > T_c} &= (U_c^+)_{\text{sp}} + A^+ (1 - T_c^-/T)^{1-\alpha_+} \end{aligned} \quad (8)$$

with  $T_c^- < T_c < T_c^+$  (see Fig. 5). Equation (8) implies a finite slope  $d\langle U \rangle / dT$  at  $T = T_c$ , and hence in Fig. 4 the slope should be unity. Instead we see slopes much smaller than unity, implying large exponents  $\alpha_-, \alpha_+$  even for  $q \geq 5$ , whose values are reasonably consistent with previous estimates where the transition was found to be of second order.<sup>(21,27-30,52)</sup>

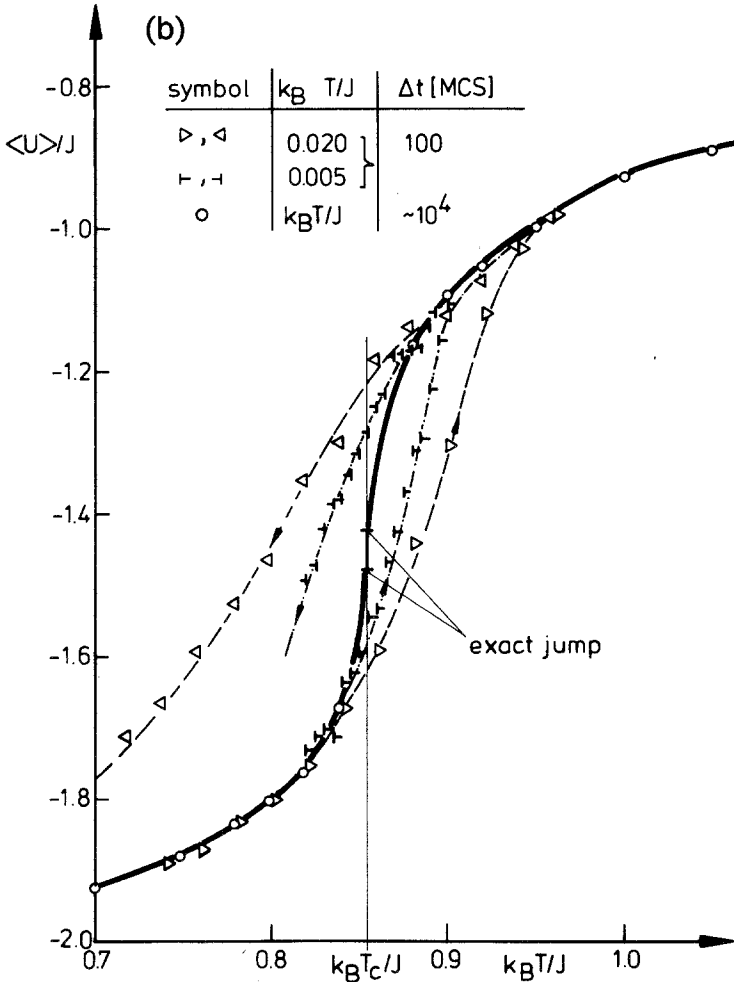


Fig. 3. Continued.

If we assume Eq. (8) to be valid and assume that  $\alpha_+ \approx \alpha_- \approx 2/3$ , as well as amplitudes  $A^+/J$  and  $A^-/J$  of order unity, and  $(U_c^-)_{sp} = (U_c^+)_{sp}$  as well as  $\Delta T \equiv T_c - T_c^- = T_c^+ - T_c$  for simplicity, we can use the exact values of the energy jump  $(U_c^+ - U_c^-)/J$  to estimate  $\Delta T$ ,

$$(U_c^+ - U_c^-)/J \approx 2(1 - T_c/T_c^+)^{1/3} \approx 2(\Delta T/T_c)^{1/3} \quad (9)$$

Hence even for  $q = 6$  we would expect a shift of the pseudospinodal singularity of no more than  $\Delta T/T_c \approx 10^{-3}$ , and the shift in the case  $q = 5$

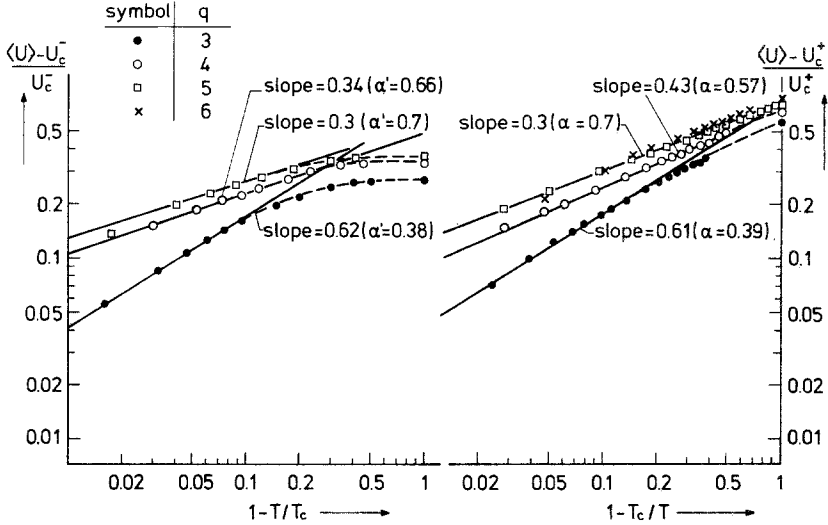


Fig. 4. Log-log plot of energy differences versus temperature for various  $q$ . Tentative estimates of the “effective” specific heat exponents are indicated. Left part refers to  $T < T_c$  and right part to  $T > T_c$ .

