Randomness-Induced Second-Order Transition in the Two-Dimensional Eight-State Potts Model: A Monte Carlo Study

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We have studied the effect of quenched, bond randomness on the nature of the phase transition in the two-dimensional eight-state Potts model. Through extensive Monte Carlo simulations, we confirm that the phase transition changes from first order to second order. A finite-size-scaling analysis of several thermodynamic quantities strongly suggests that the critical exponents fall into the universality class of the two-dimensional Ising model.

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The addition of quenched randomness to many models which exhibit second-order transitions is known to have dramatic effects on the nature of the critical behavior [1,2]. Very recently it was also suggested, on the basis of phenomenological renormalization-group arguments [3], that the addition of randomness to systems undergoing first-order transitions should alter the nature of the behavior and instead produce a second-order transition. This work, together with a more rigorous treatment of the latent heat [4], suggested that the two-dimensional q-state Potts model with $q > 4$ might be a suitable candidate for testing this prediction.

The nature of the phase transition in the two-dimensional q-state Potts model [5] has been known for some time. The transition is of first order for $q > 4$, and is continuous for $q \leq 4$ [6]. The value of the transition temperature is known for all q as are the critical exponents for $q \leq 4$. For the Potts model with quenched randomness, however, no quantitative results exist. In this Letter we present a detailed Monte Carlo study of a random-bond Potts model, verifying the above hypotheses [3,4] concerning the order of the transition as well as presenting the first estimates of the critical exponents.

The Hamiltonian of a q-state Potts model with quenched random interactions can be written as

$$-\beta H = \sum_{\langle i,j \rangle} K_{ij} \delta_{\sigma_i,\sigma_j} ,$$

where the spin σ can take on the values $1, \ldots, q$, δ is the Kronecker delta function, and the sum goes over all nearest-neighbor pairs in the system. The couplings K_{ij} are selected from two positive (ferromagnetic) values K_1 and K_2 with a strong to weak coupling ratio $K_2/K_1 = 2$. We have studied this model on the square lattice, choosing the couplings so that there are the same number of strong and weak bonds in each of the two lattice directions. This model is a restricted version of a random-bond Potts model discussed by Wu [5] which has two ferromagnetic couplings chosen randomly from the distribution

$$P(K) = p\delta(K - K_1) + (1 - p)\delta(K - K_2) .$$

For $p = 0.5$, and $K_2/K_1 = 2$, the value of K_1 at the transition can be determined by the expression [7]

$$[\exp(K_1) - 1][\exp(2K_1) - 1] = q$$

which yields $K_1^C = 0.920\,185\,27\ldots$. Although our model is a restricted version of this random-bond Potts model, we expect that the behavior of our model will be similar in the thermodynamic limit.

We performed extensive simulations of $L \times L$ lattices ($12 \leq L < 128$) with periodic boundary conditions using a "multihit" Swendsen-Wang cluster flipping method [8]. (The multihit algorithm uses multiple decorations of the Swendsen-Wang clusters to increase the speed of the simulation.) Histogram techniques [9,10] were used to determine the behavior of several thermodynamic quantities over a range of K_1. Between 6×10^5 and 1.5×10^6 Monte Carlo steps (complete lattice updates) were performed using a cluster of IBM RS/6000 model 550 workstations at the University of Georgia. For the largest system, the run length was more than 10^2 times the correlation time. Up to 40 different bond distributions were used in the configurational average over randomness for bulk properties.

The first part of our analysis was to determine the order of the phase transition. This has traditionally been difficult for systems with weak first-order transitions, but finite-size effects at first-order transitions [11] are now much better understood and different techniques for distinguishing first-order from second-order transitions have recently been developed. One of these approaches is due to Lee and Kosterlitz [12] who suggest that the size dependence of the free energy as a function of energy, $F_L(E) = -\ln P_L(E)$, where $P_L(E)$ is the probability distribution for a system of linear dimension L, can be used to determine the order of the transition even if the system size is smaller than the correlation length. Their technique makes use of the fact that for large systems the free energy at a first-order phase transition will consist of two minima of equal depth separated by a peak. (The probability distribution will therefore have two maxima separated by a minimum.) If the free-energy barrier (difference between the minima and the peak) grows with increasing system size, the transition will be first order in the thermodynamic limit while if the barrier decreases

with increasing system size, i.e., the free energy tends to a single minimum, the transition will be second order. We have used a variation of this approach to determine the order of the transition in our model; the variation is necessary because of the configurational average over randomness. We have determined the average value of the free-energy barrier by first calculating it for a given bond configuration then performing the configurational average over bond distributions. The resultant free-energy barrier $\Delta F(L)$ is plotted as a function of inverse lattice size in Fig. 1. Clearly the trend for large L is toward zero free-energy barrier which indicates that the transition has indeed changed from first to second order. For the uniform eight-state Potts model, the free-energy barrier is significantly larger [$\Delta F(L=16)\approx 1.0$] and grows with increasing system size [12]. Note that for smaller L the trend toward $\Delta F=0$ is not as clear, indicating that these systems are not yet in the asymptotic regime.

