Potts models in random fields

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The q-state Potts model is studied in the presence of random fields, which locally prefer ordering of any one of the q states. In d dimensions, the transition is expected to become first-order for $q > q_c(d)$. As in the nonrandom case, mean-field theory still yields $q_c(d)=2$ for all d. Fluctuations are argued to shift the nonrandom value, $q_c^0(d)$, into a significantly higher value, $q_c(d)$. For $q_c^0(d) < q < q_c(d)$ we thus expect random fields to turn the discontinuous transitions into continuous ones. At $d=3$ this probably includes the experimentally realizable cases $q=3$ and 4.

I. INTRODUCTION

The order of the phase transition of the q-state Potts model[1] has been the subject of intensive recent research. The transition is first-order for $q > q_c^0(d)$ and continuous for $q \le q_c^0(d)$. The critical value $q_c^0(d)$, which is universal for short-range interactions, varies with the dimensionality of the system, d. At $d=2$ it was shown exactly[2] that $q_c^0(2)=4$. Recent approximate real-space renormalization-group (RG) calculations[3] reproduced this result and gave details of the behavior for different values of q. As $d \to 1+$, Migdal-type recursion relations indicated[4] that the transition is continuous for all finite q, i.e., $q_c^0(1) \to \infty$. Indeed, it was recently shown[5] that for $d \to 1+$, $q_c^0(d)$ increases as $\exp[2/(d-1)]$. Above the upper critical dimensionality, $d > d_u = 6$, one expects the Potts model to be correctly described by mean-field theory.[6] Mean-field theory predicts that all Potts models with $q \ne 2$ should have first-order transitions due to the presence of cubic terms in the appropriate Landau free-energy expansion. Hence, $q_c^0(d)=2$ for $d > 6$. Moreover, a RG study of the model in 6-ϵ dimensions showed[7] that the transition remains first-order for $q > 2$, i.e., $q_c(6-\epsilon)=2$. Recent RG studies near four dimensions showed[8] that $q_c^0(d)=2$ for $d > 4$ and that $q_c^0(4-\epsilon)=2+\epsilon+O(\epsilon^2)$ for $d \le 4$. For $d=3$ it is now believed[9] that $q_c(3) \lesssim 3$. The critical value $q_c^0(d)$ thus seems to be a monotonically decreasing function of d changing from ∞ at $d=1$, via 4 at $d=2$ to 2 at $d=4$ (solid line in Fig. 1).

Random quenched fields (which couple linearly to the order parameter) have drastic effects on phase transitions. In particular, diagrammatic studies of the n-component spin Landau-Ginzburg-Wilson model with random fields indicate deviations from mean-field theory below six dimensions, instead of four dimensions (without random fields). The ϵ expansions of the random-field problem in $d=6-\epsilon$ dimensions are the same, to all orders, as those of the nonrandom problem in $d=4-\epsilon$ dimensions.[10–13] The situation concerning the lower critical dimensionality, d_l, below which there exists no long-range order at any finite temperature, is less clear. For rotationally invariant $O(n)$ models, the rule $d \to d-2$ also applies to d_l, which is shifted to $d_l=4$.[14] For the Ising case, $n=1$, there exist arguments yielding either $d_l=3$ (Refs. 15 and 16) or 2.[14,17–19] In any case, it is clear that random fields yield the critical behavior of an effectively reduced dimensionality, and that, therefore, the effects of fluctuations are much more severe.

The aim of the present paper is to study the effects of random fields on the order of the transitions of q-state Potts models. The model is defined in detail in Sec. II. At the level of mean-field theory (Sec. III) we tried to see if random fields strengthen or weaken the tendency of the

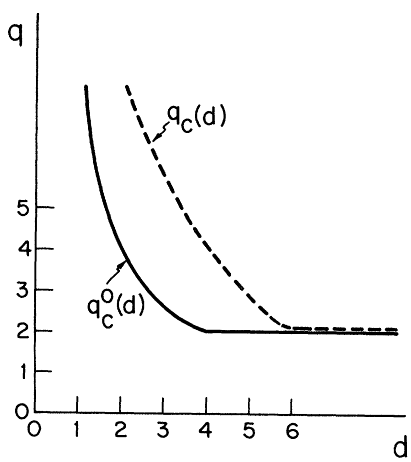

FIG. 1. Schematic plot of $q_c^0(d)$ (solid line) and $q_c(d)$ (dashed line).