would be even smaller. On the basis of this estimate we would expect to see a behavior consistent with Eq. (7) in Fig. 4 up to values  $|1 - T/T_c|$  of order  $\Delta T/T_c$ , where then a crossover to slope unity should set in. Since the reduced temperatures  $|1 - T/T_c|$  available in Fig. 4 are much larger, this behavior, which follows from Eq. (8), is also consistent with our data, although at first glance the data (Fig. 3) seem to imply that the behavior is that of Fig. 5B instead of Fig. 5A. In order to distinguish these two types of behavior, one would have to go an order of magnitude closer to  $T_c$ , which (because of finite-size rounding phenomena) would require systems of size  $N \approx 10^3 \times 10^3$ . Due to the pronounced slowing down at the transition (Section 3), this would be far beyond present computer capabilities. In the case  $q = 3$ ,  $d = 3$  current estimates for  $\alpha_+$ ,  $\alpha_-$  range from about 0.4<sup>(22)</sup> to about 0.5,<sup>(23)</sup> and  $(U_c^+ - U_c^-)/J$  is estimated to be<sup>(23)</sup> less than 0.1; hence the situation is not much better. From these findings it is also not too surprising that high-temperature series expansions as well as many real space renormalization-group calculations describe this transition for  $q \geq 5$  as second order: within the accuracy of these methods, there is no distinction among  $T_c^-$ ,  $T_c^+$ , and the true  $T_c$ .

In Fig. 6 our estimates for the free energy are shown. We obtain the



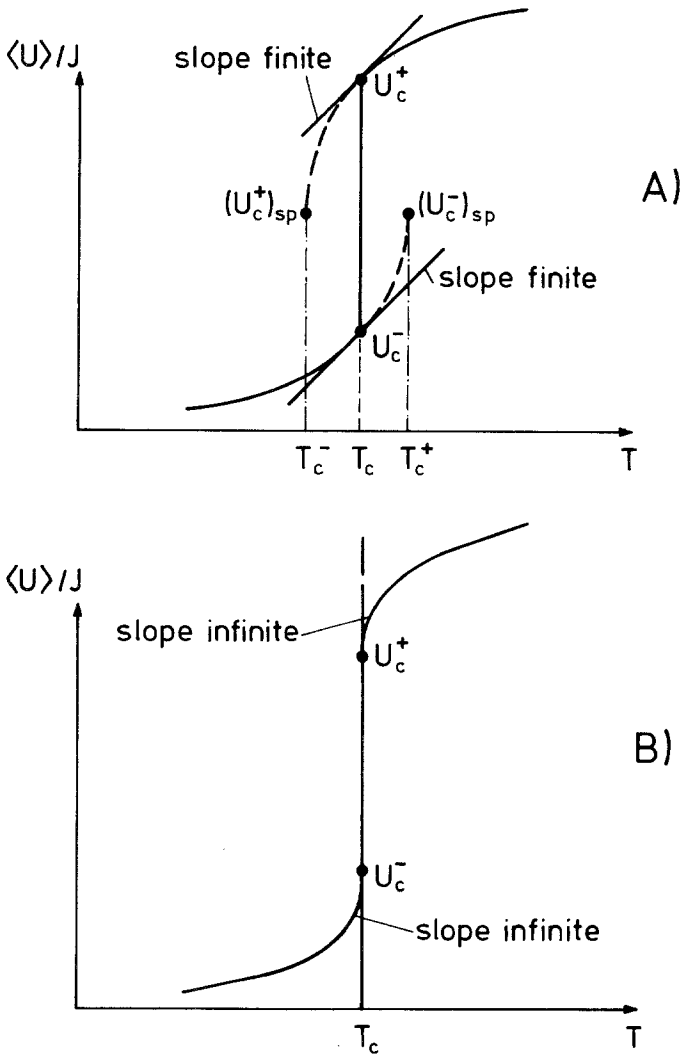


Fig. 5. Schematic variation of the energy with temperature for the case of pseudospinodal singularities (A) and a true specific heat divergence at the first-order transition (B).

free energy from integrations starting either from high or low temperatures,

$$\frac{F}{k_B T} = -\ln q + \int_0^{1/k_B T} \langle U \rangle_T d \frac{1}{k_B T} \quad (10a)$$

$$\frac{F}{k_B T} = \frac{\langle U \rangle}{k_B T} - \int_0^T \frac{d\langle U \rangle}{k dT} \frac{dT}{T} \quad (10b)$$

