Investigation of the Potts Model Using Renormalization-Group Techniques*

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We report the numerical study, using Wilson's $\eta = 0$ approximate renormalization-group recursion formula, of a continuous-spin generalization of the three-component Potts model. Previous numerical studies, based on series expansions of the partition function, have indicated strongly that the model has a phase transition of second order. This is in conflict with Landau theory which predicts that the transition be of first order. We find, in agreement with Landau theory, that our model exhibits a first-order phase transition having finite zero-field spontaneous magnetization at the transition point.

INTRODUCTION

We report the numerical study, using Wilson's $\eta = 0$ approximate renormalization-group recursion formula,[1] of a continuous-spin generalization of the Potts three-component generalized Ising model.[2,3] The problem is of interest in that previous numerical studies of the model,[4] based on high- and low-temperature series expansions of the partition function, indicate that the model most probably has a phase transition of second order. This is in conflict with the Landau theory,[5] which requires that it be of first order. We find, in agreement with Landau theory, that our model exhibits a first-order phase transition having finite zero-field spontaneous magnetization at the transition point.

The model, as first proposed by Potts,[2] is one of a general class of lattice models in which each lattice site can be occupied by any one of q different atoms having nearest-neighbor interaction energy ϵ_0 between like atoms and energy $\epsilon_1 > \epsilon_0$ between unlike atoms. The three-component Potts model is equivalent to a lattice spin system in which the spin at each lattice site is a two-dimensional vector which can point in three symmetrically placed directions, as in Fig. 1. The nearest-neighbor interaction energy between sites i and j can then be written

$$E_{ij} = -J\vec{s}_i \cdot \vec{s}_j \ . \tag{1}$$

For the two-dimensional square lattice, Potts was able to derive a dual transformation[6,7] relating the partition function at high and low temperatures and consequently determine a unique value for the critical temperature, should one exist. This class of multicomponent models was also proposed independently by Kihara, Midzuno, and Shizume,[3] who studied the nature of the critical point by means of a low-temperature series expansion of the partition function. Their study indicated that the transition was probably second order, although their analysis did not allow them to reach a definite conclusion. The three-component Potts model was studied more recently in two dimensions by Straley and Fisher,[8] extending the analysis of Kihara *et al.* to include interaction with nonzero external fields. Their study, although not conclusive, also indicated strongly that the phase transition was of second order; hence the impetus to study the model using renormalization-group techniques.

THEORY AND CALCULATIONS

To apply Wilson's recursion formula[1] we generalize this model to continuous spin at each lattice site by replacing the discrete spin distribution by the threefold symmetric continuous probability distribution $e^{-P[\vec{s}]}$, where

$$P[\vec{s}] = a(s_1^2 + s_2^2) + b(s_1^2 + s_2^2)^2 + c(s_1^3 - 3s_1 s_2^2) \ . \tag{2}$$

For $a < 0$, $b > 0$, and $c \neq 0$, we see that this distribution has three symmetrically placed maxima which break the two-dimensional rotational symmetry so as to emphasize the spin-direction choices of the discrete Potts model. Different values of the coefficient c allow one to interpolate smoothly between the symmetric XY model and the discrete Potts model in the same manner as Wilson's continuous spin interpolation between the Gaussian and Ising models.[1] By rewriting the interaction term E_{ij} as $-\frac{1}{2}J[s_i^2 + s_j^2 - (\vec{s}_i - \vec{s}_j)^2]$, which introduces the square of a (discrete) gradient, we can write the partition function for our model as a functional integral over the continuous spin variable $\vec{s}(\vec{x})$:

$$Z = \oint_{\{\vec{s}(\vec{x})\}} \exp\left\{-\int_{\vec{x}} P'[\vec{s}(\vec{x})] - \tfrac{1}{2}K\int_{\vec{x}} [\vec{\nabla}\vec{s}(\vec{x})]^2\right\} , \tag{3}$$

where

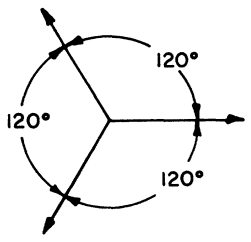

FIG. 1. The three possible spin orientations of the three-component Potts model.

