N-color Ashkin-Teller model

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We study a model Hamiltonian consisting of N Ising models coupled pairwise through a four-spin interaction K_4. When $N=2$ this model is the well-known Ashkin-Teller model which shows nonuniversal critical behavior in two dimensions in the neighborhood of $K_4=0$. To see if this behavior persists for $N\neq 2$ we perform a first-order-perturbation expansion around the decoupling point in two dimensions. As an aid in interpreting the results of this perturbation expansion we have determined the phase diagram of the system through mean-field theory and Monte Carlo studies in both two and three dimensions for $N=3$. The results show that $N=2$ is special because the coupling between Ising models is marginal over a range of values of K_4. We discuss the effect of the coupling K_4 for $N\neq 2$.

I. INTRODUCTION

Recent work in critical phenomena[1-3] has shown that the critical points and lines of many two-dimensional systems can be mapped into each other. By introducing new models we hope to find qualitatively new behavior which will enrich our understanding of critical phenomena. We have studied the model Hamiltonian

$$\begin{aligned}\mathcal{H} &= -H/kT \\ &= K_2 \sum_{\langle rr'\rangle} \sum_{\alpha=1}^{N} \sigma^{(\alpha)}(\vec{r})\sigma^{(\alpha)}(\vec{r}') \\ &\quad + \tfrac{1}{2}K_4 \sum_{\langle rr'\rangle} \sum_{\alpha\neq\beta}^{N} \sigma^{(\alpha)}(r)\sigma^{(\beta)}(r)\sigma^{(\alpha)}(r') \\ &\qquad \times \sigma^{(\beta)}(r') \quad , \end{aligned} \tag{1}$$

where α and β label different Ising spins (distinguished by their color) at a site and $\langle rr'\rangle$ denotes a nearest-neighbor bond on a lattice. For $N=1$ this is the Hamiltonian for the Ising model whereas $N=2$ gives the usual Ashkin-Teller model. The limit $N\to 0$ is relevant to problems with quenched randomness.[4] In general we could add in coupling between several colors, but these are expected to be irrelevant near $K_4=0$ which is the limit of greatest interest. These generalized models are called 2^N-state cubic models[5] since the states of the system can be represented by a vector pointing along the diagonal of an N-dimensional cube.

We have studied this model for small K_4 and arbitrary N through renormalization-group methods and specialized to the case $N=3$ to determine the phase diagram through mean-field theory and Monte Carlo studies. We begin this paper with a review of operator expansion methods in renormalization-group calculations.

II. PERTURBATION THEORY WITH A MARGINAL OPERATOR

We present a general method for deriving renormalization-group flow equations in two dimensions as a perturbation expansion in the coupling strength of a marginal operator[6,7] (the generalization to other dimensions is simple). We then apply this method to study the Hamiltonian (1) for arbitrary N, with $K_4 \sim 0$.

Consider a Hamiltonian $\mathcal{H}$ close to its critical point $\mathcal{H}^*$. Let $\{O_i\}$ be a complete set of eigenoperators of the linearized renormalization transformation (i.e., $LO_i = y_i O_i$). Following Wegner,[8] we write $\mathcal{H}=\mathcal{H}^* + \sum_i \mu_i O_i$. The renormalization-group flow equations are

$$\frac{d\mu_i}{dl} = y_i(\{\mu_k\})\mu_i \quad . \tag{2}$$

A fixed point of (2) is defined by $d\mu_i/dl = 0$ for all i. The values of the fields μ_i at a fixed point are denoted μ_i^*. In general the critical exponents $y_i(\{\mu_k^*\})$ do not vanish so we must have $\mu_i^*=0$ for a fixed point. If O_M is a marginal operator, however, $y_m(\{\mu_k^*\})=0$, so it is possible to have a line of fixed points with $\mu_M^*\neq 0$. In this case the critical exponents are functions of $\mu_M^*, y_i(0,0,\ldots,\mu_M^*,0,0,\ldots)=y_i(\mu_M^*)$. Note that $y_M(\mu_M^*)$ must vanish for all μ_M^* if the critical exponents are to vary continuously, for otherwise there could be no fixed point where $\mu_M^*\neq 0$.

The critical exponents can be evaluated using the perturbation theory developed by Kadanoff and Wegner.[7] Let $\mathcal{H}=\mathcal{H}_0 + \lambda \sum_r U(r)$, where $\mathcal{H}_0$ is a

critical Hamiltonian whose correlation functions are known and $\sum_r U(r)$ is a marginal operator in $\mathcal{H}_0$. If we wish to find the critical exponent for the operator O_i we consider the correlation function

$$\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)\rangle = \frac{1}{|\vec{r}_1-\vec{r}_2|^{2x_i}} , \tag{3}$$

where $\tilde{O}_i(\vec{r})$ is the corresponding fluctuating local operator, $x_i = d - y_i$, and $|\vec{r}_1-\vec{r}_2|$ is assumed to be much larger than the lattice spacing. We will investigate the dependence of x_i on λ.