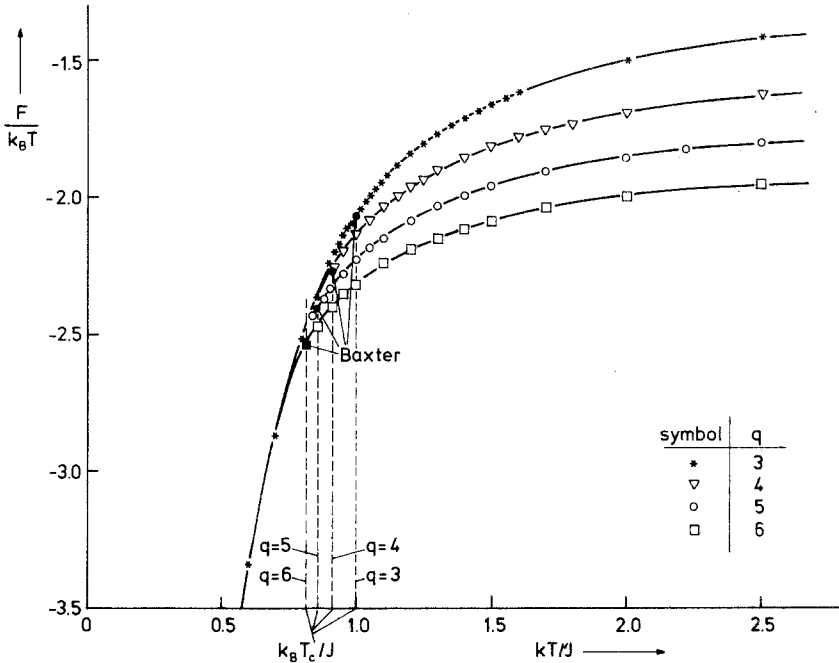


Fig. 6. Free energy  $F/k_B T$  plotted versus temperature for  $q = 3, 4, 5, 6$ . Exact critical values are calculated from Baxter.<sup>(15)</sup>

Both methods give identical results (to within an accuracy of about 0.3%), and agree with the exact results of Baxter,<sup>(15)</sup>

$$\left(\frac{F}{k_B T}\right)_{q=3} = -\frac{1}{2} \ln 3 + \int_{-\infty}^{+\infty} \frac{dx}{x} \frac{\tanh(\pi x/6) \sinh(5\pi x/6)}{\sinh \pi x} \approx -2.07 \quad (11a)$$

$$\left(\frac{F}{k_B T}\right)_{q=4} = -\ln 2 + 4 \ln \frac{\Gamma(1/4)}{2\Gamma(3/4)} \approx -2.26 \quad (11b)$$

$$\left(\frac{F}{k_B T}\right)_{q>5} = -\frac{\ln q}{2} + \Theta + \sum_{n=1}^{\infty} \frac{\exp(-n\Theta) \tanh n\Theta}{n} \quad (11c)$$

where  $\Theta = \text{arcosh}(\sqrt{q}/2)$  and the summation yields  $(F/k_B T)_{q=5} \approx -2.41$  and  $(F/k_B T)_{q=6} \approx -2.54$ .

Figures 7 and 8 show our results on the critical behavior for  $q = 3$ . The specific heat obtained from energy fluctuations and from numerical derivatives  $\partial \langle U \rangle / \partial T$  agree with each other within the accuracy (which is

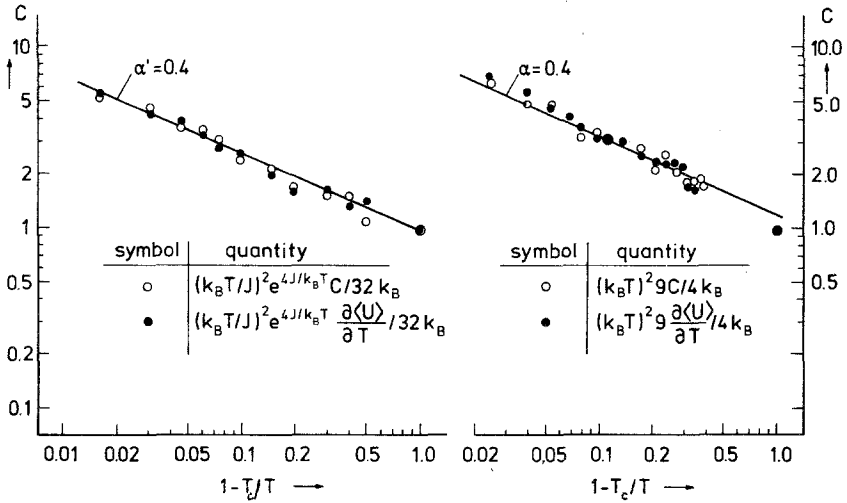


Fig. 7. Log-log plot of the specific heat versus temperature for  $q = 3$  and  $T < T_c$  [left part] as well as  $T > T_c$  [right part].