system to undergo a first-order transition. We find that the transition never becomes continuous. Going beyond mean-field theory, Sec. IV aims at estimating $q_c(d)$ in the presence of random fields. Since random fields enhance the effects of fluctuations, we expect $q_c(d)$ to increase in their presence.[20] We argue that $q_c(d)$ should now diverge to infinity at the new lower critical dimensionality d_l (probably equal to 2), and should decrease towards $q_c=2$ at $d=6$ (dashed line in Fig. 1). Section V is devoted to possible experimental realizations in which random fields may turn discontinuous transitions into continuous ones.

II. MODEL

The q-state Potts model in a random field is described by the following Hamiltonian:

$$\mathscr{H}=-\tilde{J}\sum_{\langle ij\rangle}(q\delta_{\sigma_i\sigma_j}-1)-\sum_i\sum_\alpha \tilde{H}_i^\alpha(q\delta_{\sigma_i,\alpha}-1)\ , \quad (1)$$

where σ_i is a spinlike variable at the site i of a d-dimensional lattice which can attain q different values $\sigma_i=1,2,\ldots,q$. $\tilde{J}\,(>0)$ is the ferromagnetic exchange coupling between nearest-neighbor (NN) sites i and j, and $\langle ij\rangle$ denotes a summation over NN sites only. The interaction between NN spins is $-\tilde{J}(q-1)$ (if they are in the same state) or $\tilde{J}$ (if they are in different states). The random (quenched) field $\tilde{H}_i^\alpha$ favors the state $\sigma_i=\alpha$.

In this work we consider a class of random-field distribution functions which give the same probability, $1/q$, to fields along each one of the available q states, thus preserving the permutational symmetry of the q-state Potts model. The simplest representative of this class is

$$p\{\tilde{H}_i^1\tilde{H}_i^2,\ldots,\tilde{H}_i^q\}=\tfrac{1}{q}\sum_{\alpha=1}^{q}\delta(\tilde{H}_i^\alpha-\tilde{H})\prod_{\beta\neq\alpha}\delta(\tilde{H}_i^\beta)\ . \quad (2)$$

Note that (2) assumes a constant (nonrandom) value $\tilde{H}$ for the magnitude of the field $\tilde{H}_i^\alpha$. In principle, it is possible to consider a random distribution of $\tilde{H}$ as well. However, it turns out that the most important effects follow from the random "orientation" of the field. As usual, we assume no correlations among the random fields at different sites, i.e., $P\{\tilde{H}_i^\alpha\}=\prod_i p\{\tilde{H}_i^\alpha\}$.

The average free energy per spin $\bar{F}$ is given by[21]

$$\bar{F}=\langle f\{\tilde{H}_i^\alpha\}\rangle_{\rm av}/N=\frac{1}{N}\sum_{\{\tilde{H}_i^\alpha\}}P\{\tilde{H}_i^\alpha\}f\{\tilde{H}_i^\alpha\}\ ,$$

with

$$f\{\tilde{H}_i^\alpha\}=-k_BT\ln Z\{\tilde{H}_i^\alpha\}$$
$$=-(1/\beta)\ln[\mathop{\rm Tr}_{\{\sigma_i\}}\exp(-\beta\mathscr{H}\{\sigma_i,\tilde{H}_i^\alpha\})]\ . \quad (3)$$

In (3), k_B is the Boltzmann constant, T is the temperature, $\beta=1/k_BT$, $\mathscr{H}\{\sigma_i,\tilde{H}_i^\alpha\}$ is the Hamiltonian for a given configuration of the fields $\{\tilde{H}_i^\alpha\}$, and the trace is taken over all the dynamic degrees of freedom, i.e., the spins $\{\sigma_i\}$.