A more traditional approach to determining the nature of the transition is to use finite-size-scaling (FSS) techniques [13] to extract the infinite-system behavior from finite-lattice data. When used in conjunction with histogram techniques, FSS becomes even more powerful and can provide high-resolution estimates for the critical behavior. Usually one looks at the scaling properties of the specific heat

$$C=\frac{K_1^2}{L^2}(\langle E^2\rangle-\langle E\rangle^2)$$

(E is the total energy of the system) or magnetic susceptibility to determine critical exponent ratios. For example, for sufficiently large systems, the maximum in the specific heat scales with system size like

$$C_{\max}\propto L^{a/\nu}.$$

(For a first-order transition, the specific heat diverges as L^d so a measurement of the scaling behavior of $C_{\max}$ will also provide additional confirmation of the order of the transition.) Finite-lattice transition couplings such as the location of the specific-heat maximum $K_1^C(L)$ vary with system size like

$$K_1^C(L)=K_1^C+aL^{-1/\nu}.$$

If the system sizes are not large enough, correction terms must be included in the above expressions. Of course, the order parameter

$$M=L^{-d}\max(M_1,M_2,\ldots,M_q),$$

where M_i is the number of spins in state i, can be treated in a similar fashion. It has recently been shown that other, less traditional, quantities can be used effectively in finite-size-scaling analyses [14]. For example, the logarithmic derivative of any power of the order parameter,

$$\frac{\partial \ln\langle M^n\rangle}{\partial K_1}=\frac{\langle M^n E\rangle}{\langle M^n\rangle}-\langle E\rangle,$$

scales with system size like $L^{1/\nu}$ as does the derivative of the Binder parameter $\partial V_B/\partial K_1$, where

$$V_B=1-\langle M^4\rangle/3\langle M^2\rangle^2.$$

The locations of the maxima in these derivatives also provide additional finite-lattice transition couplings.

The data were first analyzed to determine the exponent ν by studying the scaling behavior of the logarithmic derivative of M, M^2, and M^4. In Fig. 2 we plot these logarithmic derivatives as a function of system size on a log-log scale. The solid lines represent linear fits for $L\geq 28$. Results for $L<28$ were discarded because these system sizes are not yet in the asymptotic regime, as seen in Fig. 1. From these fits we conclude that the transition is second order and estimate $1/\nu=0.957\pm 0.036$ for M, 0.974 ± 0.035 for M^2, and 1.015 ± 0.032 for M^4. (The error bars are 1σ uncertainties.) Combining these results we obtain a final value $1/\nu=0.982\pm 0.017$ or $\nu=1.018\pm 0.018$. Within errors, this is identical to the $d=2$ Ising model value $\nu=1$. As a further test of the critical behavior, we plotted the specific-heat maxima as a function of lattice size on a semilogarithmic scale. The result, shown in Fig. 3, indicates that the data are well described

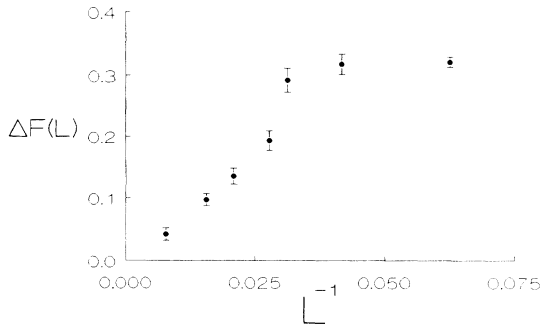

FIG. 1. Plot of the free-energy barrier $\Delta F(L)$ as a function of inverse lattice size.