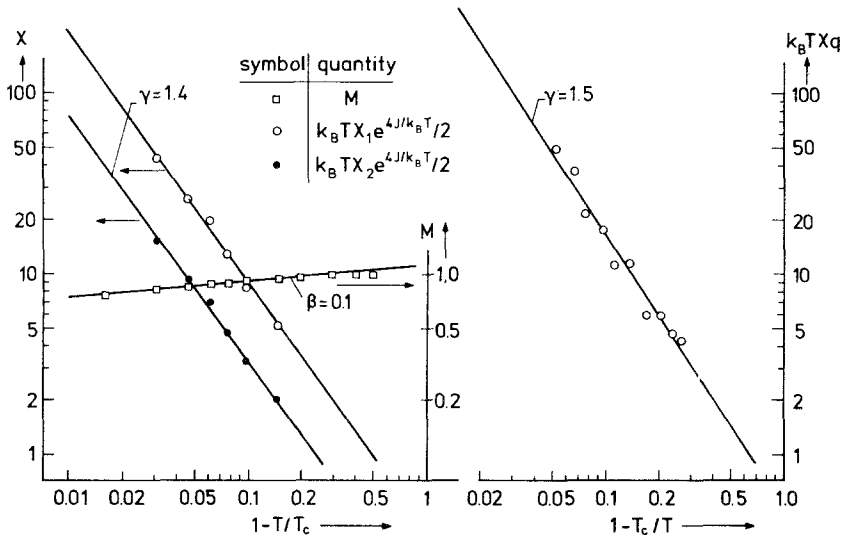


Fig. 8. Log-log plot of magnetization and susceptibility versus temperature for  $q = 3$  and  $T < T_c$  [left part] as well as  $T > T_c$  [right part].

typically about 10%), and this suggests an “effective exponent”  $\alpha \approx 0.4$  consistent with the direct analysis of the energy (Fig. 4). A higher value quoted in preliminary communications on this work<sup>(53,54)</sup> was due to insufficient statistical accuracy. We denote this exponent “effective” because the data are not extremely close to  $T_c$ , and hence (unknown) correction terms may lead to errors of systematic nature. While our estimate is reasonably close to series extrapolation results<sup>(34)</sup> and experiment,<sup>(36)</sup> it certainly does not exclude that asymptotically close to  $T_c$  the data would yield an exponent  $\alpha = 1/3$ .<sup>(38)</sup> Note that we have normalized the specific heat in Fig. 7 by such factors that it approaches unity for  $T \rightarrow 0$  or  $1/T \rightarrow 0$ , respectively. Omitting these factors would produce strong curvature on the log–log plot in the considered temperature region.

The same reservations have to be made with respect to order parameter and susceptibility as well (Fig. 8). Our estimates of the corresponding effective exponents  $\beta \approx 0.1$  and  $\gamma \approx 1.45$  agree well with series estimates.<sup>(9,22)</sup> The scaling relation  $\gamma + 2\beta (\approx 1.65) = 2 - \alpha (\approx 1.60)$  is well satisfied within our error limits, since even if systematic errors due to correction terms are absent, the statistical inaccuracy of our data implies probable relative errors of our exponents of about 5%.

As expected from our discussion of the energy, we find that specific heat and susceptibility seem to diverge at  $T_c$  even for  $q \geq 5$ . Again a distinction of “pseudospinodal singularities” and true divergences is not possible, since the expected  $T_c^-, T_c^+$  are too close to  $T_c$ . Thus we do not discuss this behavior further.

### 3. DYNAMIC PROPERTIES

The dynamics of the model is described by a master equation for the probability  $P(\mathbf{X}, t)$  of a configuration  $\mathbf{X}$  of the system,

$$\frac{dP(\mathbf{X}, t)}{dt} = - \sum_{\mathbf{X}'} W(\mathbf{X} \rightarrow \mathbf{X}') P(\mathbf{X}, t) + \sum_{\mathbf{X}'} W(\mathbf{X}' \rightarrow \mathbf{X}) P(\mathbf{X}', t) \quad (12)$$

the transition probability  $W$  being expressed in terms of the energy change  $\delta \mathcal{H}$  involved in the transition  $\mathbf{X} \rightarrow \mathbf{X}'$  as

$$W(\mathbf{X} \rightarrow \mathbf{X}') = \exp(-\delta \mathcal{H} / k_B T) \quad \text{if } \delta \mathcal{H} > 0 \quad (13a)$$

$$W(\mathbf{X} \rightarrow \mathbf{X}') = 1 \quad \text{otherwise} \quad (13b)$$

and the time  $t$  is measured in units of Monte Carlo steps/site. As changes  $\mathbf{X} \rightarrow \mathbf{X}'$  we consider random changes of  $s_i \rightarrow s_j \neq s_i$  (taken out of the values  $1, \dots, q$ ) of sites  $i$  selected at random. Nonlinear relaxation functions of

energy and magnetization are then defined as usual<sup>(43,49)</sup>

$$\phi_U^{(nl)}(t) = \frac{U(t) - U(\infty)}{U(0) - U(\infty)}, \quad \phi_M^{(nl)}(t) = \frac{M(t) - M(\infty)}{M(0) - M(\infty)} \quad (14)$$

where  $M(\infty) \equiv \langle M \rangle$  and  $U(\infty) \equiv \langle U \rangle$ . These functions are obtained straightforwardly from the “raw data” of the simulation (e.g., Figs. 1, 2). Relaxation times are found by (numerical) integration of these functions, as usual,<sup>(43,49)</sup>

$$\tau_U^{(nl)} = \int_0^\infty \phi_U(t) dt, \quad \tau_M^{(nl)} = \int_0^\infty \phi_M(t) dt \quad (15)$$