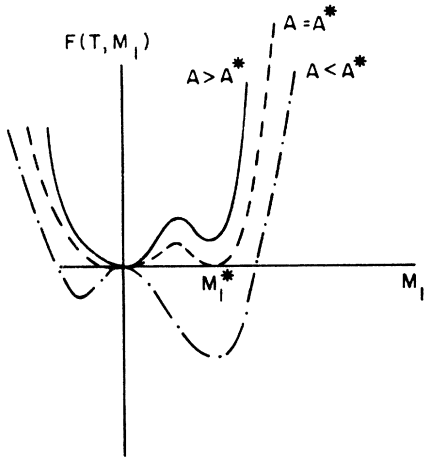

FIG. 2. Free energy $F(T, M_1)$ vs magnetization M_1 for values of $A(T) > A^*$, $A(T) = A^*$, and $A(T) < A^*$.

$$P'[\vec{s}(\vec{x})] = a'(T)[s_1^2(\vec{x}) + s_2^2(\vec{x})] + b[s_1^2(\vec{x}) + s_2^2(\vec{x})]^2 + c[s_1^3(\vec{x}) - 3s_1(\vec{x})s_2^2(\vec{x})], \quad (4)$$

and $a'(T) = a - Kd$, $K = J/k_B T$, and $\int_{\vec{x}}$ means $\int_{-\infty}^{\infty} d^d x$. The interaction is now in a form where we can use Wilson's recursion formula to study the critical behavior.

Before doing so it is instructive to study our model in the context of the Landau theory of phase transitions.[5] We assume that we can expand the free energy F as a power series in the magnetization M which exhibits the same symmetry as our original spin probability distribution. Thus

$$F(T, M) = A(T)(M_1^2 + M_2^2) + B(M_1^2 + M_2^2)^2 + C(M_1^3 - 3M_1 M_2^2). \quad (5)$$

We see immediately that, according to Landau's theory, the presence of the nonzero third-order term implies that the transition must be first order. This is because variation of the temperature parameter $A(T)$ can produce only a *discontinuous* breaking of the symmetry from the disordered to the ordered phase. This is illustrated in Fig. 2, where we have plotted $F(T, M_1)$ vs M_1 for different values of $A(T)$ for $B > 0$, $C < 0$. We see that for a certain value $A(T) = A^*$ the spontaneous magnetization, which is determined by minimizing the free energy, changes discontinuously from zero to a finite value, M_1^*, due to the presence of the CM_1^3 term in the free energy. Hence Landau's theory leads us to expect our model to have a first-order transition, in contrast to our expectations based on the numerical studies of the discrete Potts model described above.

For our model the renormalization group provides a definite answer. We recall that the recursion formulas, as derived and discussed in Ref. 1, relate the Hamiltonian for a system on a lattice with spacing L to a physically equivalent Hamiltonian for lattice spacing $2L$. For calculational convenience the recursion formulas are written for a "reduced" Hamiltonian rescaled to a lattice with unit lattice spacing and written in terms of a scaled spin variable representable, qualitatively speaking, by its values on a lattice with unit spacing.[1] The recursion formula is

$$Q_{l+1}(\vec{y}) = -2^d[\ln I_l(2^{1-d/2}\vec{y}) - \ln I_l(0)], \quad (6)$$

where $Q_{l+1}(y)$ is the dimensionless rescaled form of $P_{l+1}[s]$, and

$$I_l(\vec{z}) = \int_{-\infty}^{\infty} d\vec{y} \exp[-y^2 - \tfrac{1}{2}Q_l(\vec{y} + \vec{z}) - \tfrac{1}{2}Q_l(-\vec{y} + \vec{z})]. \quad (7)$$

Were we to start with our original Hamiltonian defined on a lattice with unit spacing, after l iterations of the recursion formulas the effective distribution function P_l would be defined on a lattice with spacing 2^l. From Ref. 1 we see that it is related to our scaled distribution function, Q_l by the relation

$$P_l[\vec{s}] = 2^{-ld}\omega Q_l[(K\rho_0/2\omega)^{1/2} 2^{l(d/2-1)}\vec{s}], \quad (8)$$

where the scale factors ρ_0 and ω are defined in Ref. 1, and the variable $\vec{s}$ is not allowed to have fluctuations over a domain of size less than 2^l. We will find this relation useful when we analyze our numerical results.

The equations were solved numerically for $d = 3$ for the initial function

$$Q_0(\vec{y}) = r_0(y_1^2 + y_2^2) + u_0(y_1^2 + y_2^2)^2 + w_0(y_1^3 - 3y_1 y_2^2). \quad (9)$$

To preserve the symmetry of the model the calculations were performed on a two-dimensional mesh of equilateral triangles. The mesh spacing was 0.4. The function $Q_l(\vec{y})$ was calculated on a hexagonally shaped domain (see Fig. 3) whose size was varied to follow the non-fixed-point behavior of the function. The domain was chosen so as to include all $\vec{y}$ for which $Q_l(\vec{y}) < 250$. The $\vec{y}$ integration was calculated over a hexagonal domain of radius 4.8. The integrals were calculated by means of the hexagonal seven-point integration formula[9] described in the Appendix. The values of $Q_{l+1}(\vec{y})$ between the mesh points were calculated by linear interpolation among the values of $Q_{l+1}(\vec{y})$ at the three vertices of the surrounding equilateral triangle. All calculations were performed using double-precision arithmetic.

