

Ising transition into an order with extensive entropy at $T=0$: Potts antiferromagnets in a magnetic field

Z. Rácz

Institute for Theoretical Physics, Eötvös University, H-1088 Budapest, Puskin utca 5-7, Hungary

T. Vicsek

*Research Institute for Technical Physics of The Hungarian Academy of Sciences,
H-1325 Budapest, P.O. Box 76, Hungary*

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The phase diagram of the $q=3$ state Potts antiferromagnet in a field is studied by exact mappings and Monte Carlo methods, and it is shown that systems with macroscopic ground-state degeneracy may exhibit conventional-type critical ordering. Our Monte Carlo data for the square-lattice case indicate a finite-temperature ordering in a range of field values where the entropy of the ground state is extensive. In a particular limit this phase transition can be shown to be of the Ising type by mapping the Potts model onto a colored, nearest-neighbor exclusion lattice gas. We also discuss the phase diagram of the body-centered-cubic Ising antiferromagnet in a field in order to show that renormalization-group arguments alone are not sufficient to restrict the diversity of possible low-temperature phases occurring in systems with a macroscopically degenerate ground state.

I. INTRODUCTION

The existence and the nature of phase transitions in systems with infinitely degenerate ground states are problems of considerable interest.¹⁻³ General principles have not yet been found and presently the accumulation of knowledge through studying particular examples is going on.

There are many examples of systems with an infinitely but not macroscopically degenerate ground state (i.e., systems with zero residual entropy per particle). They display a wide variety of ordering properties, examples being the isotropic Heisenberg ferromagnet (no transition in $d=1$ and 2 dimensions; critical ordering in $d>2$),⁴⁻⁶ the face-centered-cubic Ising antiferromagnet (first-order transition),⁷ the KDP model for the ferroelectric potassium dihydrogen phosphate (no transition),¹ the hard-square lattice gas with second-neighbor repulsion (continuous transition with critical exponents depending on the interaction),⁸ and many other models⁹⁻¹¹ with behavior not established convincingly.

The variety is smaller among the systems with a macroscopically degenerate ground state. The finite residual entropy per particle usually implies a critical point suppressed to zero temperature ($T_c=0$) as in the cases of the triangular Ising antiferromagnet¹² and the fully frustrated square-lattice Ising model¹³⁻¹⁵ or it might prevent the development of

critical correlations even at $T=0$ as in the so-called "superfrustrated" models.¹⁶

In their recent work, however, Berker and Kadanoff³ suggest that a macroscopically degenerate ground state may induce a distinct low-temperature phase with algebraically decaying correlations provided the ground state is sufficiently complex. A possible candidate for exhibiting this algebraic order was the $q=3$ -component Potts antiferromagnet on a square lattice. Initially, works based on Monte Carlo (MC) calculations¹⁷ and approximate mappings¹⁸ seemed to support the existence of some kind of order but more reliable phenomenological^{19,20} and MC (Ref. 21) renormalization-group calculations virtually excluded the possibility of finite-temperature ordering. Since the Berker-Kadanoff argument applies only above a critical dimension, the cubic Potts antiferromagnets were also studied²² but the MC results were not conclusive again and the nature of the transition remained in question.

In this paper, we provide an additional piece of information on systems with macroscopic ground-state degeneracy. Namely, we show that the extensive entropy at $T=0$ does not exclude the possibility of a finite-temperature critical ordering. The example considered is the $q=3$ -state Potts antiferromagnet in a magnetic field H . Examining the phase diagram of this model (Sec. II), we find that near the critical field $H \approx H_c$ and $T \approx 0$ the model may be mapped onto a colored, nearest-neighbor-exclusion

lattice gas which—although its ground state is macroscopically degenerate—undergoes an ordinary Ising-type transition. For the case of the square lattice, we have also carried out MC calculations to determine the phase diagram on the entire (T, H) plane (Sec. III). Finite-temperature ordering was found in the whole $0 < H < H_c$ range, in spite of the fact that the ground state is macroscopically degenerate. As a by-product, our results for the phase boundaries help to understand why MC works run into difficulties in the $H=0$ case.

Finally, Sec. IV is devoted to the phase structure of the body-centered-cubic Ising antiferromagnet in a field. By this example, we show that renormalization-group considerations alone do not restrict the variety of possible low-temperature phases in systems with macroscopic ground-state degeneracy.

II. POTTS ANTIFERROMAGNETS IN A FIELD: PHASE DIAGRAM AND MAPPINGS

The $q=3$ state Potts antiferromagnet in a field is defined by the following Hamiltonian:

$$H = J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} - H \sum_i \delta_{\sigma_i 1}, \quad (1)$$

where the Potts spins have three components ($\sigma_i = 1, 2, 3$), $\delta_{\sigma_i \sigma_j}$ is the Kronecker δ function and the nearest-neighbor coupling is positive ($J > 0$). In order to eliminate possible frustration effects arising from geometry, we shall consider only bipartite lattices which can be divided into two sublattices (A and B) with the property that all the nearest neighbors of a site on sublattice A belong to sublattice B , and vice versa.