While  $\langle M \rangle = 0$  for  $T > T_c$ , our inaccurate knowledge of  $\langle M \rangle$  for  $T < T_c$  leads to serious inaccuracies of  $\tau_M^{(nl)}$  close to  $T_c$  there. Therefore we restrict our analysis to  $T > T_c$ . Figure 9 shows a log-log plot of these relaxation times for both  $q = 3$  and  $q = 4$ . While  $\tau_M^{(nl)}$  closely follows a straight line, implying an exponent  $\Delta_M^{(nl)} \approx 1.8$ , the results for  $\tau_U^{(nl)}$  show strong curvature. Thus we consider instead the quantity  $\tau_U'^{(nl)} = \tau_U(1 - \langle U \rangle / \langle U \rangle_0)$ , which has the same critical behavior as  $\tau_U$  but removes a correction term [arising from the denominator of Eq. (14)]. For this modified energy relaxation

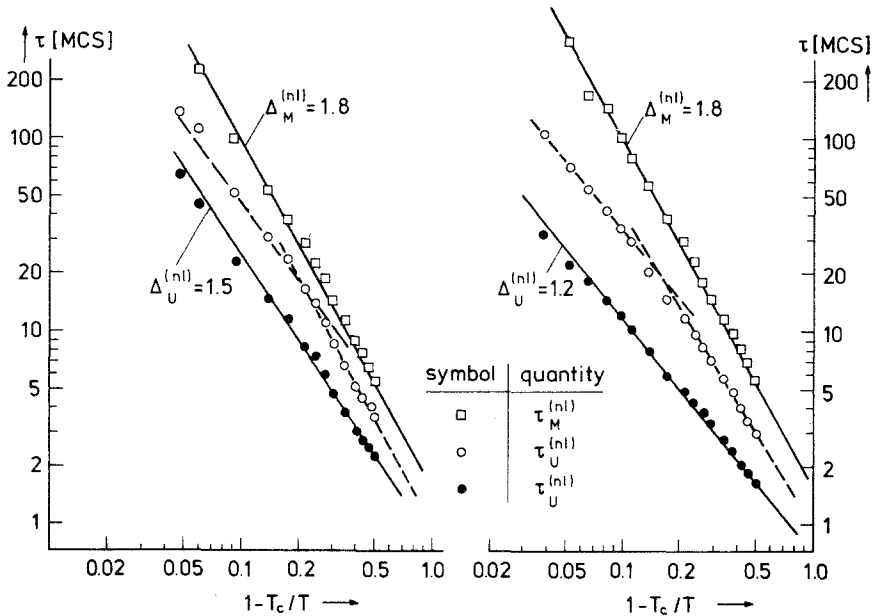


Fig. 9. Log-log plot of various nonlinear relaxation times versus temperature for  $q = 3$  [right part] and  $q = 4$  [left part].

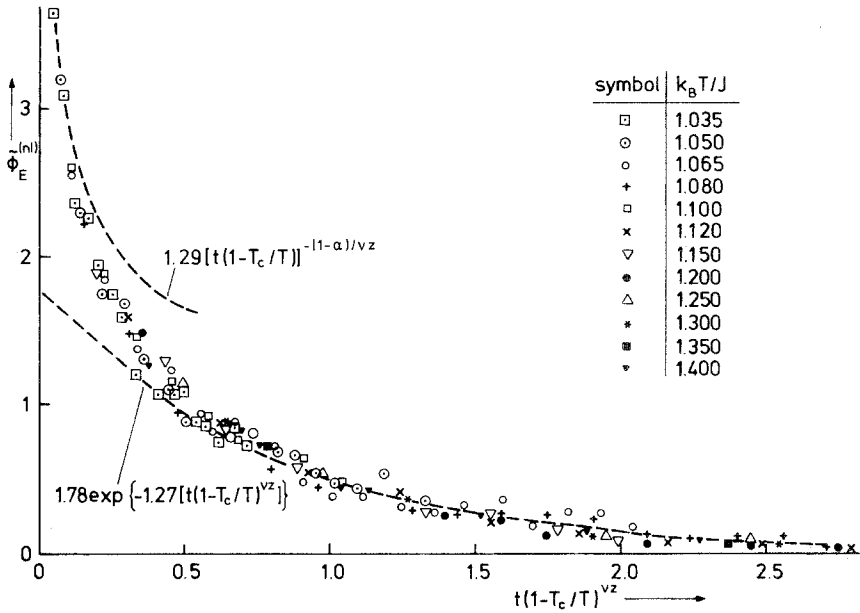


Fig. 10. Scaling plot of energy relaxation function versus time for  $q = 3$ . Exponents used are  $\alpha = 1/3$  and  $z\nu = 1.9$ . Various temperatures are shown.