Starting from the initial function of Eq. (9) with u_0 set at 0.1 and w_0 set at -0.1, the parameter r_0 was varied in an attempt to locate a fixed point of the recursion formulas. No fixed point was found. Instead we observed the transition illustrated in Figs. 4(a), 4(b), and 4(c), where we show two successive iterations of $Q_l(y_1)$ vs y_1 for values of r_0 greater than, less than, and equal to the transition

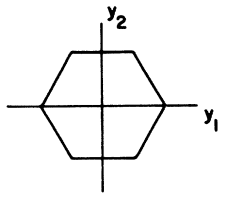

FIG. 3. Hexagonal domain of $Q_l(y)$ used in the numerical analysis.

point r^*. The values of $Q_l(\vec{y})$ for $\vec{y}$ not in one of the three symmetry-breaking directions became, in general, large and positive for large l for all r_0, increasing in value with each iteration. The value of r^* was found to be approximately -0.484188. For values of $r_0 > r^*$ the function $Q_l(\vec{y})$ for large l tended to become Gaussian, as expected for the high-temperature disordered phase.[1]

At the transition point $r_0 = r^*$, the transition function $Q_l^*(\vec{y})$ exhibits three symmetrically placed minima which compete with the minimum at the origin in determining the most probable spin orientation. With successive iterations, for large l, the positions of the minima move further away from the origin while the function itself rises increasingly sharply about the minima. The narrowing of the minima reduces the fluctuations in the spin variable, as they are then governed by the widths of the minima of the function $Q_l(\pm\vec{y}+\vec{z})$ in Eq. (7) rather than by the $-y^2$ term, which originated from the nearest-neighbor interactions. We have thus iterated the initial Hamiltonian to a lattice with spacing exceeding the correlation length. The recursion formulas can now be solved for the behavior of $Q_l(\vec{y})$ vs l in the neighborhood of a minimum by the method of saddle-point integration.[10] We get

$$Q_{l+1}(\vec{y}) \approx 2^d Q_l(\vec{y}_0) + 2Q_l''(\vec{y}_0)(\vec{y} - 2^{d/2-1}\vec{y}_0)^2, \qquad (10)$$

where $\vec{y}_0$ is the position of the minimum of $Q_l(\vec{y})$. Comparing the above equation with Eq. (8) we see that the position of the minimum remains stationary when evaluated for the unscaled distribution function $P_l[\vec{s}]$. This is indeed the case for our calculated function $Q_l^*(\vec{y})$, as is shown in Table I. The values $Q_l^*(\vec{y}_0) \neq 0$ reflect the presence of transient terms which enter through higher-order corrections to the saddle-point integral; they become negligible as l becomes large.

TABLE I. Position and magnitude of the symmetry-breaking minimum of $Q_l^*(y)$ vs l compared with the position of the minimum on the unscaled lattice.

l	y_0	$Q_l^*(y_0)$	$2^{-l(d/2-1)}y_0$
1	2.0	−1.34	1.4
2	2.4	−1.49	1.2
3	2.8	−1.56	1.1
4	2.8	−1.05	0.70
5	4.0	−0.625	0.71
6	5.6	−0.895	0.70
7	8.0	−0.247	0.71
8	11.2	−0.120	0.70

The evaluation of the spontaneous magnetization now becomes trivial, for in the absence of fluctuations we can use Landau theory on $P_l[\vec{s}]$, and the magnetization is then simply the most probable spin