The value of x_i is known at $\lambda=0$ from the properties of $\mathcal{H}_0$. If we differentiate the correlation function (3) with respect to λ we find

$$\sum_r \langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)U(\vec{r})\rangle_0 = -2\frac{dx_i}{d\lambda}\bigg|_{\lambda=0}\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)\rangle_0 \ln|\vec{r}_1-\vec{r}_2| . \tag{4}$$

This equation can be used to evaluate $(dx_i/d\lambda)|_{\lambda=0}$ if we determine the sum on the left-hand side and pick out the contribution that is proportional to $\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)\rangle_0 \ln|\vec{r}_1-\vec{r}_2|$.

Let us write the sum in Eq. (4) as an integral and introduce a cutoff $b \ll |\vec{r}_1-\vec{r}_2|$ so that the integration excludes circles of radius b around $\vec{r}_1$ and $\vec{r}_2$. Now we seek q_i such that

$$I \equiv \int d^2\vec{r}\,\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)U(\vec{r})\rangle_0 = q_i\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)\rangle_0 \ln\left|\frac{\vec{r}_1-\vec{r}_2}{b}\right| . \tag{5}$$

Differentiating (5) with respect to the cutoff we get

$$\frac{dI}{db} = \frac{-q_i}{b}\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_i(\vec{r}_2)\rangle_0 , \tag{6}$$

from the logarithmic expression, and

$$\frac{dI}{db} = -2\pi b[\langle \tilde{O}_i(0)\tilde{O}_i(\vec{r}_2-\vec{r}_1)U(b)\rangle_0 + \langle \tilde{O}_i(\vec{r}_1-\vec{r}_2)\tilde{O}_i(0)U(b)\rangle_0] , \tag{7}$$

from the integral expression. If $\langle \tilde{O}_i(\vec{r}_1-\vec{r}_2)\tilde{O}_i(0)U(b)\rangle_0$ can be expressed as $p_i/b^2\langle \tilde{O}_i(\vec{r}_1-\vec{r}_2)\tilde{O}_i(0)\rangle_0$, Eqs. (6) and (7) give $q_i = 4\pi p_i$, while Eqs. (4) and (5) give $dx_i/d\lambda = -2\pi p_i$.

Note that $\tilde{O}_i(0)$ and $U(b)$ are local operators evaluated at nearby points. According to operator expansion ideas[9] we can write

$$\tilde{O}_i(\vec{x})\tilde{O}_j(\vec{y}) = \sum_k A_{ijk}(\vec{x}-\vec{y})\tilde{O}_k\left(\frac{\vec{x}+\vec{y}}{2}\right) . \tag{8}$$

Now, the exponent for a local operator is defined by $e^{lL}\tilde{O}_i(\vec{x}) = e^{-lx_i}\tilde{O}_i(\vec{x}e^{-l})$. Applying e^{lL} to Eq. (8) we obtain

$$\exp[-(x_i+x_j)l]\tilde{O}_i(\vec{x}e^{-l})\tilde{O}_j(\vec{y}e^{-l}) = \sum_k A_{ijk}(\vec{x}-\vec{y})e^{-x_k l}\tilde{O}_k\left(\frac{\vec{x}+\vec{y}}{2}e^{-l}\right) . \tag{9}$$

Multiplying (9) by $\exp[(x_i+x_j)l]$ and requiring that the equation hold for all values of l we find

$$A_{ijk}(\vec{r}) = a_{ijk}(\vec{r}/|\vec{r}|)\,|\vec{r}|^{-(x_i+x_j-x_k)} . \tag{10}$$

Conformal covariance[10] implies that the correlation function of two operators will always vanish unless their exponents are equal. Two operators with equal indices are either identical or are said to be degenerate. We assume that we have a complete set of operators $\{O_i\}$ in which each degenerate subset has been diagonalized so that $\langle \tilde{O}_i(\vec{r}_1)\tilde{O}_j(\vec{r}_i)\rangle_0$ is proportional to δ_{ij}. Setting $\vec{x}=0$ and $\tilde{O}_j(\vec{y}) = U(b)$ in Eq. (8) we have

$$\langle \tilde{O}_i(\vec{r}_1-\vec{r}_2)\tilde{O}_i(0)U(b)\rangle_0 = \frac{a_{iui}}{b^2}\left\langle \tilde{O}_i(\vec{r}_1-\vec{r}_2)\tilde{O}_i\left(\frac{b}{2}\right)\right\rangle_0 , \tag{11}$$

where the subscript U in a_{iui} denotes the marginal operator U. Recalling that $b \ll |\vec{r}_1-\vec{r}_2|$, we find $p = a_{iui}$ and

$$\frac{dx_i}{d\lambda} = -2\pi a_{iui} . \tag{12}$$

Now consider the Hamiltonian given by Eq. (1). We can write the fluctuating local-energy density on color α as

$$\epsilon^{(\alpha)}(r) = \frac{1}{2}\sum_{j(r)}\sigma^{(\alpha)}(r)\sigma^{(\alpha)}(j(r)) - \bar{\epsilon}^{(\alpha)} ,$$