III. MEAN-FIELD THEORY

In the mean-field approximation one assumes that the local order parameter, $\delta_{\sigma_i,\alpha}-1/q$, acquires a nonzero average value in one of the available q states, for instance, $\langle\delta_{\sigma_i,\alpha}-1/q\rangle=Q\delta_{\alpha,1}$. In that case,

$$f\{\tilde{H}_i^\alpha\}=CN(q-1)\tilde{J}Q^2/2-(1/\beta)\sum_i\ln\{\mathop{\rm Tr}_{\{\sigma_i\}}\exp[\beta C\tilde{J}Q(q\delta_{\sigma_i,1}-1)+\beta\tilde{H}_i^\alpha(q\delta_{\sigma_i,\alpha}-1)]\}\ , \quad (4)$$

where C is the coordination number. The trace has different values for $\sigma_i=1$ and for $\sigma_i\neq1$, and one finds

$$f\{\tilde{H}_i^\alpha\}=CNJQ^2/2-(1/\beta)\sum_i\ln\left[\exp\{\beta[CJQ+\tilde{H}_i^\alpha(q\delta_{\alpha,1}-1)]\}+\sum_{\gamma=2}^{q}\exp\{\beta[-CJQ/(q-1)+\tilde{H}_i^\alpha(q\delta_{\alpha,\gamma}-1)]\}\right]\ , \quad (5)$$

where $J=(q-1)\tilde{J}$. Averaging (5) with (2) and summing over γ we obtain the mean-field average free energy,

$$\bar{F}=CJQ^2/2-G(Q,H)\ , \quad (6)$$

where $H=(q-1)\tilde{H}$ and

$$G(Q,H)=(1/q\beta)\ln\{\exp[\beta(CJQ+H)]+(q-1)\exp[-\beta(CJQ+H)/(q-1)]\}$$
$$+[(q-1)/q\beta]\ln(\exp\{\beta[CJQ-H/(q-1)]\}+\exp\{\beta[-CJQ/(q-1)+H]\}$$
$$+(q-2)\exp\{-\beta(CJQ+H)/(q-1)\})\ . \quad (7)$$

The solution $Q=0$ will have the lowest free energy for sufficiently high temperature and (random) fields. As the temperature is lowered, one finds an additional solution $Q\neq0$, with lower free energy, by minimizing $\bar{F}(Q)$ and equating the minimum to $\bar{F}(0)$.

If the transition is continuous or weakly first-order, we can find the transition point by expanding (6) in powers of Q around $Q=0$. Writing

$$\bar{F}=F_0+F_1Q+\tfrac{1}{2}rQ^2+wQ^3+uQ^4+O(Q^5)\ , \quad (8)$$

the coefficients are found to be

$$F_0=-(1/\beta)\ln[e^{\beta H}+(q-1)e^{-\beta H/(q-1)}] , \quad (9)$$

$$F_1=0 , \quad (10)$$

$$r(\tau)=(CJ/T)(T-T_c),\ \ T_c=T_c(0)(1-\tau^2),\ \ T_c(0)=CJ/k_B(q-1) , \quad (11)$$

$$w(\tau)=w(0)(1-\tau)^2(1+2\tau),\ w(0)=\beta^2C^3J^3(2-q)/6(q-1)^2 , \quad (12)$$

$$u(\tau)=u(0)(1-\tau)\{1+\tau+[6/(q^2-6q+6)][-(q^2-5q+5)\tau^2+(q^2-3q+3)\tau^3]\} , \quad (13)$$

$$u(0)=\beta^3C^4J^4(q^2-6q+6)/24(1-q)^3 ,$$

$$\tau=(e^{\beta H}-e^{-\beta H/(q-1)})/(e^{\beta H}+(q-1)e^{-\beta H/(q-1)}) , \quad (14)$$

$$\beta H\equiv x=[(q-1)/q]\ln\{[1+(q-1)\tau]/(1-\tau)\} .$$

Note that τ is a monotonically decreasing function of $x=\beta H$, i.e., $1\geq\tau\geq 0$ for $\infty\geq x\geq 0$.

