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First-Order Phase Transitions and the Three-State Potts Model

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We have used the Monte Carlo renormalization-group method to study the three-state Potts model in three and four dimensions. In both cases, we find a first-order transition without an associated discontinuity fixed point. The transition in three dimensions is "almost second order" in the sense that some evidence was found for the existence of second-order fixed points associated with singularities in the metastable region just beyond the first-order transition.

The three-dimensional, three-state, ferromagnetic Potts model[1] is described by

$$H = K_{\mathrm{nn}} \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \tag{1}$$

where $\sigma_i = 1$, 2, or 3, the sum is over the nearest-neighbor pairs, and K_{nn} includes a factor of $-1/k_{\mathrm{B}}T$. It is expected to describe the critical properties of a number of physical systems such as ferromagnets with cubic anisotropy in a magnetic field.[2] Although Landau theory predicts a first-order phase transition (which is certainly correct for sufficiently high dimensionality), the transition is known to be second order in two dimensions.[3] Several attempts have been made to determine the nature of the transition in three dimensions, but it proved to be difficult to find, theoretically or experimentally, an unambigous answer to the problem,[4-20] although the experimental results point to a first-order transition.[21,22]

We have studied the three-state Potts model in both three and four dimensions using the Monte Carlo renormalization-group (MCRG) method.[23-26] We have been able to determine that the transition is first order in both cases. In addition, the rather novel position-space renormalization-group flows obtained from the MCRG analysis have clarified the nature of these first-order transitions (including the existence of metastable branches) and explained the difficulties encountered by other methods. We believe that these results should have broad application to the general theory of first-order transitions.

The usual description of first-order transitions in the context of position-space renormalization-group theory (which includes the MCRG) was first given by Nienhuis and Nauenberg.[27] They showed that a *sufficient* condition for a first-order transition is the existence of a "discontinuity fixed point," characterized by an eigenvalue of the linearized RG transformation equal to b^d, where b is the scale factor and d is the dimensionality. The existence of such a fixed point in an RG analysis is necessary to describe the divergence of the susceptibility along the coexistence line in the $d=3$ Heisenberg model.[28-30] A discontinuity fixed point describing the low-temperature phase of the $d=2$ Ising model has also been found by the MCRG method[25] as predicted by Klein, Wallace, and Zia,[31] who linked it to the presence of essential singularities in the free energy as a function of the magnetic field.

In contrast to this traditional picture, we find that there is *no discontinuity fixed point* associated with the first-order transition in either three or four dimensions. Instead, the MCRG analysis for the ordered phase in both the stable *and metastable* regions resulted in flows toward the strong-coupling fixed point, while the corresponding MCRG flows for the disordered phase approached the weak-coupling fixed point. This implies that the first-order transition corresponds to a simple crossing of two branches of the free energy—the thermodynamic properties can be analytically continued through the first-order transition into the metastable phases without encountering any singularities associated with the transition.

We also find evidence that the transition in the three-dimensional Potts model is "almost second order" in the sense that there are second-order fixed points which could, in principle, be reached from the metastable regions. Experiments on such a system would show thermodynamic properties (in the stable phases) that are describable by power-law singularities with the apparent location of the singularity in the metastable region just beyond the first-order transition.

A schematic diagram of the MCRG flows for the disordered phase is presented in Fig. 1. The vertical axis shows the nearest-neighbor coupling and the horizontal axis represents all other possible interactions. The solid lines are flows from the stable phase that eventually go to the weak-coupling fixed point. The flow from K_1 (the first-order transition temperature) is not qualitatively different from flows immediately above or below—it is only distinguished by having a free energy equal to that of the ordered phase at the same temperature.

Table I contains MCRG data for the renormalized, nearest-neighbor correlation functions of the simple-cubic ($d=3$) Potts model at its transition temperature ($K_1=0.550$) for both the ordered and disordered phases. The numbers reflect the shrinking lattice size as well as the renormalized coupling constants, but the trends toward strong- or weak-coupling fixed points are still clear.

Table II contains MCRG values for the even- and odd-eigenvalue exponents of the linearized RG transformation[24,25] for the same MC simulations used in Table I. The renormalized Hamiltonians are clearly moving in different directions

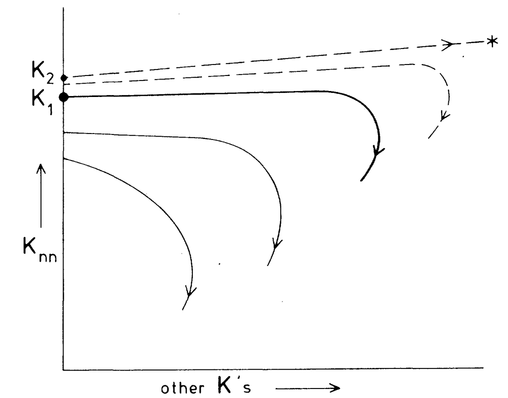

FIG. 1. Schematic RG flow diagram for the disordered branch of the three-dimensional, three-state, nearest-neighbor, Potts model. K_1 is the nearest-neighbor coupling at the first-order transition. The solid lines represent flows from the stable phase and dashed lines from the metastable phase. K_2 is the apparent second-order transition point in the metastable region.