where $j(r)$ denotes the nearest neighbors of r, and $\bar{\epsilon}^{(\alpha)}$ is the average energy density on α. The Hamiltonian becomes

$$\mathcal{H} = \mathcal{H}_0 + K_4\sum_r U(r) + K_4\sum_r V(r) , \tag{13}$$

where

$$\mathcal{H}_0 = K_2\sum_{\langle rr'\rangle}\sum_{\alpha=1}^{N}\sigma^{(\alpha)}(\vec{r})\sigma^{(\alpha)}(\vec{r}') ,$$

$$U(\vec{r}) = \frac{1}{2}\sum_{\alpha\neq\beta}^{N}\epsilon^{(\alpha)}(\vec{r})\epsilon^{(\beta)}(\vec{r}) ,$$

and

$$V(\vec{r}) = \frac{1}{2}\sum_{\alpha\neq\beta}^{N}[\epsilon^{(\alpha)}(\vec{r})\bar{\epsilon}^{(\beta)} + \epsilon^{(\beta)}(\vec{r})\bar{\epsilon}^{(\alpha)}] + \text{const} .$$

$V(r)$ simply renormalizes the coupling constant in

H_0 and will not be considered further.

To determine the critical index of U when $\lambda=0$ we compute the correlation function[11]

$$\langle U(\vec{r}_1)U(\vec{r}_2)\rangle_0=\frac{1}{2}\sum_{\alpha\neq\beta}^{N}\langle\epsilon^{(\alpha)}(\vec{r}_1)\epsilon^{(\alpha)}(\vec{r}_2)\rangle_0\langle\epsilon^{(\beta)}(\vec{r}_1)\epsilon^{(\beta)}(\vec{r}_2)\rangle_0=\frac{2N(N-1)}{\pi^4|\vec{r}_1-\vec{r}_2|^4}\ . \tag{14}$$

Thus $X_u(0)=2$ and we identify U as a marginal operator when $\lambda=0$.

All that remains is to compute the operator expansion coefficients a_{iui}. In addition to the marginal operator U we consider: energy density,

$$E(\vec{r})=\frac{1}{\sqrt{N}}\sum_{\alpha=1}^{N}\epsilon^{(\alpha)}(\vec{r})\ ;$$

polarization,

$$P(\vec{r})=\frac{1}{2}\sum_{\alpha=2}^{N}\sigma^{(\alpha)}(\vec{r})\sigma^{(\beta)}(\vec{r})\ ;$$

crossover operator,

$$C(\vec{r})=\frac{1}{\sqrt{N}}\left[\epsilon^{(1)}(\vec{r})-\sum_{\alpha=2}^{N}\epsilon^{(\alpha)}(\vec{r})\right]\ .$$

We will determine a_{EUE} to illustrate the technique. Consider Eq. (8) with $\tilde{O}_i(\vec{x})=E(\vec{x})$ and $\tilde{O}_j(\vec{y})=U(\vec{y})$ multiplied on both sides by $E(\vec{z})$. Recalling that $\langle\tilde{O}_i(\vec{r}_1)\tilde{O}_j(\vec{r}_2)\rangle_0=0$ unless $x_i=x_j$, we find

$$\langle E(\vec{x})U(\vec{y})E(\vec{z})\rangle_0=\frac{a_{EUE}}{|\vec{x}-\vec{y}|^2}\left\langle E\left(\frac{\vec{x}+\vec{y}}{2}\right)E(\vec{z})\right\rangle_0\ .$$

Using[11]

$$\langle\epsilon^{(\alpha)}(\vec{r}_1)\epsilon^{(\beta)}(\vec{r}_2)\rangle_0=\frac{2\delta_{\alpha\beta}}{\pi^2|\vec{r}_1-\vec{r}_2|^2}\ , \tag{15}$$

and taking $|\vec{z}-[(\vec{x}+\vec{y})/2]|\gg|\vec{x}-\vec{y}|$ we find $a_{EUE}=2(N-1)/\pi^2$. By similar manipulations we obtain $a_{CUC}=-2(N-1)/\pi^2$, $a_{PUP}=1/2\pi^2$, and $a_{UUU}=4(N-2)/\pi^2$.

Together with Eq. (12) these results show that, to first order in K_4,

$$X_U=2-\frac{8(N-2)}{\pi}K_4\ ,\quad X_E=1-\frac{4(N-1)}{\pi}K_4\ ,$$
$$X_L=\frac{4(N-1)}{\pi}K_4\ ,\quad X_P=\frac{1}{4}-\frac{1}{\pi}K_4\ . \tag{16}$$

The renormalization flow equations for K_2 and K_4 become

$$\frac{dK_4}{dl}=\frac{8(N-2)}{\pi}K_4^2\ , \tag{17}$$

$$\frac{d(K_2-K_2^*)}{dl}=\left[1+\frac{4(N-1)}{\pi}K_4\right](K_2-K_2^*)\ . \tag{18}$$

We can see immediately that, except when $N=2$, $U(r)$ is a marginal operator only at $\lambda=0$. Equations (17) and (18) predict that for $N>2$ and $K_4\gtrsim 0$ the flow will be to larger K_4, while for $K_4\lesssim 0$ the flow will be towards $K_4=0$. For $N<2$ the situation is just the reverse. When the flow is away from K_4 there are two alternatives for the nature of the phase transition. If K_4 continues to grow without bound, the transition is likely to be first order. Alternatively, higher-order corrections to Eq. (17) may lead to a new fixed point at finite K_4 in which case the transition will be continuous and most likely not in the Ising universality class.

