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Exact Results for a Dilute Potts Model

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Exact results are obtained for the annealed, dilute, q-component Potts model on the decorated square lattice. The phase diagram is found to consist of a high-temperature region, a low-temperature region, and a two-phase region in between which arises only for $q > 4$; exact expressions for the phase boundary and the critical probability are derived. At the critical point the specific heat is generally finite and has a cusp; the slope of the cusp is finite for $q = 4$ and infinite (vertical) for $q = 2$ and 3.

KEY WORDS: Dilute Potts model; phase diagram; critical probability; specific heat.

1. INTRODUCTION

Recently there has been considerable theoretical interest in the problem of the random Potts model, a statistical mechanical model in which the sites of a lattice are occupied at random by atoms interacting with Potts interactions. As in any disordered system, this randomness can be either quenched or annealed. In a quenched system, which is mathematically more difficult to deal with, the atoms are frozen in position, while in an annealed system the atoms are in thermal equilibrium with the surroundings. The latter fact makes the annealed system more tractable to analysis.

The annealed model is also of interest in its own right, for it is related to other problems of physical interest. Murata[1] has shown that the dilute Potts model leads to a Hamiltonian formulation of the problem of site percolation in a lattice gas. The statistical mechanical model of polymer gelation proposed by Coniglio *et al.*[2] can also be considered in a similar fashion.

The annealed random Potts model has been considered by Niehuis *et al.*[3] using the renormalization group. More recently, Turban[4] studied a

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related problem of quenched bond disorder in the Potts model under an "effective interaction approximation." Both of these studies are approximate in nature. In this paper we consider an annealed random Potts model for which exact results can be obtained. We derive, in particular, its exact phase diagram and the behavior of the specific heat near the critical point.

The model is defined in Section 2. We show in Section 3 that this random model is reducible to a regular Potts model. From this equivalence we obtain in Section 4 its exact phase diagram. The critical behavior of the specific heat and other properties of this model are discussed in Section 5.

2. MODEL DESCRIPTION

Consider the decorated square lattice shown in Fig. 1, constructed by inserting decorating sites into the bonds of a square lattice. To distinguish the decorating sites from those on the original lattice, we shall denote the inserted sites by the index α and the original square lattice sites by the index i. Consider next a lattice gas on this decorated lattice subject to the condition that (i) all sites i are occupied by atoms, and (ii) the sites α can be either occupied or empty. Two atoms occupying nearest neighboring sites interact with a Potts interaction.

As in a lattice gas, the Hamiltonian $\mathscr{H}$ takes the form

$$-\mathscr{H}/kT = K \sum_{(i,\alpha)} t_\alpha \delta_{i\alpha} + \Delta \sum_\alpha t_\alpha \tag{1}$$

Here T is the temperature; $t_\alpha = 0, 1$ is a random variable associated with the site α; Δ is the chemical potential of each occupied site; and the first summation in (1) is taken over all nearest neighbors. Also

$$\delta_{i\alpha} = \delta(\lambda_i, \lambda_\alpha) \tag{2}$$

where $\lambda_i, \lambda_\alpha = 1, 2, \ldots, q$ specify the Potts states. For simplicity we shall assume $q \geqslant 1$. The system is ferromagnetic (antiferromagnetic) for K positive (negative).

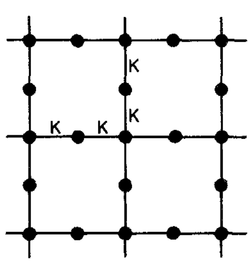

Fig. 1. The decorated square lattice.

For $q = 2$ this model reduces to the model of dilute ferromagnetism introduced by Syozi.[5,6] As we shall see, the generalization to general q leads to new features not found in the dilute Ising system.

The grand partition function of the present model takes the form

$$\Xi(\Delta, K) = \sum_{t_\alpha = 0,1} \sum_{\lambda_i = 1}^{q} \sum_{\lambda_\alpha = 1}^{q} e^{-\mathscr{H}/kT} \tag{3}$$

where it is understood that the summation over the q states of λ_α arises only for $t_\alpha = 1$, namely when the site α is occupied. Since the physical variable that actually enters the picture is p, the fraction, or concentration, of the occupied decorating sites, the chemical potential Δ is to be eliminated through the relation

$$p = \frac{\partial}{\partial \Delta} z(\Delta, K) \tag{4}$$

where

$$z(\Delta, K) = \lim_{N \to \infty} (2N)^{-1} \ln \Xi(\Delta, K) \tag{5}$$

N being the number of sites of the square lattice. Similarly, the energy per decorating site is

$$U(p, K) = -\frac{\partial}{\partial K} z(\Delta, K) \tag{6}$$

where $\Delta = \Delta(p, K)$ obtained from (4) is to be substituted *after* the differentiation. The phase boundary is now defined to be the surface in the (p, q, T) space on which $U(p, K)$ becomes singular in K. Finally, the temperature derivative of $U(p, K)$ at constant p yields the specific heat

$$c(p, K) = -\frac{K}{T} \frac{\partial}{\partial K} U(p, K) \tag{7}$$

3. REDUCTION TO A REGULAR POTTS MODEL

Analysis of the random model (1) relies on the fact that the decorated bonds together with the decorating sites α can be replaced by equivalent single Potts interactions. This equivalence is given in Fig. 2, which shows a decorated bond replaced by a single interaction of strength K^*. Writing

$$A \exp(K^* \delta_{ij}) = 1 + \sum_{\lambda_\alpha = 1}^{q} \exp[K(\delta_{i\alpha} + \delta_{j\alpha}) + \Delta] \tag{8}$$