The phase diagram of the model defined by Eq. (1) is drawn schematically on Fig. 1. Its characteristic features—some of which are quite obvious—will be discussed throughout this section.

A. $H \rightarrow -\infty$

All the configurations with a spin being in the states $\sigma_i = 1$ are excluded, so the system becomes an Ising antiferromagnet. Thus, in the limit $H \rightarrow -\infty$, the system undergoes an Ising-type critical ordering at a finite temperature for dimensions $d > 1$.

B. $-\infty < H < 0$

The spin state $\sigma_i = 1$ is still energetically unfavorable and the doubly degenerate ground state is the same as that of an Ising antiferromagnet. Since the ground state and the symmetry of the order parameter are not changed as the $H = -\infty$ restriction is

lifted, universality implies that the phase transition for all $H < 0$ should be of the Ising type.

Of course, the behavior of the ordering line as $H \rightarrow 0$ —poses a problem since the ground state becomes macroscopically degenerate at $H=0$. This problem has been investigated²³ for the case of the square lattice using Müller-Hartmann and Zittarz's interface method²⁴ and an ordering temperature going to zero as $H \rightarrow 0$ was found.

For the square lattice, an exact result is also available. Taking the limit $T \rightarrow 0$, $H \rightarrow 0$ with $H/T = a$, one can map the Potts antiferromagnet onto a lattice gas with all the lattice sites occupied by colored particles and with nearest-neighbor exclusion of the same colors being the interaction between the particles.²⁵ There are three colors for the $q=3$ Potts model and the parameter a is related to the fugacities of those colors with two of the colors having the same fugacity. The lattice-gas problem is exactly solvable and the critical value of a is $a^* = 0$, imply-

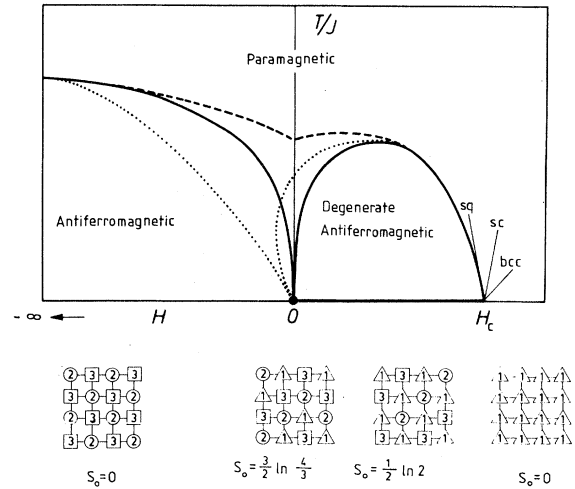


FIG. 1. Schematic plot of three possible phase diagrams of the $q=3$ -state Potts antiferromagnets in a magnetic field. Solid lines with no finite-temperature ordering at $H=0$ are expected to describe the square-lattice case. If two critical lines meet in a bicritical point ($T_c > 0, H=0$) (dashed lines), a first-order transition should take place between the $H < 0$ and $H > 0$ phases for $T < T_c$. Bulging of the phase boundary (dotted line) would result in a finite-temperature transition at $H=0$, but the ordering would be incomplete even at $T=0$. Straight lines at the point $H=H_c$ correspond to the slopes of the phase boundaries for various geometries (sq, square lattice, sc, simple cubic lattice, bcc, body-centered-cubic lattice). Typical spin-state configurations and the corresponding values of the residual entropy s_0 are also shown for the square-lattice case. (The field favors state 1.)

ing that the phase boundary of the $q=3$ square-lattice Potts antiferromagnet starts out of the $(T=0, H=0)$ point with an infinite slope.

It is worth mentioning that the phase boundary obtained by the interface method has a finite slope at $(T=0, H=0)$. The situation is, perhaps, comparable to the case of the triangular Ising antiferromagnet in a field. There is no ordering in zero field¹² and it follows from scaling arguments²⁶ that the phase boundary should approach the $(T=0, H=0)$ point with an infinite slope. At the same time, calculations based on the interface method give only a finite slope.²⁷

C. $H=0$

The ground state is macroscopically degenerate. A lower bound for the residual entropy per spin s_0 can be given by counting the following ground-state configurations. Let all spins on sublattices A be in state 1. Then the $N/2$ sites of the sublattice B can be independently occupied by spins in the states 2 and 3. The number of such configurations is $W=2^{N/2}$, thus $s_0 \geq \frac{1}{2} \ln 2$.

