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Finite-Size Effects and Phase Transition in the Three-Dimensional Three-State Potts Model

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The three-state Potts model in three dimensions is studied by Monte Carlo and finite-size scaling techniques. Using a histogram method recently proposed by Ferrenberg and Swendsen, the finite-size dependence for the maximum of the specific heat is found to scale with the volume of the system, indicating that the phase transition is of first order. The value of the latent heat per spin and the correlation length at the transition are estimated.

KEY WORDS: Potts model; first-order phase transition; finite-size effects; Monte Carlo simulations; latent heat; correlation length.

The knowledge of the finite-size dependence of the various thermodynamic quantities in the neighborhood of a phase transition provides a very useful way to compute, using numerical techniques and appropriate extrapolation, the properties of infinite systems. In this paper we investigate the finite-size effects at a temperature-driven phase transition in the three-state Potts model in three dimensions. Numerical simulations here performed show that the maximum of the specific heat scales with the volume of the system in the thermodynamic limit, indicating that the phase transition of the model is first order. We use a finite-size scaling form for the behavior of the maximum of the specific heat valid for all volumes to estimate the latent heat and correlation length at the transition point.

In an infinite system the singularities observed in a second-order phase transition can be traced back to the divergence of the correlation length, which leads to the well-known universal behavior characterized by a critical region and critical exponents. The singularities occurring in a first-order phase transition are, however, due to phase coexistence only. The

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correlation length does not diverge and is actually of the order of a few lattice spacings and discontinuous at the transition. The amount of energy necessary to convert one phase into the other is the latent heat of the transition. Although the origin of the singularities is physically different for both types of transitions, the finite-size effects induce a rounding of the transition region and also a shift of the transition temperature, thereby leading to ambiguities in the identification of the order of the transition and location of the transition point. In a second-order phase transition the correlation length is limited by the size L of the system, leading to a scaling prediction for the rounding and shifting of the transition temperature to decrease as $L^{-1/\nu}$ and for the maximum of the specific heat to diverge as $L^{\alpha/\nu}$. First-order transitions are rounded and shifted, decreasing as L^{-d}, with the maximum of the specific heat growing as L^{d}.(1) These results can be used to diagnose the type of phase transition and to locate the temperature transition point in the thermodynamic limit by studying finite systems. Finite-size effects at a first-order phase transition have recently been observed experimentally in adsorbed oxygen films.(2)

Several attempts have been made both experimentally and theoretically to determine the nature of the phase transition in the three-state Potts model. Earlier theoretical attempts(3–13) proved to be difficult to find an unambiguous answer to the problem. More recent works, however, have shown that the system undergoes a weak first-order phase transition at a temperature of about $K_B T_c/J \simeq 1.817 \pm 0.001$. The principal difficulty in identifying the nature of the transition was the apparent divergence of the correlation length in the vicinity of the transition point, which is a characteristic of a second-order phase transition. This problem has recently attracted interest because of its similarities with the results for the finite-temperature phase transition in QCD.(16)

This model has been extensively studied by different techniques. Earlier studies were done by high-temperature series analysis,(3-6) mean field theories,(7) renormalization group techniques,(8-10) and Monte Carlo simulations.(11–13) Recent calculations have been done mostly by numerical simulation using multilattice microcanonical simulation(14) and Monte Carlo techniques.(15)

The model investigated here is described by the following Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) - H \sum_i \delta(\sigma_i, 1) \qquad (1)$$

where $\langle i, j \rangle$ indicates the sum over all pairs of nearest neighbor interactions. $\sigma_i = 1, 2, \ldots, q$ specifies one of the q states of a spin at site i. The symbol $\delta(\sigma_i, \sigma_j)$ is the Kronecker δ-function, $J > 0$ is the interaction energy between two spins, and H is the applied magnetic field. An extensive review of the static properties of the q-state Potts model in all dimensions is found in ref. 17.