When the flow is toward $K_4=0$ the critical behavior is almost certainly in the Ising universality class. This behavior may be unstable, however, as can be seen from the following example.

When $N=4$ the complete set of marginal operators is

$$O_1=\frac{1}{\sqrt{6}}(\epsilon^1\epsilon^2+\epsilon^1\epsilon^3+\epsilon^1\epsilon^4+\epsilon^2\epsilon^3+\epsilon^2\epsilon^4+\epsilon^3\epsilon^4)\ ,$$

$$O_2=\frac{1}{\sqrt{12}}(2\epsilon^1\epsilon^2-\epsilon^1\epsilon^3-\epsilon^1\epsilon^4-\epsilon^2\epsilon^3-\epsilon^2\epsilon^4+2\epsilon^3\epsilon^4)\ ,$$

$$O_3=\frac{1}{2}(\epsilon^1\epsilon^3-\epsilon^1\epsilon^4-\epsilon^2\epsilon^3+\epsilon^2\epsilon^4)\ ,$$

$$O_4=\frac{1}{\sqrt{2}}(\epsilon^1\epsilon^3-\epsilon^2\epsilon^4)\ ,$$

$$O_5=\frac{1}{\sqrt{2}}(\epsilon^1\epsilon^4-\epsilon^2\epsilon^3)\ ,$$

$$O_6=\frac{1}{\sqrt{2}}(\epsilon^1\epsilon^2-\epsilon^3\epsilon^4)\ .$$

These operators are chosen so that $\langle O_iO_j\rangle_0=\delta_{ij}$ and $\langle O_iO_jU\rangle_0=m_i\delta_{ij}$. We find that O_1, the original marginal operator, is the only marginally irrelevant operator for $K_4<0$. O_2 and O_3 are relevant and tend to drive the system towards being two decoupled Ashkin-Teller models. The remaining operators are truly marginal to first order in K_4. Thus it is possible that the system will behave like two decoupled Ashkin-Teller models rather than four decoupled Ising models when $N=4$ and $K_4<0$ if Hamiltonian (1) is slightly perturbed.

The remainder of this paper will be devoted to a study of the phase diagram of this system through mean-field, Monte Carlo, and ϵ-expansion techniques. In determining the phase diagram we hope to establish the nature of the fixed points of the renormalization flow equations.

III. MEAN-FIELD THEORY

To gain insight into the possible fixed points for flow away from $K_4=0$, we have studied the Hamiltonian (1) in the mean-field approximation (exact in ∞ dimensions) and through an $\epsilon=4-d$ expansion in an attempt to sneak down in dimensionality towards $d=2$. Mean-field calculations have been performed before in the case $N=2$,[12] so we will concentrate on the case $N=3$.

We write a single-site effective Hamiltonian

$$\mathcal{H}_{mf}(r)=\sum_{\alpha=1}^{3}h_\alpha(r)\sigma^\alpha(r)+\frac{1}{2}\sum_{\alpha\neq\beta}^{3}h_{\alpha\beta}(r)\sigma^\alpha(r)\sigma^\beta(r)\ , \tag{19}$$

where

$$h_\alpha(r)=\tfrac{1}{2}K_2\sum_{j(r)}\langle\sigma^\alpha[j(r)]\rangle\ ,$$

and

$$H_{\alpha\beta}(r)=\tfrac{1}{2}K_4\sum_{j(r)}\langle\sigma^\alpha[j(r)]\sigma^\beta[j(r)]\rangle\ ,$$

and $j(r)$ are the nearest neighbors of r. The single-site partition function is $Z(r)=\sum_{\{\sigma^{(\alpha)}(r)\}}e^{\mathcal{H}_{mf}}$ and the free energy is approximately

$$F=-\sum_r\ln Z(r)+K_2\sum_{\langle rr'\rangle}\sum_{\alpha=1}^{3}\langle\sigma^\alpha(r)\rangle\langle\sigma^\alpha(r')\rangle$$
$$+\tfrac{1}{2}K_4\sum_{\langle rr'\rangle}\sum_{\alpha\neq\beta}^{3}\langle\sigma^\alpha(r)\sigma^\beta(r)\rangle\langle\sigma^\alpha(r')\sigma^\beta(r')\rangle\ . \tag{20}$$