The square-lattice case has been studied intensively. The residual entropy per spin,

$$s_0 = \frac{3}{2} \ln \frac{4}{3}, \quad (2)$$

is known exactly from works on the ice model²⁸ and on the three-coloring problem.²⁵ Although MC calculations¹⁷ and universality arguments¹⁸ pointed towards a possible finite-temperature ordering, it is now quite well established that the only critical point of this system is at $T=0$. Actually, Berker and Kadanoff's Migdal-type renormalization-group result also suggests an algebraic order only in dimensions $d \geq 3$.

In $d=3$, MC results are available for the simple cubic and the body-centered-cubic lattices.²² Although there are indications of a continuous transition taking place at a finite temperature, these MC simulations are susceptible to the same type of uncertainties as in case of the square lattice; so the nature of the transition (if it exists at all) is not established reliably. We shall return to this question in Sec. III.

D. $0 < H < H_c = mJ$

For $H > 0$, there is a competition between the field aligning all the spins into state 1 and the antiferromagnetic interactions favoring different spin states on neighboring sites. The antiferromagnetic interactions dominate for $0 < H < H_c = mJ$, where m is the number of nearest neighbors of a site. The ground state is characterized by all the spins being

in state 1 on one of the sublattices while spins on the other sublattice having an independent choice between states 2 and 3. The number of such configurations is $W=2 \times 2^{N/2}$, and thus the ground state is macroscopically degenerate and

$$s_0 = \frac{1}{2} \ln 2. \quad (3)$$

The MC calculations of Sec. III indicate that, in spite of the macroscopic ground-state degeneracy, a finite-temperature ordering takes place at least in the square-lattice case (Figs. 1 and 3). As to the nature of the symmetry breaking, the MC results indicate that the essential feature of the ordering is the breaking of the twofold sublattice symmetry. In other words, the other parameter is presumably the difference in the number of spin-1 states on the two sublattices and the degeneracy arising from flipping the spins between states 2 and 3 is irrelevant. If this is true then the ordering is again in the universality class of a simple Ising antiferromagnet. As we shall see below, the existence of this type of ordering is supported by our results on the behavior of the system near the critical field H_c , where the ordering temperature goes to zero.

E. $H = H_c + aT$, $T \rightarrow 0$

Most of our new and nontrivial results in Sec. II are related to this limit so we shall discuss it in detail. In the limit $H = H_c + aT$ and $T \rightarrow 0$, the Potts antiferromagnet is reduced to a colored, nearest-neighbor-exclusion lattice gas and—as it is shown below—the fugacity z of the lattice gas is related to the slope a of approaching the $(T=0, H=H_c)$ point. Then, by studying the lattice gas, we gain information on the phase structure of the Potts antiferromagnet²⁹: A phase boundary which has a slope a^* at the $(T=0, H=H_c)$ point can be determined from the lattice-gas model since it has a phase transition at the corresponding $z^*=z(a^*)$. As it turns out, the colored, nearest-neighbor-exclusion lattice gas also serves as a very simple and easily understandable example of models in which the ground state is macroscopically degenerate, but nevertheless, undergoes a continuous ordering at a finite fugacity.

To see the correspondence between the Potts antiferromagnet and the colored lattice gas, consider the ferromagnetic configuration with all the spins being in state 1. The energy of this configuration is

$$E_F = N \left[\frac{m}{2} J - H \right]. \quad (4)$$

Now, let us turn n nonneighboring spins into states 2 or 3. Since

$$H = H_c + aT = mJ + aT,$$

the temperature-independent term in the increase of the magnetic energy, nH_c , is canceled by the decrease in the energy of the nearest-neighbor interaction, $-nmJ$, and so the change of energy can be written as

$$\delta E = E - E_F = n(-mJ + H) = naT. \quad (5)$$

Thus, choosing E_F as the zero of the energy scale, the contribution of such a configuration into the partition function,

$$P = e^{-na}, \quad (6)$$

becomes temperature independent.

In all the other possible configurations, there are neighboring spins among the n spins turned out of state 1. Then the decrease of the energy of the nearest-neighbor interactions is smaller than nmJ so the term nH_c is not canceled by it and the change of the energy is of the following form:

$$\delta E = E - E_F = naT + lJ, \quad (7)$$

where l is a positive integer. As a consequence, the Boltzmann weight of configurations with neighboring spins in states 2 or 3,

$$P = e^{-na - (lJ/T)}, \quad (8)$$

is negligible in the limit $T \rightarrow 0$.