By following Ferrenberg and Swendsen$^{(18),2}$ Let us rewrite the Hamiltonian (1) in the form

$$-\beta H = K \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) + h \sum_i \delta(\sigma_i, 1) \equiv KE + hM \tag{2}$$

where K is a dimensionless coupling constant in which we have absorbed the usual factor of $1/K_B T$, and $h = H/K_B T$. The partition function can now be written as

$$Z(K, h) = \sum_{E,M} N(E, M) \exp(KE + hM) \tag{3}$$

where $N(E, M)$ is the number of states for the system with energy E and magnetization M. The probability distribution of E and M for a given temperature and field is given by

$$P_{(K,h)}(E, M) = N(E, M) \exp(KE + hM)/Z(K, h) \tag{4}$$

so that the average of any thermodynamic quantity can be evaluated as

$$\langle A(E, M) \rangle_{(K,h)} = \sum_{(E,M)} A(E, M)\, P_{(K,h)}(E, M) \tag{5}$$

The probability distribution can be found numerically, by using Monte Carlo simulation to generate the histogram of values of E and M. The histogram properly normalized is an estimate of $P(K, h)$ for a point (K, h) in the parameter space. The great advantage of the method is that the estimated probability distribution for a given point (K, h) can be used to generate the probability distribution for a different point (K', h') in the parameter space, that is,

$$P_{(K',h')}(E, M) = \frac{P_{(K,h)}(E, M) \exp[(K' - K)E + (h' - h)M]}{\sum_{E,M} P_{(K,h)}(E, M) \exp[(K' - K)E + (h' - h)M]} \tag{6}$$

One should emphasize that the above relation is exact and any errors are due to the numerical determination of the number of states $N(E)$. The denominator of Eq. (6) is in fact an approximation for the partition func-

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[2] See refs. 19 for earlier work using the histogram method. Further discussion of the present method is found in ref. 20, which should also be consulted for a more complete list of work using the histogram method.

tion. Since we are interested in quantities that involve the various moments of the energy distribution, we shall restrict the phase space to one dimension involving only the energy E.

Before we report our numerical results, let us first review the main results of the theory of finite-size scaling at temperature-driven first-order phase transition, proposed by Challa *et al.*(1) The starting point is the Landau theory of thermodynamic fluctuations.(21) In this approach the probability distribution $P(E)$ of finding the system in a single phase with internal energy E is a Gaussian centered about the infinite-lattice energy E_0, namely

$$P(E)=\frac{A}{\sqrt{C}}\exp\left(-\frac{L^d(E-E_0)^2}{2K_B T^2 C}\right) \tag{7}$$

where A is a normalization constant and C is the specific heat at temperature T. In the thermodynamic limit the probability distribution $P(E)$ is a δ-function centered at E_0. Because of phase coexistence at a first-order phase transition, one can assume that the probability distribution $P(E)$ is a superposition of Gaussians centered at the energies of each phase. Let E_+ (E_-) be the internal energy at the transition in the high (low)-temperature phase. If the temperature is shifted by a small amount $\Delta T = T - T_c$, the probability distribution can be written as

$$P(E)=\frac{a_+}{\sqrt{C_+}}\exp\left[-\frac{[E-[E_+ + C_+\,\Delta T)]^2 L^d}{2K_B T^2 C_+}\right] + \frac{a_-}{\sqrt{C_-}}\exp\left[-\frac{[E-(E_- + C_-\,\Delta T)]^2 L^d}{2K_B T^2 C_-}\right] \tag{8}$$

where C_+ and C_- are the discontinuities of the specific heat at the critical temperature, that is,

$$C_\pm \underset{T\to T_c^\pm}{=} \lim C(T) \tag{9}$$

The weights a_+ and a_- are functions of the free energy difference $\Delta F = F_+ - F_-$ of the two phases:

$$a_\pm = \sqrt{C_\pm}\,\exp(\pm x) \tag{10}$$

with

$$x = -(\Delta F/2K_B T)L^d, \qquad \Delta F = -(E_+ - E_-)\Delta T/T_c$$

In the special case when the transition occurs from a disordered state to a q-fold degenerate ordered state (as in the q-state Potts model), the expression for the probability distribution is identical to Eq. (8) except for $a_- = q(C_-)^{1/2}\exp(-x)$. From Eq. (8) it is straightforward to compute the moments of the energy distribution. In particular, the specific heat is given by

$$C_L(T) = \frac{a_+ C_+ + a_- C_-}{a_+ + a_-} + \frac{a_+ a_-[(E_+ - E_-) + (C_+ - C_-)\,\Delta T]^2}{K_B T^2 (a_+ + a_-)^2} L^d \tag{11}$$

From the above expression one finds that the maximum of the specific heat occurs at

$$\frac{T_c(L) - T_c}{T_c} = \frac{K_B T_c \ln[q(C_-/C_+)^{1/2}]}{E_+ - E_-} L^{-d} \tag{12}$$

where $T_c(L)$ and T_c are the transition temperatures of the finite and infinite systems, respectively. The maximum of C_L behaves as

$$C_L^{\max} \simeq \frac{(E_+ - E_-)^2}{4K_B T_c^2} L^d + \frac{C_+ + C_-}{2} \tag{13}$$

From the above results one can see that the effect of finite size is to shift the temperature by an amount given by Eq. (12) and that it approaches the infinite-temperature value as L^{-d}. The specific heat, on the other hand, diverges as L^d with a slope proportional to the square of the latent heat. We now proceed to describe the numerical results.

We have performed Monte Carlo simulations in the three-dimensional three-states Potts model at the infinite-lattice transition temperature $T_c = 1.817 \pm 0.001$ and zero magnetic field, for lattice sizes between $L = 3$ and $L = 15$. As initial condition we have take a configuration where all spins are in the same state $\sigma_i = 1$ and let the system evolve toward equilibrium under Glauber dynamics. The spins are flipped with the transition probability $p = \exp[-\Delta E/K_B T_c]/[1 + \exp(-\Delta E/K_B T_c)]$, where ΔE denotes the change in the energy for a spin flip.

The histogram of values of E was accumulated after discarding an appropriate number of Monte Carlo steps (MCS). Typical observation time was 2.5×10^5 to 10^6 MSC/spin, with the first 10^4 MCS/spin discarded to allow for thermalization.

The thermodynamic quantities calculated in the present simulation are the specific heat per spin, calculated from the energy fluctuation:

$$C/K_B = \beta^2[\langle E^2 \rangle - \langle E \rangle^2]/N \tag{14}$$

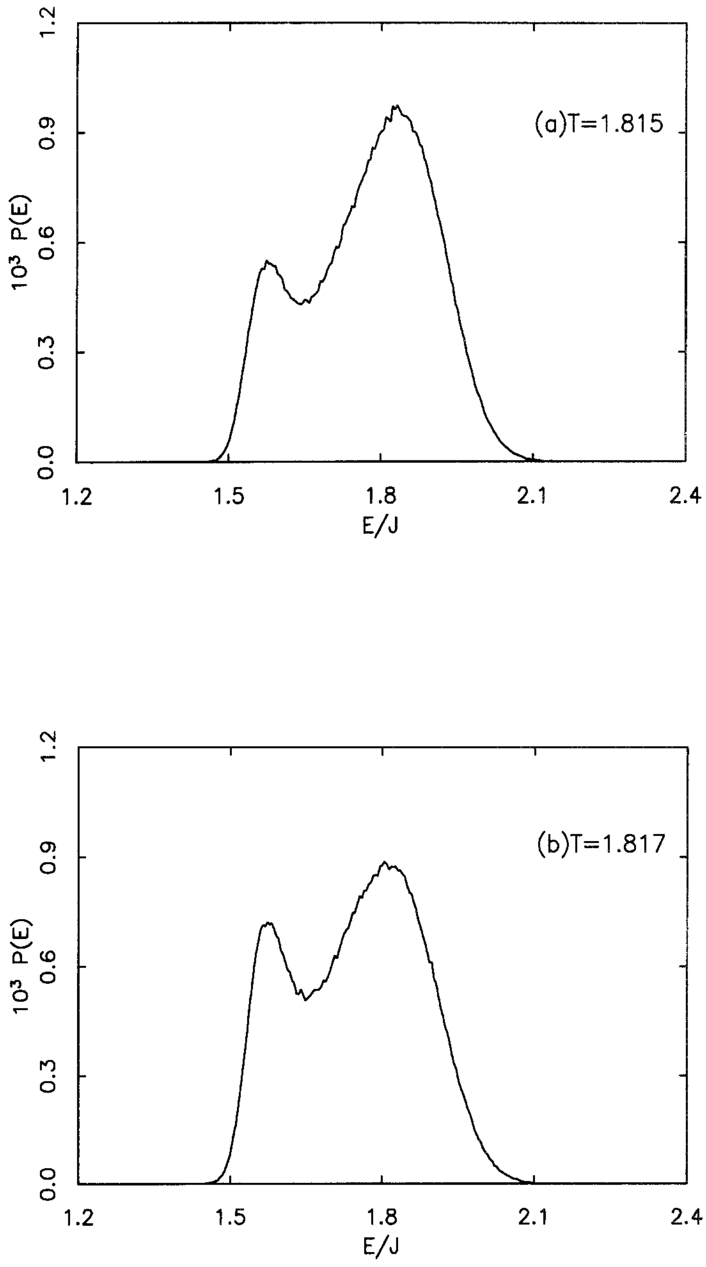

Fig. 1. Distribution of the internal energy per spin for a sequence of three temperatures and lattice size $L = 15$.

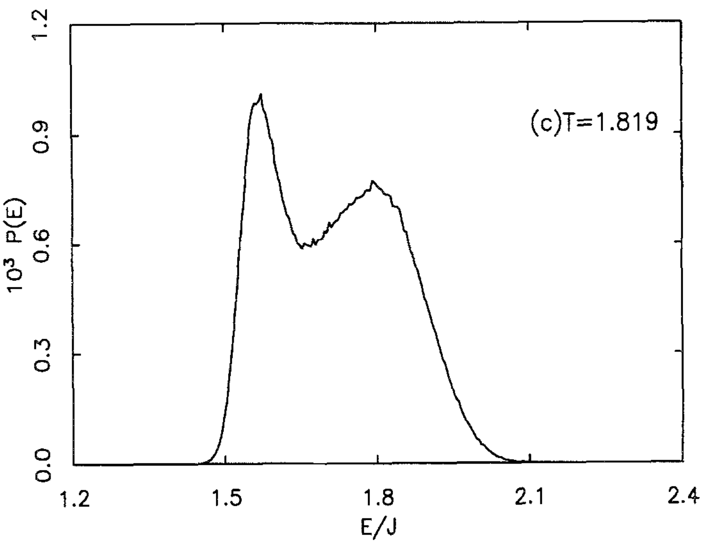

FIG. 1—*Continued.*

and the reduced fourth-order cumulant V_L, defined by

$$V_L = 1 - \frac{\langle E^4 \rangle}{3\langle E^2 \rangle^2} \tag{15}$$

For a first-order phase transition, V_L takes on a value 2/3 for low and high temperatures, tending toward a nontrivial value of[1]

$$V_L \underset{L\to\infty}{=} \frac{2}{3} - \frac{1}{3}\left[\frac{E_+^2 - E_-^2}{E_+^2 + E_-^2}\right]^2 \tag{16}$$

at T_c, where E_+ and E_- are the discontinuities of the internal energy at the transition point. Using the estimates of Wilson and Vause[14] for the internal energy discontinuities $E_+ = -1.7831(8)$ and $E_- = -1.5862(6)$, we obtain for the cumulant at T_c the value $V_L = 0.663$.