The averages are given by the formulas

$$\langle\sigma^\alpha(r)\rangle=\sum_{\substack{\text{configs}\\ \text{at } r}}\sigma^\alpha(r)e^{\mathcal{H}_{mf}}\Big/Z(r)\ ,$$
$$\langle\sigma^\alpha(r)\sigma^\beta(r)\rangle=\sum_{\substack{\text{configs.}\\ \text{at } r}}\sigma^\alpha(r)\sigma^\beta(r)e^{\mathcal{H}_{mf}}\Big/Z(r)\ . \tag{21}$$

These equations can be solved if we make some assumptions about the relationship between averages at r and averages at r'. We will only consider $K_2>0$, so we will always assume $\langle\sigma^\alpha(r)\rangle=\langle\sigma^\alpha(r')\rangle$. For $K_4>0$ we assume $\langle\sigma^\alpha(r)\sigma^\beta(r)\rangle=\langle\sigma^\alpha(r')\sigma^\beta(r')\rangle$, while for $K_4<0$ we also consider staggered products. With these assumptions we look for solutions of Eqs. (21). The solution which gives lowest free energy is taken to be the true mean-field solution.

A. $K_4>0$

The mean-field phase diagram for the $N=3$ model is shown in Fig. 1. This diagram gives a suggestive picture of what to expect in high dimensions, but we expect substantial differences in the two-dimensional phase diagram. For $x>0$ each color of spins orders with a sign which is independent of the sign of the other colors. As a consequence all products are ordered with $\mathrm{sgn}(\langle\sigma^\alpha\sigma^\beta\rangle)=\mathrm{sgn}(\langle\sigma^\alpha\rangle\langle\sigma^\beta\rangle)$ and $\langle\sigma^1\sigma^2\rangle\langle\sigma^2\sigma^3\rangle\langle\sigma^3\sigma^1\rangle>0$. In analogy with the usual ($N=2$) Ashkin-Teller model we call this phase the Baxter phase.

As the temperature is increased, for $x<3$ (to the left of point C), there is a transition directly from the Baxter phase to the paramagnetic phase. At $x=0$ (point A) we recognize this as an Ising transition at $K_2=K_c^I$ in the three decoupled Ising models. The Ising transition continues up to point B, where the four-spin coupling becomes important. The transition is first order along BC.

Near point D we can study the model through second-order perturbation theory in $K_2=K_4/x$. When $K_2=0$ the Hamiltonian (1) becomes

$$\mathcal{H}=K_4\sum_{\langle rr'\rangle}[\tau_{12}(r)\tau_{12}(r')+\tau_{23}(r)\tau_{23}(r')$$
$$+\tau_{12}(r)\tau_{23}(r)\tau_{12}(r')\tau_{23}(r')]\ , \tag{22}$$

where $\tau_{\alpha\beta}(r)=\sigma^\alpha(r)\sigma^\beta(r)$. This is the Hamiltonian for the $N=2$ Ashkin-Teller model at $x=1$, which is also the Hamiltonian of the four-state Potts model. From Ref. 12 we know that the transition, which occurs at $K_4=K_c^P$, is second order in two dimensions and first order in higher dimensions. Adding a small K_2 term does not alter the Hamiltonian to second order in K_2, beyond reducing the coupling strength:

$$K_{\text{eff}}=K_4-K_2^2\ . \tag{23}$$

Thus we expect that near D we will have a first-order transition between the paramagnetic phase and a phase in which products of colors are ordered: $\langle\sigma^\alpha\sigma^\beta\rangle\neq0$, $\langle\sigma^\alpha\rangle=0$, and $\langle\sigma^1\sigma^2\rangle\langle\sigma^2\sigma^3\rangle\langle\sigma^3\sigma^1\rangle>0$.

Near point E we expect that $\langle\sigma^\alpha\sigma^\beta\rangle=\pm1$ for all products. Thus $\sigma^\alpha(r)=\pm\sigma^\beta(r)$ with high probability and the Hamiltonian takes the form

$$\mathcal{H}=3K_2\sum_{\langle rr'\rangle}\sigma^\alpha(r)\sigma^\alpha(r')+\text{const}\ . \tag{24}$$

This shows that there will be an Ising-like transition at $K_2=\frac{1}{3}K_c^I$, where each color orders conforming to the requirement $\mathrm{sgn}(\langle\sigma^\alpha\rangle)\mathrm{sgn}(\langle\sigma^\beta\rangle)=\mathrm{sgn}(\langle\sigma^\alpha\sigma^\beta\rangle)$.

B. $K_4<0$

For $K_4\ll0$ it is energetically unfavorable to have the products of colors ordered ferromagnetically, so we must consider states with a staggered product magnetization, $\langle\sigma^\alpha\sigma^\beta\rangle_{\text{AF}}$. In this case the system divides itself into two sublattices A and B with points on sublattice A (or B) being the nearest neighbors of

points of sublattice B (or A). The product $\sigma^\alpha\sigma^\beta$ alternates in sign between the sublattices.