Thus we arrive at the following lattice-gas picture. If a lattice site is occupied by a spin in states 2 or 3 then this site is considered to be occupied by a particle which may have two colors corresponding to states 2 or 3. The contribution of a configuration into the partition function is given by Eq. (6) if no nearest-neighbor sites are occupied; otherwise its contribution is zero. This means that, independently of colors, the interaction between the particles is a nearest-neighbor-exclusion interaction and every occupied site carries a factor $\exp(-a)$, i.e., the fugacity of the lattice gas is related to the ratio $a = (H - H_c)/T$ by

$$z = e^{-a}. \quad (9)$$

The ground state of this colored lattice gas is macroscopically degenerate. One of the sublattices is fully occupied in the limit $z \rightarrow \infty$, and every occupied site may have two different colors. Since the color of an occupied site is independent from the others, the number of ground-state configurations, $W = 2 \times 2N/2$, is equal to that of the Potts antiferromagnet for $0 < H < H_c$. This equality is not surprising since the limit $z \rightarrow \infty$ corresponds to approaching the $(T=0, H=H_c)$ point along the $T=0$ axis from the $H < H_c$ side.

In spite of the macroscopic ground-state degeneracy, the lattice gas undergoes an Ising-type transi-

tion at a finite fugacity. To show the existence of the transition, let us write the partition function of the lattice gas as

$$Z = \sum_{n=0}^{N/2} A_n 2^n z^n, \quad (10)$$

where A_n is the number of ways n lattice sites can be chosen so that none of them are nearest neighbors and the factor 2^n follows from the 2^n different ways the n -occupied sites can be colored.

Introducing $\xi = 2z$, the partition function can be rewritten in the form

$$Z = \sum_{n=0}^{N/2} A_n \xi^n. \quad (11)$$

This sum, however, is the partition function of the colorless, nearest-neighbor-exclusion lattice gas with fugacity ξ . Thus, apart from an irrelevant change of scale $\xi = 2z$, the colored and the colorless lattice gases display the same thermodynamic behavior. Physically, this is the consequence of the fact that the color is just an internal degree of freedom not affecting the interaction of the particles.

The phase transition in the colorless lattice gas is well understood.³⁰⁻³² At low densities (small values of ξ), the system is disordered. Above a critical value of the fugacity ($\xi > \xi^*$), however, the density of particles becomes so large that, as a result of the nearest-neighbor exclusion, the particles are mainly constrained to one of the sublattices, i.e., the symmetry between the two sublattices is broken. Accordingly, the transition is expected to belong to the Ising universality class. Indeed, for the square-lattice case the existence of the ordering is well established ($\xi^* = 3.7960 \pm 0.0001$) (Refs. 29 and 33) and the critical exponents of the order parameter ($\beta = 0.1249 \pm 0.0001$) (Ref. 29) and of the correlation length ($\nu = 0.999 \pm 0.001$) (Ref. 30) are known to a high accuracy. Less is known about the simple cubic and body-centered-cubic models³⁴ but there is no doubt about the existence of a phase transition in them.

Since z^* is related to the slope a^* of the phase boundary of the $q=3$ Potts antiferromagnet at the $(T=0, H=H_c)$ point, and $z^* = \xi^*/2$, results for the colorless lattice gas imply the existence of the Potts phase boundary. Also, it is now established that, at least in the limit $T \rightarrow 0$, the phase transition across this phase boundary is of Ising type although the ground state of the system is macroscopically degenerate.

The values of a^* for different lattices can be found in Table I. There, besides the bipartite lattices, one can find the triangular lattice as well. Although the gross features of the phase diagram of

TABLE I. Slope of the phase boundary (a^*) of the $q=3$ Potts antiferromagnets at the ($T=0, H=H_c$) point. The estimates are from calculations of the critical fugacity ζ^* of the corresponding hard-core lattice gases (Refs. 30, 34, and 35). The accuracy of the estimates are given between parentheses in units of the last significant digit.

Lattice	$a^* = -\ln(\zeta^*/2)$
Honeycomb	-1.37(1)
Square	-0.6408(1)
Simple cubic	0.60(7)
Body-centered-cubic	0.95(7)
Triangular	-1.7129...

the triangular Potts antiferromagnetics are different from that shown in Fig. 1, the lattice-gas mapping around the upper critical field $H_c = 6J$ is the same as for the bipartite lattices. The resulting hard-hexagon problem has been solved by Baxter³⁵; thus

$$a^* = -\ln\left[\frac{1}{4}(11+5\sqrt{5})\right] \quad (12)$$

is exactly known in this case. It is worth mentioning that changing to the triangular lattice changes the universality class of the transition. The ground state of the hard-hexagon model is threefold degenerate and its ordering belongs to the universality class of the $q=3$ Potts ferromagnet. Consequently, the triangular Potts antiferromagnet in the limit $H=H_c+aT, T \rightarrow 0$ and the $q=3$ Potts ferromagnet are in the same universality class.