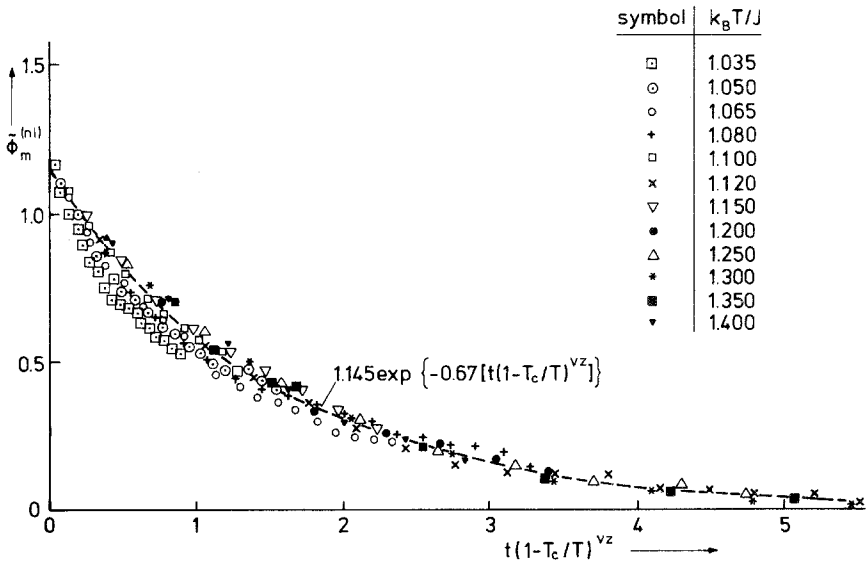


Fig. 11. Scaling plot of order parameter relaxation function versus time for  $q = 3$ . Exponents used are  $\beta = 1/9$  and  $z\nu = 1.85$ . Various temperatures are shown.

time, most of the curvature on the log-log plot is removed, and an exponent estimate  $\Delta_U^{(nl)} \approx 1.2$  results. Both exponents should be related via the dynamic scaling law<sup>(47,49)</sup>

$$\Delta_M^{(nl)} - \Delta_U^{(nl)} = 1 - \alpha - \beta \quad (16)$$

which gives  $\Delta_M^{(nl)} - \Delta_U^{(nl)} \approx 0.57$  for  $q = 3$ , using  $\beta \approx 0.1$  and  $\alpha = 1/3$ , while  $\Delta_M^{(nl)} - \Delta_U^{(nl)} \approx 0.25$  for  $q = 4$ , using  $\beta \approx 0.08$  (consistent with our direct observations of  $M$  for  $q = 4$  not shown here) and  $\alpha = 2/3$ . It appears that Eq. (16) is reasonably well obeyed. Our estimates would imply that the exponent  $\Delta \equiv \nu z \approx 1.9$ , independent of  $q$  within our accuracy (this holds even for the Ising case,  $q = 2$ ).<sup>(43)</sup> As with respect to static quantities, we should consider this value as an estimate of an effective exponent only, since correction terms cannot be excluded. Note that for  $q \geq 3$ ,  $\Delta$  differs strongly from  $\gamma$ , and hence there is a clear violation of the “conventional theory” of slowing down, which implies  $\Delta = \gamma$ .<sup>(43)</sup>

A more detailed test of dynamic scaling is performed using  $\phi_U^{(nl)}(t)$  and  $\phi_M^{(nl)}(t)$  and defining the functions<sup>(49)</sup>

$$\tilde{\phi}_U^{(nl)} = (1 - T_c/T)^{\alpha-1} \phi_U^{(nl)}(t), \quad \tilde{\phi}_M^{(nl)} = (1 - T_c/T)^{-\beta} \phi_M^{(nl)}(t) \quad (17)$$

which no longer should depend on the two variables  $t$ ,  $1 - T_c/T$  separately but rather only on a single variable  $\tilde{t} = t(1 - T_c/T)^{\nu z}$ . Figures 10 and 11 show that within our accuracy this type of scaling actually works, and hence the scaling functions  $\tilde{\phi}_U^{(nl)}(\tilde{t})$  and  $\tilde{\phi}_M^{(nl)}(\tilde{t})$  can be estimated. One expects that<sup>(48-50)</sup>

$$\tilde{\phi}_U \propto \tilde{t}^{-(1-\alpha)/\nu z}, \quad \tilde{t} \ll 1 \quad (18a)$$

$$\tilde{\phi}_U \propto \exp(-c_1 \tilde{t}), \quad \tilde{t} \gg 1 \quad (18b)$$

$$\tilde{\phi}_M \propto \tilde{t}^{-\beta/\nu z}, \quad \tilde{t} \ll 1 \quad (18c)$$

$$\tilde{\phi}_M \propto \exp(-c_2 \tilde{t}), \quad \tilde{t} \gg 1 \quad (18d)$$

where  $c_1$  and  $c_2$  are constants of order unity. While our data provide some evidence for relations (18a) and (18b), it turns out that  $\tilde{\phi}_M$  is fitted nearly completely by Eq. (18d): due to the smallness of  $\beta$ , extremely small  $\tilde{t}$  (but nevertheless large  $t$ ) are required to actually see the power-law decay of the order parameter relaxation (18c). Note also that due to the scatter of the data the plots in Figs. 10 and 11 are not very sensitive to the precise values of the exponents  $\alpha$ ,  $\beta$ , and  $\nu z$  used.