Consider first the limit $K_2=0$. The Hamiltonian can be written

$$\mathcal{H}=-K_4\sum_{\langle rr'\rangle}[\tau'_{12}(r)\tau'_{12}(r')+\tau'_{23}(r)\tau'_{23}(r') -\tau'_{12}(r)\tau'_{23}(r)\tau'_{12}(r')\tau'_{23}(r')]\ , \quad (25)$$

where $\tau'_{\alpha\beta}(r)=S(r)\sigma^\alpha(r)\sigma^\beta(r)$ and $S(r)=+1(-1)$, when r is on sublattice $A(B)$. This is identical to the Hamiltonian for the $N=2$ model at $x=-1$, and can also be interpreted as an antiferromagnetic four-state Potts model. From Refs. 12 and 13 we know that this model will be disordered for all $K_4<0$ in two dimensions, but that in three or more dimensions there will be a transition to a state with a single staggered product ordered. This transition is in the Heisenberg model universality class.[13] In mean-field theory the transition occurs at $K_4=-K_c^I$.

For any $x<-1$ there is a transition from paramagnetism to the single staggered-product phase (phase IV) as K_2 is increased. Once the system is in the staggered-product phase the only additional ordering that can occur is for the remaining color to order ferromagnetically. This is a continuous phase transition both in two dimensions and in mean-field theory. The transition, which occurs at $K_2=K_c^I$ in mean-field theory, has an Ising-like order parameter.

With these observations we can understand most of the $x<0$ phase diagram. The line GF is a second-order transition in the ferromagnetically ordered color. The line HJ is the Heisenberg universality class in three dimensions but occurs at $K_4=-K_c^I$ in the mean-field theory. At point I, where these lines intersect, four phases touch. Phase III has only a single color ordered, phase IV has a single staggered product ordered, phase V has one staggered product and the remaining color ordered, and phase VII is paramagnetic. Phases analogous to III and IV were found in the $N=2$ model.[12]

The remaining transitions are first order. Along JF there is a first-order phase transition from phase III to the Baxter phase. As the temperature is lowered, the large entropy of phase III becomes insufficient to ensure stability and the system orders into either phase V or the Baxter phase. There is a first-order transition between the Baxter phase and phase V along JK. At $T=0$ the point $x=-\frac{1}{2}$ is highly degenerate. Many configurations can be found with energy equal to the ground-state energy [for arbitrary N we expect to find analogous behavior at $x=(1-N)^{-1}$]. In particular, the Baxter phase at $x=-\frac{1}{2}$ has the same energy as a configuration with only two colors and their product ordered ferromagnetically. This latter configuration has higher entropy, so at finite temperature we expect to find a phase characterized by this configuration. In Fig. 1 it is labeled phase VI and occupies a narrow region between points K and L.

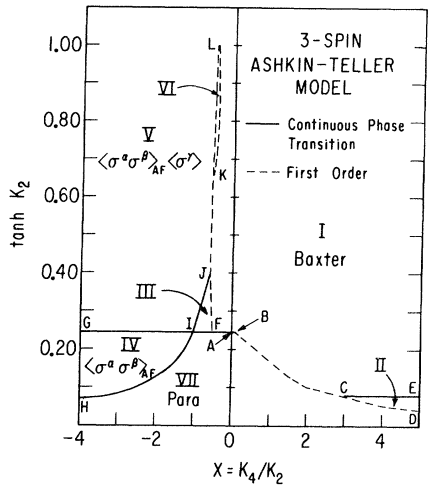

FIG. 1. Mean-field-theory phase diagram of the $N=3$ model. In phase II all products of colors are ordered. In phase III a single color is ordered. In phase VI two colors and their product are ordered. In phases IV and V the quantities shown are the only nonvanishing order parameters.

IV. MONTE CARLO RESULTS

The importance sampling Monte Carlo technique was applied to the Hamiltonian (1) for $N=3$ in two and three dimensions. The same method was used here as in the $N=2$ model and is described in Appendix A of Ref. 12. The size of the lattice was $10\times10\times10$ in three dimensions and 30×30 or 40×40 in two dimensions. Periodic boundary conditions were imposed, and both random and ordered searches were carried out. The equilibrium nature of the final states was confirmed by starting with a variety of initial configurations.

A. Three dimensions

Figure 2 shows our proposed phase diagram for the $N=3$ model in three dimensions. In Sec. III we discussed perturbation expansions which described the behavior at points D, E, and H. At point A we know that the system behaves like three decoupled Ising models, but K_4 is a relevant coupling in three dimensions so it can completely alter the nature of the phase transitions in the neighborhood of A.