It may be of interest to note that the lattice-gas mapping around $T \approx 0$ and $H \approx H_c$ can be carried out generally for a q -component Potts antiferromagnet. The only difference from the $q=3$ case is that the 2^n factor in the partition function [Eq. (10)] is replaced by $(q-1)^n$, i.e., the particles of the nearest-neighbor-exclusion lattice gas may take on $q-1$ different colors. The colors, however, play a role only in scaling the fugacity to that of the colorless nearest-neighbor-exclusion lattice gas [$\zeta = (q-1)z$], and thus, in the neighborhood of the ($T=0, H=H_c$) point, the critical exponents of Potts antiferromagnets are independent of q .

F. $H > H_c$

The ground state is ferromagnetic: All spins are state 1. Since the ground state is not degenerate, phase transition is not expected in this region except slightly above H_c . As can be seen from Table I, a^* is positive for the simple cubic and the body-centered-cubic lattices. Thus, for those lattices, the degenerate antiferromagnetic phase discussed in Sec. II E bulges above the critical field (see Fig. 1). As a

consequence, decreasing the temperature in the region $H \geq H_c$, one can observe first an ordering, then a disordering transition. A similar phenomenon is known to occur in the body-centered-cubic Ising antiferromagnet near its critical field.^{33,36}

III. MONTE CARLO SIMULATIONS FOR THE SQUARE LATTICE

We carried out MC calculations in order to detect the phase transition predicted in Sec. II and to make the schematic phase diagram (Fig. 1) more quantitative. The simplest case of the square lattice was studied and we concentrated mainly on locating the critical temperatures as a function of the magnetic field $T_c(H)$. Besides, some additional calculations were carried out with the purpose of understanding the transitionlike behavior at nonzero temperatures in the fieldless case.

A possible choice for the order parameter of the $q=3$ state antiferromagnetic Potts model is²²

$$M = \frac{1}{N} \sum_{k=1}^3 M_k, \quad (13)$$

with

$$M_k = \left| \sum_{i \in A} \delta_{\sigma_i, k} - \sum_{i \in B} \delta_{\sigma_i, k} \right|, \quad (14)$$

where A and B stand for the two sublattices and k denotes the Potts states. This order parameter is a simple generalization of the sublattice magnetization in Ising antiferromagnets. It is equal to unity for both kinds of sublattice orderings expected to appear in the $H < 0$ and the $0 < H < H_c$ regions in the limit $T \rightarrow 0$, and it is obviously equal to zero in a completely disordered system. In our simulations, lowering the temperature, we observed a quick increase of $M(T)$ from a low value $M \approx 0.1$ to 1.0 in a narrow region of temperatures depending on the field $T_c(H)$ (Fig. 2). This relatively sharp transition has been observed without any remarkable fraction of defects in the new phase. (Note that for $H=0$ the situation is quite different because in that case calculations show a saturation of the order parameter near the value $M \approx 0.64$.) Unfortunately, it would have required prohibitively large computing times to calculate the critical exponents associated with the transition detected by the sudden change in the order parameter. It can be seen, however, that the behavior of M for $H > 0$ is very similar to that in the $H < 0$ region, where a simple Ising transition should take place (Fig. 2).

The MC runs were typically carried out on 50×50 cells with periodic boundary conditions. The subsequent configurations were generated by flipping spins according to a standard MC technique

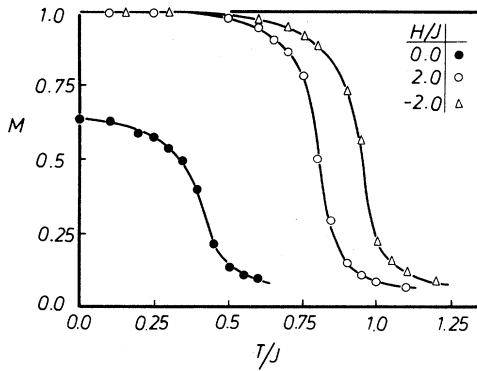


FIG. 2. Order parameter M of the $q=3$ state square-lattice Potts antiferromagnet as a function of the reduced temperature T/J for three values of the magnetic field H . Data for the $H=0$ case are taken from Ref. 17.

described in Ref. 37. Of course, a finite-cell, finite-time MC calculation suffers from the well-known problems: The transition is less sharp, the corresponding critical temperatures are usually higher than those of the infinite system, and it cannot be guaranteed that true equilibrium was reached. In order to investigate the finite-size effects we made several 32×32 runs as well, without finding any significant change in the transition temperatures. In addition, our simulations starting from various initial configurations lead to the same final order-parameter values; therefore, the finite-time effects seem to be also irrelevant.