The results for larger  $q$  are qualitatively very similar to the case  $q = 3$ . Figure 12 summarizes the (apparent?) divergences associated with the first-order transition for  $q = 5$ .

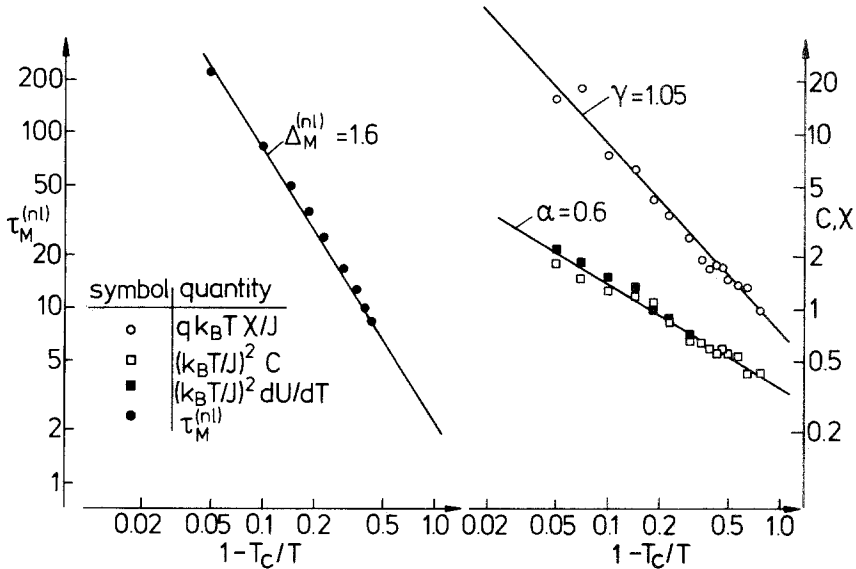


Fig. 12. Log-log plot of the relaxation time versus temperature [left part] and susceptibility and specific heat [right part] for  $q = 5$ .

#### 4. CONCLUSIONS

The phase transition of the  $q$ -state Potts model on the square lattice was studied for  $q = 3, 4, 5, 6$  by Monte Carlo methods. The data obtained are nicely consistent with the exact critical temperatures, energies, and free energies (Figs. 3 and 6). We estimate "effective" critical exponents for  $q = 3$  as  $\alpha \approx 0.4$ ,  $\beta \approx 0.1$ ,  $\gamma \approx 1.45$ , in rough agreement with high-temperature series extrapolations and real space renormalization and the scaling relation  $2 - \alpha = \gamma + 2\beta$ . The transition for  $q = 5, 6$  is found to be a very weakly first-order transition: specific heat and susceptibility diverge either right at the transition temperature  $T_c$  or at "pseudospinodal" temperatures  $T_c^+$ ,  $T_c^-$ , which are no more apart from  $T_c$  than about  $\Delta T/T_c \approx 10^{-3}$ . The implication of our results for related studies of the three-dimensional systems is that great care is needed for the accurate estimate of the magnitude of jumps at first-order transitions.

A kinetic Potts model is introduced in about the same way as the kinetic Ising model, defining time evolution in terms of a suitable master equation. This time evolution is directly realized by the Monte Carlo process. It is shown that within the framework of this kinetic model we find no metastable states even in the case of first-order transitions, but pronounced critical slowing down. The exponent  $\nu\gamma$  associated with the slow-



ing down is estimated to be about 1.9, independent of  $q \geq 2$  within our accuracy. This result would imply a pronounced departure from the conventional slowing down ( $z\nu = \gamma$ ) for  $q \geq 3$ . The exponents associated with nonlinear relaxation of the order parameter and energy are estimated and found to be consistent with dynamic scaling. The associated scaled relaxation functions also are estimated.

## ACKNOWLEDGMENTS

The author is indebted to D. D. Betts, H. J. Hermann, L. P. Kadanoff, E. K. Riedel, and R. J. Swendsen for sending relevant preprints. He thanks A. Aharony for stimulating discussions, and T. Burkhardt and D. Stauffer for a careful reading of the manuscript.