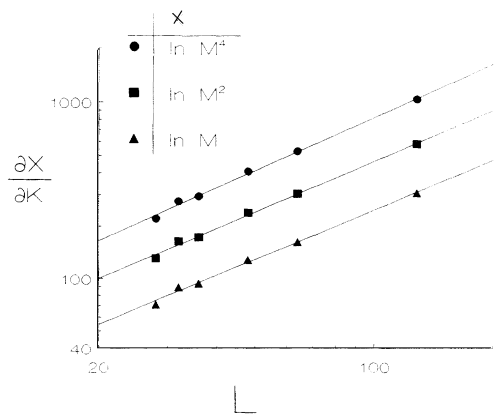

FIG. 2. Log-log plot of the size dependence of logarithmic derivatives of the order parameter. The solid lines are linear fits including systems with $L\geq 28$. Errors in the individual points are comparable to the symbol size.

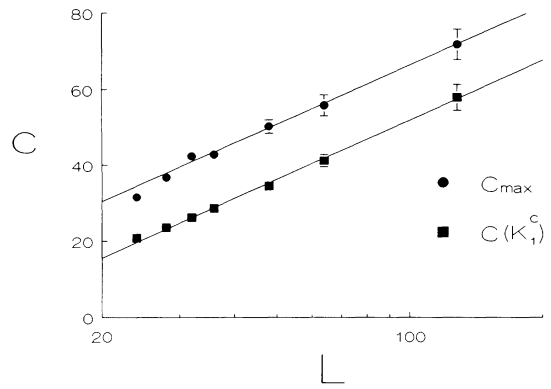

FIG. 3. Semilogarithmic plot of the specific heat vs lattice size for the maximum value of the specific heat as well as the specific heat at the infinite-lattice critical point K_c^f. The solid lines are linear fits including data for $L \geq 28$. Where not shown, error bars are smaller than the symbols.

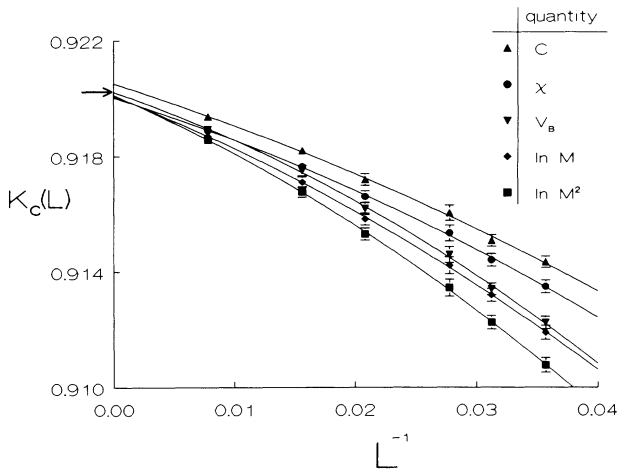

FIG. 4. Size dependence of the estimates for finite-lattice critical couplings $K_c^f(L)$ for various thermodynamic quantities. The solid curves are fits to the finite-size-scaling form including the lowest-order correction term. The arrow shows the location of the exact transition temperature.

by a linear fit (the solid line) for systems larger than $L=28$ as would be expected for a two-dimensional Ising model.

The locations of the peaks in the derivatives of the various thermodynamic functions occurred at different values of K, but all of the positions moved to larger K as the lattice size increased. Using $\nu=1$ and a correction term which varied as L^{-2}, we fitted the positions of the maxima using finite-size-scaling theory. The result, plotted in Fig. 4, showed that for $L \geq 28$ all of the positions could be well fitted with an extrapolated value of $K_c=0.9202 \pm 0.0003$ in excellent agreement with the "exact" value quoted earlier. If we analyze the behavior of the moments of the order parameter at K_c, we find that from M, $\beta/\nu=0.118 \pm 0.008$ and from M^2, $2\beta/\nu=0.247 \pm 0.006$. These values also agree quite well with the 2D Ising result $2\beta/\nu=0.25$. Previous work has shown that several different models which have second-order transitions in the pure system, but fall into different universality classes, apparently have Ising critical behavior when impurities are present [2]. It is intriguing that the introduction of quenched randomness into a model with a first-order transition also yields critical behavior which is indistinguishable from that of the Ising model.

In summary, the result of rather extensive simulations for the $q=8$ Potts model in two dimensions with two kinds of randomly distributed ferromagnetic bonds is that a second-order transition with Ising exponents results. It is, of course possible, that there are small deviations from 2D Ising behavior, particularly in the form of logarithmic corrections, which are simply too small for us to detect. Any significant improvement would require at least an order of magnitude more computer time or some other method, such as Monte Carlo renormalization group. We know of no theoretical predictions of the anticipated critical behavior and would encourage theoretical effort to explain our findings.

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