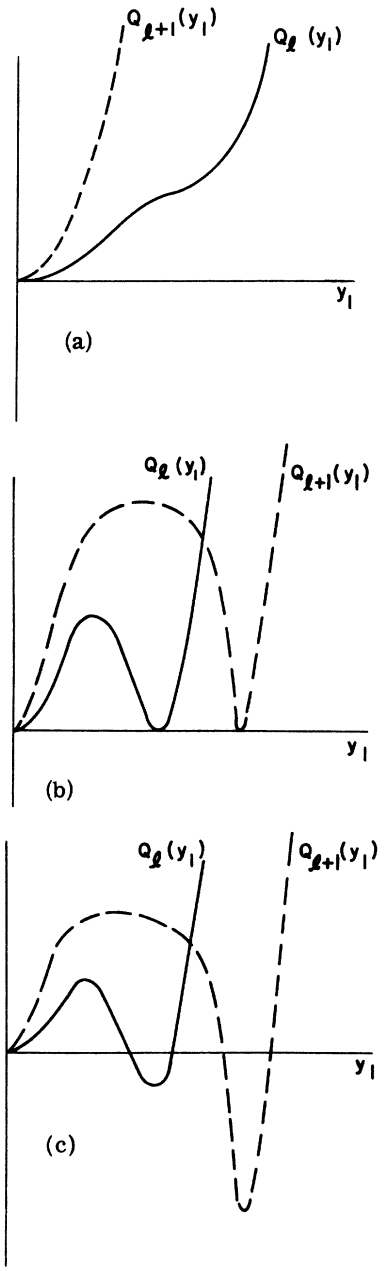

FIG. 4. (a) Two successive iterations of $Q_l(y_1)$ vs y_1 for $r_0 > r^*$. (b) Two successive iterations of $Q_l(y_1)$ vs y_1 for $r_0 = r^*$. (c) Two successive iterations of $Q_l(y_1)$ vs y_1 for $r_0 < r^*$.

TABLE II. Scaled magnetization $M^*(w_0)/(K\rho_0/2\omega)^{1/2}$ for three values of the symmetry-breaking parameter w_0.

w_0	$M^*(w_0)/(K\rho_0/2\omega)^{1/2}$
0.01	0.019
0.05	0.48
0.10	0.70

TABLE III. Integration weights w_i for the domain points (x_i, y_i) of the seven-point integration formula.

(x_i, y_i)	w_i
(0, 0)	21/36
$(\pm\frac{1}{2}h, \pm\frac{1}{2}h\sqrt{3})$	5/72
$(\pm h, 0)$	5/72

value scaled back to the original system size. By adding a small external magnetic field to break the symmetry of the system, we can make any one of the three symmetric minima the most probable. The magnitude of the spontaneous magnetization can be read off from Table I as $M^* = 0.70(K\rho_0/2\omega)^{1/2}$.

The magnetization of the low-temperature phase can be analyzed in the same manner, the only change from the above being that $Q_i(\vec{y}_0) < 0$ rather than $= 0$ in Eq. (10). The spontaneous magnetization is observed to increase with decreasing temperature as expected. It will not be discussed further here.

The spontaneous magnetization at the transition point was also calculated for two other values of the symmetry-breaking parameter, $w_0 = -0.05$ and -0.01. The results, as summarized in Table II, allow us to infer that the spontaneous magnetization varies continuously from zero as a function of the symmetry-breaking parameter:

$$M^*(w_0) \propto (w_0)^{\delta^*}, \tag{11}$$

where δ^* is approximately 0.56. Thus the phase transition appears to be of first order for all $w_0 \neq 0$.

Although we have demonstrated that the phase transition of our model is first order, one may still wish to question whether it is physically equivalent to the Potts model. We have also examined continuous spin distributions with the alternate nonanalytic form

$$P'[\vec{s}] = (A - B\cos 3\theta)(s_1^2 + s_2^2) + C(s_1^2 + s_2^2)^2, \tag{12}$$

θ being the angle of $\vec{s}$ with respect to the s_1 axis, which allows one to *continuously* break the symmetry away from the origin by variation of A. A discontinuous first-order transition was still obtained from the recursion formulas, indicating that the nature of the transition is a general feature of systems with threefold symmetry. We also examined our original model for $d = 4$ using Wilson's recursion formula, and for $d = 2$ using the recursion formula of Baker[11] with his parameter η arbitrarily set equal to $\frac{1}{4}$.[12] In both cases the transition proved to be of first order, indicating its generality with respect to dimensionality. Thus the Potts-model transition, within the context of the approximate $\eta = 0$ renormalization-group recursion formulas, is found generally to be of first order. Whether this conclusion will be changed by an *exact* renormalization-group analysis is an open question.[13]

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APPENDIX

Formula for the seven-point integration over a hexagonal domain H of radius h:

$$\frac{1}{\frac{3}{2}\sqrt{3}\,h^2}\iint_H f(x,y)\,dx\,dy = \sum_{i=1}^{7} w_i f(x_i, y_i) + R, \tag{1}$$

where the weights w_i are given for the points (x_i, y_i) in Table III, and $R = O(h^4)$.

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