Equation (10), $F_1=0$, follows directly from the permutational symmetry of (2). The fact that $w\neq 0$ for $q\neq 2$ implies that within mean-field theory the transition is always first-order.[22,23] Note that w decreases monotonically with βH, approaching zero as $\beta H\to\infty$. For $q=2$, $w=0$ and one recovers the Ising model in a random field.[21]

For $1<q<3-\sqrt{3}\simeq 1.268$ and for $q>3+\sqrt{3}\simeq 4.732$ we find that $u(0)<0$, and higher-order terms are needed for stability. This does not affect the experimentally relevant values $q=2$, 3, and 4. In addition, u decreases with increasing τ, and becomes negative for $\tau<\tau^*(q)$ [with $\tau^*(q)\simeq 0.577$, 0.542, and 0.465 for $q=2,3$ and 4, respectively].

Truncating (8) at quartic order, we indeed find a first-order transition at

$$r_p(\tau)=\frac{w^2(\tau)}{2u(\tau)} , \quad (15)$$

with the discontinuity

$$\Delta Q(\tau)=-\frac{w(\tau)}{2u(\tau)} . \quad (16)$$

The explicit dependence of r_p and of ΔQ on τ may give us an indication on the effects of the random fields. For both $q=3$ and 4, r_p first decreases with increasing τ, and then starts to increase due to the approach of $u(\tau)$ to zero at $\tau^*(q)$. One should clearly include higher-order terms in the latter regime. A similar analysis of ΔQ is even less conclusive: ΔQ increases with τ for $q=3$, and shows an initial decrease with τ for $q=4$ (turning to an increase as τ^* is approached). One can thus not make any general statements in regard to the "strength" of the first-order transition in the presence of the random fields.

In any case, it is clear from Eq. (12) that $w(\tau)$ never changes sign as function of τ. One will thus never encounter an "accidental" continuous transition in the presence of the random fields.

Similar qualitative results were found when we averaged over the *magnitude* of H, e.g., with a square or with an exponential distribution.

We now return to Eq. (7) and consider directly the low-temperature limit, $\beta\to\infty$. In this limit, Eq. (6) reduces to

$$\bar{F}=\begin{cases}CJQ^2/2-CJQ, & H<CJQ\\ CJQ^2/2-H, & H>CJQ .\end{cases} \quad (17)$$

This yields the paramagnetic phase, $Q=0$ (with $\bar{F}=-H$) for $H>CJ/2$, and a ferromagnetic phase, $Q=1$ (with $\bar{F}=-CJ/2$) for $H<CJ/2$. The transition at zero temperature is thus always strongly first-order, occurring at $H=CJ/2$.

IV. FLUCTUATIONS

In the absence of random fields, fluctuations yield nonclassical critical exponents for the Potts model below six dimensions. Similarly, $q_c^0(d)$ deviates from 2 below four dimensions. We now consider the ϵ expansions of these quantities in $6-\epsilon$ and $4-\epsilon$ dimensions, respectively. These ϵ expansions are based on diagrammatic perturbation expansions in w, u, etc. Expanding also in the random fields, the most divergent diagrams can be shown to be treelike (with a random field at the end of each branch). Repeating the arguments of Aharony *et al.*[10] and Young[12] there exists an exact mapping of each of these diagrams onto one in the nonrandom expansion, provided that d is replaced by $d-2$. One can now repeat the calculations of Priest and Lubensky[6] and find that the random-field Potts-model exponents deviate from their mean-field values below eight dimensions, with, e.g., $2\nu=1+\epsilon/7+O(\epsilon^2)$ in $d=8-\epsilon$ dimensions. One can similarly repeat all the steps used by Aharony and Pytte[8] and find that $q_c(d)=2$ for $d>6$, while $q_c(d)=2+\epsilon+O(\epsilon^2)$ in $d=6-\epsilon$ dimensions. It is not clear if one may extend these statements beyond the asymptotic regime near $d=6$. If one could, then we would be led to the conclusion that $q_c(d)=q_c^0(d-2)$. In particular, this would imply that the new lower critical dimensionality is equal to 3, and that $q_c(d)\to\infty$ as $d\to 3+$.