TABLE I. Nearest-neighbor correlation functions for the renormalized configurations of the three-dimensional, three-state Potts model at its first-order transition temperature. Data for both ordered and disordered states were taken from MC simulations at a coupling $K_1=0.550$ (with ordered and random starting configurations, 200 MC steps per site to reach equilibrium, and averages over 2000 MC steps per site, for a $32\times32\times32$ lattice with periodic boundary conditions). RG iteration 0 refers to averages over the unrenormalized configurations.

	C_{nn}	
RG iteration	Ordered state	Disordered state
0	0.580	0.529
1	0.629	0.503
2	0.753	0.482
3	0.922	0.453

TABLE II. Even and odd MCRG eigenvalue exponents obtained from the same MC simulations of the ordered and disordered states of the three-state, three-dimensional Potts model described in Table I. The scale factor for the RG transformation is $b=2$, and block spins are assigned by majority rule, using predetermined sites as "tie breakers" when necessary. Missing entries correspond to complex eigenvalues.

RG iteration	Number of interactions	y_1^e Ordered	y_1^e Disordered	y_1^o Ordered	y_1^o Disordered
1	1	1.65	1.53	2.51	2.41
	2	1.75	1.62	2.41	2.42
	3	1.75	1.62	2.33	2.42
2	1	2.05	1.61	2.73	2.32
	2	2.06	1.70	2.32	2.33
	3	2.05	1.72	...	2.34
3	1	2.45	1.52	3.12	2.21
	2	2.31	1.66	...	2.23
	3	2.40	1.67	3.27	2.23

toward different fixed points. On the other hand, the changes in the eigenvalue exponents are fairly slow, which is consistent with being close to fixed points in the metastable region. The data are not nearly good enough to give estimates of the eigenvalue exponents for the metastable fixed points, but it may be worth noting the proximity of both to the Ising critical values ($y_1^e \approx 1.6$, $y_1^o \approx 2.5$).[32]

The first-order nature of the transitions can, of course, also be seen by standard MC methods. Figure 2 shows hysteresis data for the three-dimensional, nearest-neighbor correlation function C_{nn} plotted against the coupling strength K_{nn} for lattices with linear dimensions $N=24$ and $N=32$ and periodic boundary conditions. The circles show averages over intervals of 100 Monte Carlo steps per site and the arrows on the dashed lines indicate the development of the system for successive intervals. The solid lines show the stable branches and are only drawn to quide the eye.[33]

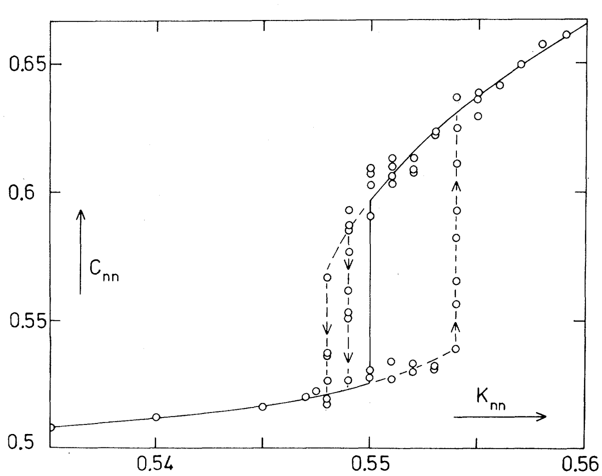

FIG. 2. Hysteresis data for the nearest-neighbor correlation function of a simple-cubic Potts model. Circles represent averages over 100 MC steps per site on $24\times24\times24$ and $32\times32\times32$ lattices.

Since one would expect the apparent second-order transitions to be limits of stability of the metastable phases, it is interesting to note that the strong-coupling series of Miyashita, Betts, and Elliott[20] suggested a singularity near $K=0.5475$, while Straley's[17] weak-coupling series suggested a singularity near $K=0.5535$. Both numbers are in reasonable agreement with the hysteresis shown in Fig. 2.

The first-order transition in the four-dimensional hypercubic Potts model occurs at $K_1=0.3875\pm0.0010$ and is qualitatively similar to the three-dimensional case. Further details of the calculations for both cases will be presented elsewhere.

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[32]It is difficult to obtain accurate data in the metastable region because of the large "almost critical" fluctuations and the tendency to nucleate the competing stable phase within a few hundred MC steps per site. Consequently, our data in this region provide only a qualitative confirmation of the picture we have presented. It is possible that a different MC algorithm that suppresses the nucleation of the stable phase would allow more accurate calculations to be made in the metastable region.

[33]The results of standard MC methods have been confirmed by L. Jacobs and C. Rebbi (private communication) using a different algorithm on a 32× 32× 30 lattice. They also investigated the first-order nature of the transition by using mixed starting configurations in which half the system was ordered and the other half random.