To obtain a point of the phase boundary, the order parameter [Eqs. (13) and (14)] was determined either by lowering the temperature in small steps at a fixed value of the magnetic field or by decreasing the field at a fixed temperature. Then the critical fields and temperatures were determined from the maximum of the following quantities:

$$\left[\frac{\partial M(T, H)}{\partial H} \right]_T \quad \text{and} \quad \left[\frac{\partial M(T, H)}{\partial T} \right]_H.$$

Obtaining one value of the critical temperature required typically 1200–1500 MC steps per spin (MCS/S). As a check of the method we made several simulations in the region $H \approx H_c$ and $T \approx 0$, where the behavior of the phase boundary is well known from the mapping onto the hard-square lattice gas (see Sec. II). The hard-square lattice-gas results imply a value $a^* \approx 0.64$ for the slope of the phase boundary, while our numerical data lead to the estimation $a^* \approx 0.57$, which is in accord with the theory.

Results shown on Fig. 3 suggest that the transition temperature is suppressed to zero in the fieldless system and the phase boundaries lie rather close

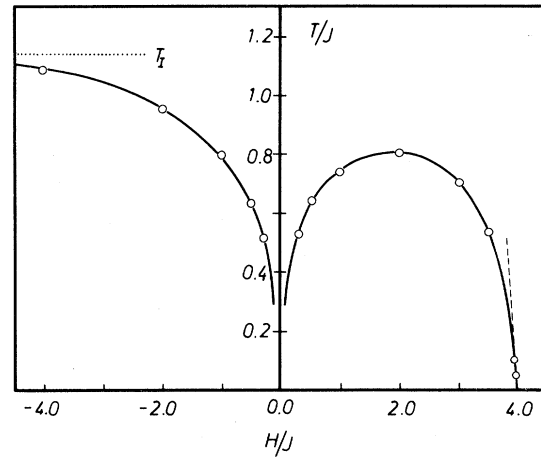


FIG. 3. Critical temperatures of the $q=3$ state square-lattice Potts antiferromagnet as a function of the magnetic field determined from MC simulations. Dotted line shows the well-known Ising transition temperature in the limit $H \rightarrow -\infty$, while dashed line corresponds to the slope of the phase boundary as calculated from lattice-gas mapping.

to the $H=0$ axis for temperatures $T \lesssim 0.4J$. The possibility of a nonzero transition temperature, however, is not entirely excluded. In that case, ($H=0$, $T=T_c$) would be a bicritical point (Fig. 1., dashed lines), and a first-order transition would be expected to take place between the low-temperature phases existing in the $H < 0$ and $H > 0$ regions.³⁸ In our MC simulations aimed at clarifying this point, however, the characteristic two-time-scale relaxation³⁹ accompanying such transitions could not be detected.

The shape of the phase boundary might be the reason for the inconclusive results of Grest and Banavar¹⁷ concerning the transition at $T \neq 0$. Configurations obtained by MC simulations in the region between the two nearby phase boundaries ($T < 0.4J$) are dominated by the large fluctuations having the symmetry of the $H < 0$ and $0 < H < H_c$ ground states, thus giving in average an apparent nonzero order parameter in a finite system.

An analogous situation arises in the triangular Ising antiferromagnet, where $T=0$ is the only critical point¹² for $H=0$, and the T - H phase diagram has a similar shape to that of the $q=3$ square-lattice Potts antiferromagnet for $H > 0$. Correspondingly, an order-parameter definition analogous to Eqs. (13) and (14) results in a plot (Fig. 4) showing an apparent transition in contrast to the exact result.

Similar arguments may be applied to the three-dimensional $q=3$, $H=0$ case,²² where at low temperatures M is saturated near the value 0.9 and the

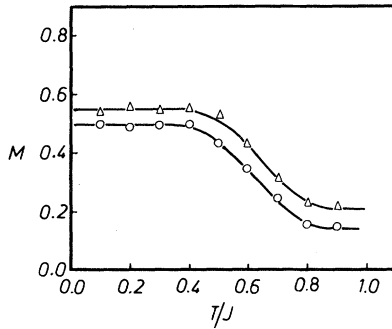


FIG. 4. Order parameter M of the triangular Ising antiferromagnet as a function of the reduced temperature for $H=0$ from MC simulations of 30×30 (Δ) and 54×54 (\circ) lattices.

symmetry of the ordered state is the same as that of the ground state in the region $0 < H < H_c$. A higher value of the order parameter does not necessarily mean a true transition. It may be due to the fact that the phase boundary for $H > 0$ is closer to the $H=0$ axis than the phase boundary in the region $H < 0$. In this case we expect those fluctuations to be dominant which have the symmetry of the ground state in the region $0 < H < H_c$. From the definition (13) and (14) it follows that domination of one kind of fluctuation results in a greater order parameter. This effect is further enhanced if finite-size cells are studied.