For $x\geq0$ the phase diagram is very similar to the one predicted by mean-field theory. The low-temperature phase is the Baxter phase in which each color and each product of colors has a nonvanishing average. Between the Baxter and paramagnetic

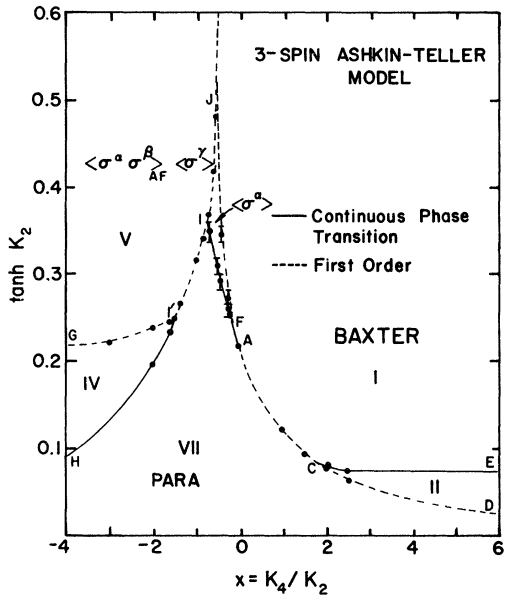

FIG. 2. Monte Carlo results for the $N=3$ model in three dimensions. The labeling of the phase is consistent with Fig. 1, with the exception that the $\langle\sigma^{\alpha}\rangle$ phase was not clearly like either phase III or phase VI. Solid points indicate where the Monte Carlo simulations were performed.

phases and to the right of point C ($x=1.75\pm0.1$) there is a phase analogous to phase II of the mean-field-theory phase diagram in which all products of two colors are ordered. The mean-field-theory differed in that C was further to the right and there was a short line, AB, of second-order phase transitions before the first-order line, BC.

For $x<0$ there are more substantial differences from the mean-field-theory predictions. At low temperatures we find the phase with one color and the staggered product of the remaining two being the only nonvanishing averages (phase V). This ordering is not perfect, however—even at $T=0$ $\langle\sigma^{\gamma}\rangle$ and $\langle\sigma^{\alpha}\sigma^{\beta}\rangle_{\mathrm{AF}}$ are slightly less than 1.0. This is because it is possible to find sites where a pair of colors can be flipped simultaneously with no change in energy. For all $x<-0.5$, $\langle\sigma^{\alpha}\sigma^{\beta}\rangle_{\mathrm{AF}}=\langle\sigma^{\gamma}\rangle\approx0.94$ at $T=0$. Note that we still have $\langle\sigma^{1}\sigma^{2}\sigma^{3}\rangle_{\mathrm{AF}}=1.0$ at low temperature since flipping two colors at a single site leaves the triple product unchanged.

Mean-field theory predicted a tetracritical point (I in Fig. 1), where the low-temperature phase met the paramagnetic phase. In our Monte Carlo simulation we find instead a line II′ of first-order transitions. To the left of I′ there is a phase (phase IV) with only one staggered product having nonzero average, as was expected from our analysis of point H in Sec. III.

To the right of the point I there is a phase tentatively labeled $\langle\sigma^{\alpha}\rangle$. It was difficult to distinguish unambiguously whether the system has a single color ordered (as in phase III of the mean-field theory), or two colors ordered (as in phase VI of the mean-field theory). For some runs the ordering was like that of phase VI. These states seemed to be metastable, however, so we assume that the ordering should be like that of phase III. No conclusive evidence for the existence of phase VI was found in three dimensions.

Note that the transitions along GI' and IJ are first order. In mean-field theory these transitions were second order, so the first-order nature must be due to strong local fluctuations. The transition along FJ is probably weakly first order. There was no apparent discontinuity in the energy but there was evidence for the presence of metastable states indicative of a first-order transition. Note that a similar problem was found in this region of the phase diagram of the $N=2$ model.[12]

B. Two dimensions

Figure 3 shows our proposed phase diagram for the $N=3$ model in two dimensions. As in three dimensions, the behavior near points E, D, and G is known through the effective Hamiltonians derived in Sec. III, and A is the decoupling point where we know there must be an Ising transition. For $x>0$ the only difference between two and three dimensions is the

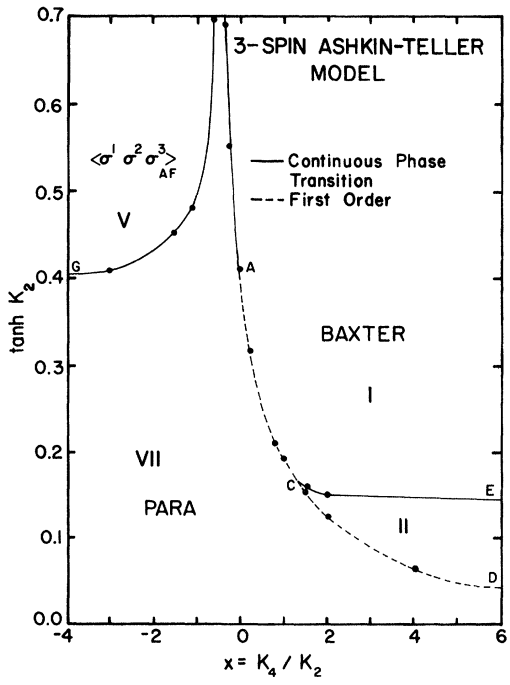

FIG. 3. Monte Carlo results for the $N=3$ model in two dimensions. Solid points indicate where the Monte Carlo simulations were performed.

location of point C ($x = 1.35 \pm 0.5$) in two dimensions.