It is now widely believed that the shift $d\to d-2$ should not be applied for the Ising model at low dimensionalities.[14,17,18] These arguments may be directly generalized to any discrete spin model, and in particular to the q-state Potts model. At low temperatures, the random fields will break the system into domains, where in each domain the spins point along the local average field, provided $d<2$. This identification of d_l as 2 seems not to be modified even if roughening of the domain boundary is allowed for.[17] In fact, it has been suggested that $d\to d'=d-2+\eta(d')$, rather than $d\to d-2$.[10,24] This yields

$d_l=2$ and leads to the line $q_c(d)=q_c^0(d')$ shown in Fig. 1. Even if all of these detailed quantitative statements are not fully justified, we believe that the line $q_c(d)$ will be similar to that drawn in Fig. 1. In particular, $q_c(d)$ should approach infinity at d_l (equal to 2), and 2 at $d=6$. Any reasonable interpolation between these two limits will imply that $q=3$ and probably $q=4$ are below $q_c(3)$, so that the transitions in these cases may turn second-order by the application of random fields.

It should be noted that the fact that $3<q_c(3)$ does not necessarily mean that the transition of the random-field three-state Potts model is continuous. Rather, the transition may become continuous for some range of values of the random field.

V. EXPERIMENTAL REALIZATIONS AND CONCLUSIONS

Our first conclusion is that random fields should destroy long-range order for all Potts models in two dimensions. There exist many realizations of these models for adsorbed layers,[25] and random fields are easily generated on them by, e.g., randomizing the substrate and thus creating random local chemical potentials. Experiments (real or computer) can be made to verify the disappearance of long-range order.

Regarding three dimensions, the most interesting case seems to be $q=3$, since $q_c^0(3)<3<q_c(3)$. The application of a random field is expected to turn the first-order transition into a continuous one via a tricritical point. One experimental realization of this model occurs in $SrTiO_3$, when it is stressed along [111].[26] The coupling to strain degrees of freedom involves terms in the Hamiltonian of the form $\sum_{\alpha,\beta}A_{ij}^{\alpha\beta}Q_i^\alpha Q_j^\beta$, where $\vec{Q}$ is the three-component antiferrodistortive order parameter. Impurities will generate local random strains, i.e., random values of $A_{ij}^{\alpha\beta}$, with $[A_{ij}^{\alpha\beta}]_{av}=0$. Under [111] stress one has ordering of the [111] component of $\vec{Q}$, $\langle Q_{[111]}\rangle$, generating a three-state Potts term in the two components perpendicular to it, $\langle Q_{[111]}\rangle[(Q^1)^3-3Q^1(Q^2)^2]$. The random $A_{ij}^{\alpha\beta}$'s will then generate random linear terms of the form $\tilde{A}^i\langle Q_{[111]}\rangle Q^i$, $i=1,2$, which act as random fields. An increase in the concentration of the impurities, or an increase in the [111] stress (and therefore in $\langle Q_{[111]}\rangle$), may then turn the transition at which Q^1 and Q^2 order into a continuous one.

The mixed antiferromagnet $Fe_{1-x}Co_xCl_2$ (Ref. 27) provides another possible realization of $q=3,d=3$. The Hamiltonian describing the magnetic transitions includes terms of the form $wS_i^zS_i^x[(S_i^x)^2-3(S_i^y)^2]$, where $\vec{S}_i$ is the three-component staggered magnetization. Moreover, the impurities generate[28] random anisotropy terms, e.g., $A_{ij}S_i^zS_j^x$, with $[A_{ij}]_{av}=0$. Again, ordering of S^z generates a $(q=3)$-state Potts model in a random field.

It has recently been suggested[29] that phase transitions induced by a uniform magnetic field directed along [111] in certain type-I fcc antiferromagnets (such as NdSb, NdAs, CeAs, and others) provide a physical realization of the $(q=4)$-state Potts model in $d=3$ dimensions. By diluting these antiferromagnets in the presence of the uniform field it may be possible to generate random fields.[30] Assuming that $q_c(3)>4$ (Fig. 1), then increasing the strength of the uniform field will probably change the order of the transition from first-order to continuous.

We expect that similar effects should occur in any system which undergoes a first-order transition in three dimensions and a continuous one in lower dimensions. The strong random-field fluctuations, which cause an effective reduction in the dimensionality of the system, should induce the crossover from first-order to continuous transitions predicted in this work.

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