On the basis of our studies of the phase boundaries, we suggest another possible explanation for the incomplete ordering at $H=0$ with a true transition at a finite temperature. In principle, it is possible that the phase boundary starting at the $(T=0, H=H_c)$ point first crosses the $H=0$ axis at a temperature $T_c > 0$ and then arrives at the $(T=0, H=0)$ point, showing a bulging as in the $H \approx H_c$ region. This type of bulging results in an incomplete ordering in the body-centered-cubic Ising antiferromagnet at its critical field.³⁶ We think this problem should be clarified by further MC calculations in three dimensions. Also a numerical study of the critical exponents and the ground-state entropy of the three-dimensional $q=3$, $H=0$ case would be of interest.

IV. FINAL REMARKS

In closing, we discuss how to reconcile Berker and Kadanoff's argument³ with the existence of ordinary critical phenomena in systems with a macroscopically degenerate ground state.

Berker and Kadanoff's main *observation* is that a macroscopically degenerate ground state of suffi-

cient complexity is not invariant under rescaling transformations or, in other words, the $T=0$ point is not a fixed point of approximate or exact renormalization-group transformations. They add an assumption to this observation: They assume that the possible phase transformations are adequately described by a one-parameter renormalization group (only the temperature is affected by the rescaling). Under this assumption, they find constraints on the possible orderings in systems with a macroscopically degenerate ground state, namely, low-temperature phases with algebraically decaying correlations may exist in such systems, but the usual second-order transitions are excluded.

The problematic point in Berker and Kadanoff's argument is the *assumption*. We show below that the constraints on the possible phase structure follow from the use of a one-parameter renormalization-group transformation. Enlarging the parameter space, one might obtain new features in the phase diagram and it can be shown that renormalization-group ideas do not contradict the existence of critical ordering in systems with macroscopic ground-state degeneracy.

The example which we consider is the body-centered-cubic Ising antiferromagnet in a field. The ground state of this system is macroscopically degenerate at the critical field H_c , where H_c is the value of the field for which the energies of the ferromagnetic and antiferromagnetic configurations are equal. As it has been mentioned in Sec. II F, the phase boundary of this system bulges above H_c . Thus, cooling the system at $H=H_c$ (dotted line in Fig. 5), it undergoes a continuous transition at a finite temperature although its ground state is macroscopically degenerate. The only strange feature of the transition is that the antiferromagnetic ordering is not complete³⁶ as $T \rightarrow 0$. Clearly, a one-parameter renormalization-group calculation with the magnetic field fixed at H_c would not reproduce the above features. It is natural, however, to allow

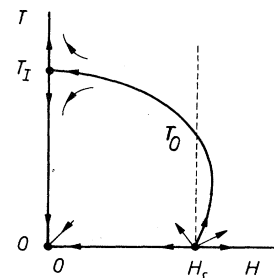


FIG. 5. Possible flow diagram of a two-parameter renormalization-group transformation for the body-centered-cubic Ising antiferromagnet in a field.

the magnetic field to be renormalized as well; then the resulting flow diagram of a two-parameter renormalization-group calculation might look as shown on Fig. 5. A similar fixed-point structure has been found in simple real-space renormalization-group approximations for Ising antiferromagnets on different lattices.^{40,41}

The meaning of Fig. 5 is quite obvious. The $(T=T_0, H=H_c)$ point is attracted to the Ising fixed point $(T=T_I, H=0)$, so the ordering properties of the system with a macroscopically degenerate ground state $(H=H_c)$ are determined by the field-less case, i.e., the system undergoes an ordinary Ising-type transition at $T=T_0$. Actually, as more sophisticated approximations reveal,⁴²⁻⁴⁵ the fixed-point structure shown in Fig. 5 should be more complicated. The magnetic field is a relevant perturbation^{42,46} and there are additional fixed points along the critical line connecting the $(T=0, H=H_c)$ point with the Ising fixed point. This complication, however, does not change the main point of our argu-

ment, namely, that the type of ordering which might occur in the $H=H_c$ case is not restricted *a priori* by the possible fixed-point arrangements.

Thus, the conclusion of this section, and also of the whole paper, is that the macroscopic ground-state degeneracy does not seem to restrict the variety of low-temperature orderings. In particular, we have shown that a system with macroscopic ground-state degeneracy may exhibit the usual critical transition into a low-temperature phase with simple order parameter and exponentially decaying correlations.