For $-\frac{1}{2} < x < 0$ the Baxter phase is stable at low temperatures. Exactly at $x = -\frac{1}{2}$ the model remains paramagnetic for all T. It seems likely that this behavior will be quite general with an N color model being paramagnetic for all T at $x = 1/(1-N)$. We find a second-order transition between the Baxter and paramagnetic phases. This is consistent with the perturbation expansion described in Sec. II where we have predicted that the transition should be in the same universality class as point A which is known to have an Ising transition.

We would like to point out one difficulty that arose in the Monte Carlo simulation near $x = 1/(1-N)$ in both the $N = 2$ and 3 models. Because the transition temperatures are so low the equilibrium time becomes too long for us to trust our results for the magnetization. For instance, in the $N = 2$ model the transition temperature is known[2] and the $\langle \sigma^\alpha \rangle$ phase is believed to be unstable. However, on heating the system from low temperatures the simulations showed a $\langle \sigma^\alpha \rangle$ phase which appeared near the known transition temperature and became paramagnetic at a higher temperature. The state seemed to be metastable with a very small energy difference from the paramagnetic state. We feel that the simulations should not be trusted since a $\langle \sigma^\alpha \rangle$ phase is difficult to incorporate into what has been established regarding the $N = 2$ model in two dimensions.[2] Recognizing this difficulty, we choose to identify the transition temperatures in the $N = 3$ model by the heat-capacity maximum instead of the vanishing order parameters, since it is known that the energy and heat capacity are correctly given by the Monte Carlo simulations even in cases where the time is too short to determine the order parameter correctly. This is found to be the case for spin-glass systems.[15]

For $x < -\frac{1}{2}$ there is only one ordered phase. No color or product of two colors orders either ferromagnetically or antiferromagnetically, however $\langle \sigma^1 \sigma^2 \sigma^3 \rangle_{\mathrm{AF}}$ was nonzero. There is no intermediate $\langle \sigma^\alpha \sigma^\beta \rangle_{\mathrm{AF}}$ phase, as can be seen by noting that the Hamiltonian (25) is paramagnetic in two dimensions[13] for all $K_4 < 0$. When the system was initially placed in a configuration with $\langle \sigma^1 \rangle = \langle \sigma^2 \sigma^3 \rangle_{\mathrm{AF}} = 1$ at $T = 0$ single-spin flips were never observed and the system remained ordered. If, however, we allow for more than a single color to flip at one time on a given site the system quickly disorders both colors and products of two colors by flipping two colors simultaneously. In three dimensions multiple-spin flips produced only a slight disordering. Note that this process leaves $\tau_{123}(r) = \sigma^1(r)\sigma^2(r)\sigma^3(r)$ invariant. Since the ordering is AF Ising-like in the variable $\tau_{123}(r)$ we believe that this transition is in the Ising model universality class, and we note that for $K_4 \ll 0$ the transition occurs at $K_2 = K_c^{\mathrm{I}}$. This result is somewhat surprising because the Hamiltonian (1) does not treat $\tau_{123}(r)$ as a natural-order parameter.

V. $\epsilon = 4 - d$ EXPANSION

Returning to arbitrary N, we transformed the Hamiltonian (1) to continuous-spin variables. A perturbation expansion in K_4 yields the effective Hamiltonian

$$\mathcal{H} = \int d^b x \left[-\frac{1}{2} \left[\sum_{i=1}^{N} (\nabla \sigma^i)^2 + r_2 \sum_{i=1}^{N} \sigma_i^2 \right] \right] + \frac{1}{2} A 8 z^3 K_2^2 K_4 \sum_{i<j=1}^{N} \sigma_i^2 \sigma_j^2 \ , \tag{26}$$

where A is the average of $\sigma_i^2 \sigma_j^2$, and z is the coordination number of the lattice. This Hamiltonian is well known and is the generalized Cubic model.[14] For $K_4 > 0$ this model shows a first-order transition, whereas for $K_4 < 0$ there is some N_c for which flow will be to a Cubic fixed point when $N > N_c$ and to a Heisenberg fixed point when $N < N_c$. N_c is given approximately by $N_c \approx (4 + 3.176\epsilon)/(1 + 1.294\epsilon)$. This gives $N_c \approx 2.9$ in two dimensions, but its accuracy for $\epsilon = 2$ is questionable.

VI. CONCLUSION

The major problem addressed in this paper was determining the nature of the phase transitions in two dimensions of Hamiltonian (1) in the four cases, $N > 2$ and $K_4 > 0$, $N > 2$ and $K_4 < 0$, $N < 2$ and $K_4 > 0$, and $N < 2$ and $K_4 < 0$. By determining the phase diagram for $N = 3$ we have established that the transition will be first order when $N > 2$ and $K_4 > 0$. The Monte Carlo studies and the perturbation expansion indicate that the transition will be continuous, and most likely in the Ising universality class, when $N > 2$ and $K_4 < 0$, and when $N < 2$ and $K_4 > 0$. The nature of the phase transition when $N < 2$ and $K_4 < 0$ is still unknown. If we interpret this model as an $O(N)$ model with symmetry-breaking terms we are led to speculate that the transition will be continuous and possibly in a new universality class.

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