In Fig. 1 we show the distribution of the internal energy per spin for three different temperatures after about 10^6 MCS through a 15^3 lattice. The results show a double-peak structure in a small temperature range around $T = 1.817$ which is an indication of a first-order phase transition. Another indication that the transition is of first order is given by the temperature dependence of the fourth-order cumulant V_L as shown in Fig. 2. The value of V_L at T_c as the lattice size increases approaches the infinite value of $V_L = 0.663$ as obtained from Eq. (16). In Fig. 3 the maximum of the specific

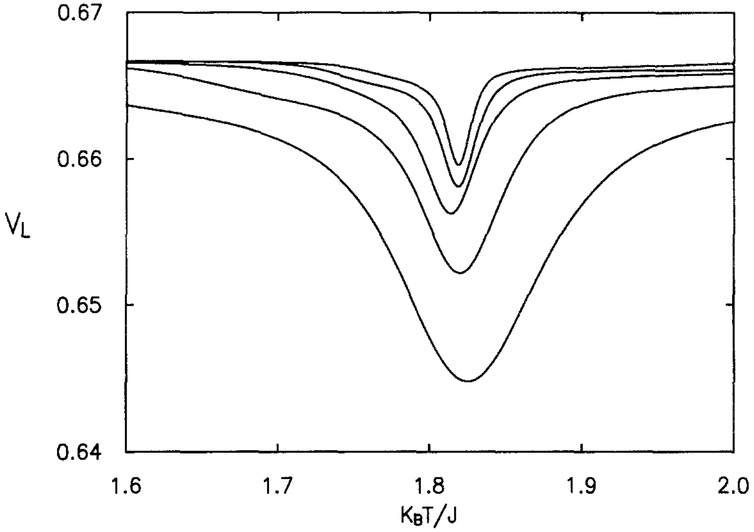

Fig. 2. Temperature dependence of the fourth-order cumulant for the energy for lattice sizes $L=7$, 9, 11, 13, and 15. The lowermost curve corresponds to $L=7$ and the uppermost to $L=15$.

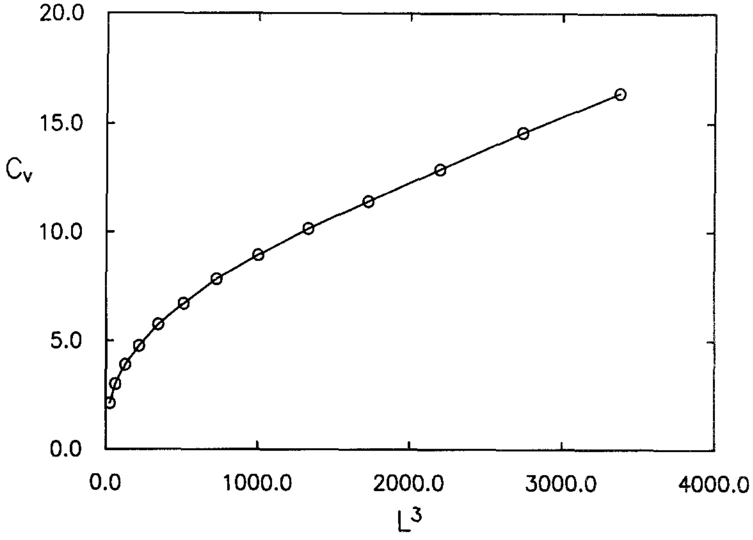

Fig. 3. Dependence of the specific heat maximum on L^3 for lattice sizes between $L=3$ and $L=15$. The solid line is a guide to the eye.