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- ¹E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 1, p. 331.
- ²G. Toulouse, *Commun. Math. Phys.* **2**, 115 (1977).
- ³A. N. Berker and L. P. Kadanoff, *J. Phys. A* **13**, L259 (1980).
- ⁴N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**, 1133 (1966).
- ⁵G. A. Baker, G. S. Rushbrook, and P. W. Wood, in *Phase Transitions and Critical Phenomena*, Ref. 1, Vol. 3, p. 245.
- ⁶A. M. Poljakov, *Phys. Lett.* **59B**, 82 (1975).
- ⁷M. K. Phani, J. L. Lebowitz, M. H. Kalos, and C. C. Tsai, *Phys. Rev. Lett.* **42**, 577 (1979).
- ⁸W. Kinzel and M. Schick, *Phys. Rev. B* **24**, 324 (1981).
- ⁹F. H. Ree and D. A. Chesnut, *Phys. Rev. Lett.* **18**, 5 (1967).
- ¹⁰W. Kinzel, W. Selke, and F. Y. Wu, *J. Phys. A* **14**, L399 (1981).
- ¹¹K. Binder and D. P. Landau, *Phys. Rev. B* **21**, 1941 (1980).
- ¹²G. H. Wannier, *Phys. Rev.* **79**, 357 (1950).
- ¹³J. Villain, *J. Phys. C* **10**, 1717 (1977).
- ¹⁴G. Andre, R. Bidaux, J.-P. Carten, R. Conte, and L. de Seze, *J. Phys. (Paris)* **40**, 479 (1979).
- ¹⁵G. Forgács, *Phys. Rev. B* **22**, 4473 (1980).
- ¹⁶A. Sütő, *Z. Phys. B* **44**, 121 (1981).
- ¹⁷G. S. Grest and J. R. Banavar, *Phys. Rev. Lett.* **46**, 1458 (1981).
- ¹⁸J. L. Cardy, *Phys. Rev. B* **24**, 5128 (1981).
- ¹⁹M. P. Nightingale and M. Schick, *J. Phys. A* **15**, L39 (1982).
- ²⁰M. P. M. den Nijs, M. P. Nightingale, and M. Schick, *Phys. Rev. B* **26**, 2490 (1982).
- ²¹C. Jayaprakash and J. Tobochnik, *Phys. Rev. B* **25**, 4890 (1982).
- ²²J. R. Banavar, G. S. Grest, and D. Jasnow, *Phys. Rev. Lett.* **45**, 1424 (1980); *Phys. Rev. B* **25**, 4639 (1982).
- ²³T. Temesvári, *J. Phys. A* **15**, L625 (1982).
- ²⁴E. Müller-Hartmann and J. Zittarz, *Z. Phys. B* **27**, 261 (1977).
- ²⁵R. J. Baxter, *J. Math. Phys.* **11**, 3116 (1970).
- ²⁶W. Kinzel and M. Schick, *Phys. Rev. B* **23**, 3435 (1981).
- ²⁷J. Dóczy-Réger and P. C. Hemmer, *Physica (Utrecht) A* **108**, 531 (1981).
- ²⁸E. H. Lieb, *Phys. Rev. Lett.* **18**, 692 (1967).
- ²⁹Similar ideas have already been applied to Ising antiferromagnets in a field: R. J. Baxter, I. G. Enting, and S. K. Tsang, *J. Stat. Phys.* **22**, 465 (1980), and also in Ref. 33.
- ³⁰D. S. Gaunt and M. E. Fisher, *J. Chem. Phys.* **43**, 2840 (1965).
- ³¹L. K. Runnels and L. L. Combs, *J. Chem. Phys.* **45**, 2482 (1966).
- ³²F. H. Ree and D. A. Chesnut, *J. Chem. Phys.* **45**, 3983 (1966).
- ³³Z. Rácz, *Phys. Rev. B* **21**, 4012 (1980).
- ³⁴D. S. Gaunt, *J. Chem. Phys.* **46**, 3237 (1967).
- ³⁵R. J. Baxter, *J. Phys. A* **13**, L61 (1980).
- ³⁶D. P. Landau, *Phys. Rev. B* **16**, 4164 (1977); T. E. Shirley, *ibid.* **16**, 4078 (1977).
- ³⁷K. Binder, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979), p. 1.
- ³⁸M. E. Fisher and D. R. Nelson, *Phys. Rev. Lett.* **32**, 1350 (1974).
- ³⁹D. P. Landau and K. Binder, *Phys. Rev. B* **18**, 2328

- (1978).
- ⁴⁰W. Kinzel, Phys. Rev. B 19, 4584 (1979).
- ⁴¹Z. RÁCZ and M. F. Collins, Phys. Rev. B 21, 229 (1980).
- ⁴²B. Nienhuis and M. Nauenberg, Phys. Rev. B 13, 2021 (1976).
- ⁴³G. D. Mahan and F. H. Claro, Phys. Rev. B 16, 1168 (1977).
- ⁴⁴N. Jan, J. Phys. C 12, 3771 (1979).
- ⁴⁵B. Schuh, Z. Phys. B 31, 55 (1978).
- ⁴⁶M. P. Nightingale, Phys. Lett. 59A, 486 (1977).