## REFERENCES

1. R. B. Potts, *Proc. Camb. Phil. Soc.* **48**: 106 (1952).
2. T. Kihara, Y. Midzuno, and T. Shizume, *J. Phys. Soc. Japan* **9**:681 (1954).
3. S. Alexander, *Phys. Lett. A* **54**:353 (1975).
4. E. Domany and E. K. Riedel, *J. Appl. Phys.* **49**:1315 (1978).
5. A. N. Berker, S. Ostlund, and F. A. Putnam, *Phys. Rev. B* **17**:3650 (1978).
6. D. Mukamel, M. E. Fisher, and E. Domany, *Phys. Rev. Lett.* **37**:565 (1976).
7. B. Barbara, M. F. Rossignol, and P. Bak, *J. Phys. C* **11**:L183 (1978).
8. (a) A. Aharony, K. A. Müller, and W. Berlinger, *Phys. Rev. Lett.* **38**:33 (1977); (b) B. K. Das and R. B. Griffiths, Carnegie-Mellon University preprint.
9. J. P. Straley and M. E. Fisher, *J. Phys. A* **6**:1310 (1973).
10. P. M. Levy and J. J. Sudano, *Phys. Rev. B* **18**:5087 (1978).
11. G. R. Golner, *Phys. Rev. B* **8**:3419 (1973).
12. D. J. Amit and A. Sherbakov, *J. Phys. C* **7**:L96 (1974).
13. R. G. Priest and T. C. Lubensky, *Phys. Rev. B* **13**:4159 (1976).
14. R. K. P. Zia and D. J. Wallace, *J. Phys. A* **8**:1495 (1977).
15. R. J. Baxter, *J. Phys. C* **6**:L445 (1973).
16. R. V. Ditzian and L. P. Kadanoff, *J. Phys. A* **12**:L229 (1979).
17. R. V. Ditzian and J. Oitman, *J. Phys. A* **7**:L61 (1974).
18. I. G. Enting, *J. Phys. A* **7**:1617 (1974).
19. I. G. Enting and C. Domb, *J. Phys. A* **8**:1228 (1975).
20. J. P. Straley, *J. Phys. A* **7**:2173 (1974).
21. D. Kim and R. I. Joseph, *J. Phys. A* **8**:891 (1975).
22. S. Miyashita, D. D. Betts, and C. J. Elliott, *J. Phys. A* **12**:1605 (1979).
23. H. J. Herrmann, *Z. Physik B* **35**:171 (1979).
24. H. W. J. Blöte and R. H. Swendsen, *Phys. Rev. Lett.* **43**:799 (1979).
25. B. Chu, M. F. Schoenes, and M. E. Fisher, *Phys. Rev.* **185**:219 (1969).
26. R. H. Swendsen, *Phys. Rev. Lett.* **42**:859 (1979).
27. T. W. Burkhardt, H. J. F. Knops, and M. den Nijs, *J. Phys. A* **9**:L179 (1976).
28. C. Dasgupta, *Phys. Rev. B* **15**:3460 (1977).
29. M. P. M. den Nijs and H. J. F. Knops, *Physica* **93A**:441 (1978).
30. M. P. M. den Nijs, *Physica* **95A**:449 (1979).

31. A. Aharony, *J. Phys. A* **10**:389 (1977).
32. B. W. Southern, *J. Phys. A* **10**:L253 (1977).
33. B. Nienhuis, A. N. Berker, E. K. Riedel, and M. Schick, *Phys. Rev. Lett.* **43**:737 (1979); see also T. Burkhardt, preprint.
34. T. de Neef and I. G. Enting, *J. Phys. A* **10**:801 (1977).
35. R. Zwanzig and J. D. Ramshaw, *J. Phys. A* **10**:65 (1977).
36. M. Bretz, *Phys. Rev. Lett.* **38**:501 (1977).
37. I. G. Enting, *J. Phys. A* **8**:L35 (1975).
38. M. P. M. den Nijs, *J. Phys. A* **12**:1857 (1979).
39. K. Binder, ed., *Monte Carlo Methods in Statistical Physics* (Springer, Berlin, 1979).
40. D. P. Landau and K. Binder, *Phys. Rev. B* **17**:2328 (1978).
41. B. Nienhuis and M. Nauenberg, *Phys. Rev. Lett.* **35**:477 (1975).
42. H. Müller-Krumbhaar and K. Binder, *J. Stat. Phys.* **8**:1 (1973).
43. E. Stoll, K. Binder, and T. Schneider, *Phys. Rev. B* **8**:3266 (1973).
44. S. T. Chui, private communication.
45. M. Suzuki, *Int. J. Magnetism* **1**:123 (1971).
46. Z. Racz, *Phys. Rev. B* **13**:263 (1976).
47. M. E. Fisher and Z. Racz, *Phys. Rev. B* **13**:5039 (1976).
48. K. Binder, D. Stauffer, and H. Müller-Krumbhaar, *Phys. Rev. B* **12**:5261 (1975).
49. R. Kretschmer, K. Binder, and D. Stauffer, *J. Stat. Phys.* **15**:267 (1976).
50. R. Bausch, E. Eisenriegler, and H. K. Janssen, *Z. Physik B* (1979).
51. K. Binder and H. Müller-Krumbhaar, *Phys. Rev. B* **9**:2328 (1974).
52. I. G. Enting, *J. Phys. A* **7**:2181 (1974).
53. K. Binder, in *Proceedings of the 4th EPS Gen. Conf., York, 1978* (Institute of Physics, London, 1979), p. 164.
54. K. Binder, in *Ordering in Strongly-Fluctuating Condensed-Matter Systems*, T. Riste, ed. (Plenum Press, New York, to be published).