heat is plotted against the volume of the system. Each point shown in Fig. 3 has been calculated from the average of ten independent runs each measured using 2.4×10^5 MCS/spin. The error bars estimated from the dispersion of $C_L^{\max}$ obtained by ten independent runs are about 1 % or less and smaller than the size of the open circles. The onset of the asymptotic behavior, that is, the maximum of the specific heat scaling with the volume, as predicted by Eq. (13), is already seen for large lattice size. Since the fuly asymptotic behavior has not been reached for the lattices used in our simulation, we cannot use the data presented in Fig. 3 together with Eq. (13) directly to extract information about the latent heat and specific heat singularities at the transition point. In order to do that, we must include correction to scaling terms in Eq. (13). We find by using a nonlinear square fitting that the data are best fitted if an L-dependent exponential term is also added to the terms present in Eq. (13), as was done for the two-dimensional Potts model.(18) Figure 4 shows the maximum of the specific heat against L along with the nonlinear best fit, using

$$C_L^{\max} = \alpha L^3 + \beta + \gamma \exp(-L/l) \tag{17}$$

where α is proportional to the square of the latent heat, as seen from

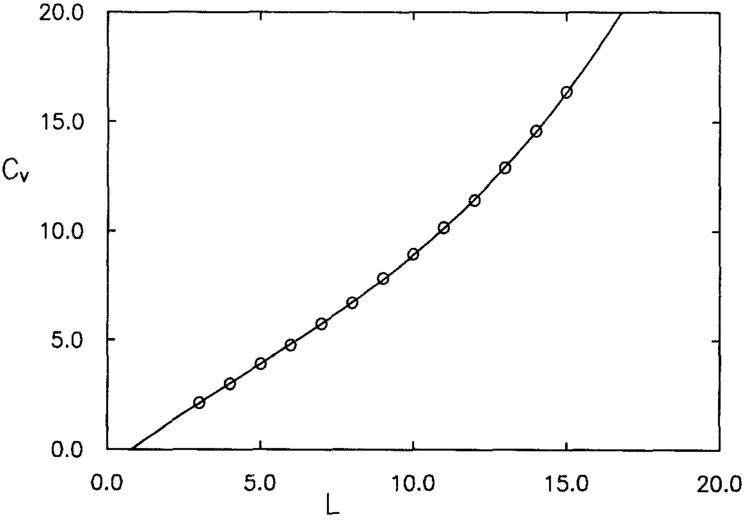

Fig. 4. Plot of the maximum of the specific heat against L. The points correspond to the Monte Carlo simulation. The continuous line is the nonlinear best fitting using Eq. (17).

Eq. (13), and l is a measure of the correlation length. The best-fitted values for the above parameters are

$$\alpha = 0.0023 \pm 0.0001, \qquad \beta = 12.9 \pm 2.0$$
$$\gamma = -13.8 \pm 1.9, \qquad l = 12.8 \pm 2.7$$

The errors above come from two sources: the statistical error in computing the raw data and the uncertainty in fitting by Eq. (17), with the latter having the largest magnitude. This gives for the latent heat $E_+ - E_- = 0.17 \pm 0.04$, which is in fairly good agreement with the value $\Delta E = 0.1969(9)$ obtained by multilattice microcanonical simulation.(14) Using the results of the present simulation and the specific heat discontinuity found by Wilson and Vause,(14) we estimate the specific heat of the ordered phase as $C_- = 17.4 \pm 2.3$ and for the disordered phase as $C_+ = 8.4 \pm 1.8$.

In summary, we have carried out Monte Carlo simulations to study the three-state Potts model in a cubic lattice. The calculations show that the system undergoes a weak first-order phase transition. By using finite-size scaling, we estimate the latent heat, the correlation length, and the values of the specific heat at the transition for both ordered and disordered phases.

The histogram technique used in the present work has been shown to be very useful to locate the heights and positions of narrow peaks of thermodynamic quantities near first-and second-order phase transitions. In a second-order phase transition a single Monte Carlo simulation is sufficient to obtain information about the thermodynamic functions over a range of temperature in the neighborhood of the critical point.(18) In a first-order phase transition, however, this information is not readily available due to the breaking of symmetry at the transition point.

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