Fig. 2. Equivalence of a decorated bond with a single interaction of strength K^*.

we obtain the following relation valid for a periodic lattice:

$$\Xi(\Delta, K) = [A(\Delta, K)]^{2N} Z(K^*) \tag{9}$$

where $Z(K^*)$ is the partition function of a Potts model on the square lattice whose Hamiltonian is $-\mathscr{H}/kT = K^* \sum_{ij} \delta_{ij}$. Explicitly from (8), we have

$$A(\Delta, K) = 1 + e^{\Delta}(e^{2K} + q - 2) \tag{10}$$

$$e^{K^*} = \frac{1 + e^{\Delta}(e^{2K} + q - 1)}{1 + e^{\Delta}(2e^{K} + q - 2)} \geqslant 1 \tag{11}$$

Note that (11) implies K^* ferromagnetic for all K. The concentration of the occupied decorating sites given by (4) now takes the form

$$p = \frac{2e^K + q - 2}{e^{-\Delta} + 2e^K + q - 2}[1 - E(K^*)] + \frac{e^{2K} + q - 1}{e^{-\Delta} + e^{2K} + q - 1} E(K^*) \tag{12}$$

where

$$E(K^*) = \lim_{N\to\infty} (2N)^{-1} \frac{\partial}{\partial K^*} \ln Z(K^*) \tag{13}$$

Finally, eliminating Δ between (11) and (12), we obtain

$$\frac{v^2}{2v + q} = \frac{v^*[1 + v^{*-1} - E(v^*)]}{p(1 + v^{*-1}) - E(v^*)} \tag{14}$$

where we have introduced the convenient variables $v = e^K - 1$, $v^* = e^{K^*} - 1$. Equation (14) is the key expression which relates v^* to v. Also, by combining (6) and (9) with (11), we obtain the following explicit expression for the energy:

$$U(p, K) = \frac{2(1 + v)v^*}{v^2 - qv^*} + E(v^*)\frac{v(1 + v)v^*(v^2 - vv^* - qv^*)}{(v^2 - qv^*)(v^2 - qv^* + v^2v^*)} \tag{15}$$

where, again, $v^* = v^*(p, K)$ is to be obtained from (14).

4. EXACT PHASE DIAGRAM

We are now in a position to derive the exact phase diagram for the decorated system. We observe from (15) that the phase boundary in the (p, q, T), or (p, q, K^{-1}), space is the trajectory along which either v^* or $E(v^*)$ is nonanalytic in v. Now $v^*(v)$ obtained from (14) also implicitly contains $E(v^*)$. Hence we need only to focus on the function $E(v^*)$.

It has been established that, for $v^* \geqslant 0$ and $q \geqslant 1$ at least, $E(v^*)$ has a unique singularity at $v = \sqrt{q}$.[7,8] It follows from (14) that the phase boundary is

$$\frac{v_c^2}{2v_c + q} = \frac{\sqrt{q}(1 + q^{-1/2} - E_c)}{p(1 + q^{-1/2}) - E_c} \tag{16}$$

where $E_c = E(\sqrt{q})$. Other established properties of $E(v^*)$ are the following[9]:

For $q \leqslant 4$, $E(v^*)$ is continuous at $v^* = \sqrt{q}$ with the critical value

$$E_c = \tfrac{1}{2}(1 + q^{-1/2}) \tag{17}$$

For $q \geqslant 4$, $E(v^*)$ has a jump discontinuity at $v^* = \sqrt{\mathrm{q}}$ with the limiting values

$$E_c = E(\sqrt{q}\pm) = \tfrac{1}{2}(1 + q^{-1/2})[1 \pm \Delta(q)] \tag{18}$$

where

$$\Delta(q) = \tanh(\tfrac{1}{2}\theta) \prod_{n=1}^{\infty} (\tanh n\theta)^2 \tag{19}$$

$$2 \cosh \theta = \sqrt{q} \tag{20}$$

Equation (16) in conjunction with (17) and (18) now determines the exact phase diagram for the decorated system. We consider the ferromagnetic and antiferromagnetic cases separately.

4.1. Ferromagnetic Interactions

For $K > 0$ or $v_c > 0$, the left-hand side of (16) is always positive. Also, $E(v^*) \leqslant 1$; hence the phase boundary extends only to the region

$$p(1 + q^{-1/2}) \geqslant E_c \tag{21}$$

Using the values of E_c given by (17) and (18), we obtain the following critical probability:

$$\begin{aligned} p_c(q) &= \tfrac{1}{2}, & q \leqslant 4 \\ &= \tfrac{1}{2}[1 - \Delta(q)], & q \geqslant 4 \end{aligned} \tag{22}$$

The critical probability has the meaning that there is no transition for $p < p_c(q)$. Note that the critical probability happens to coincide with the threshold probability of bond percolation[10] for all $q \leqslant 4$, a property unique to the square lattice.

For $q \leqslant 4$, the critical condition (16) assumes the explicit expression

$$e^{K_c} = 1 + \frac{\sqrt{q}}{2p - 1}\{1 + [1 + \sqrt{q}(2p - 1)]^{1/2}\} \tag{23}$$

which for $q = 2$ reduces to

$$\cosh K_c = 1 + \sqrt{q}/(2p - 1) \tag{24}$$

This is the established result for the dilute Ising model.[5,6] For $q > 4$, the critical surface splits into two branches when the two values of E_c in (18) are substituted into (16). The two branches coalesce at $p = 1$, however.

The phase diagram of the ferromagnetic decorated model is constructed in Fig. 3. It is seen that the phase space is divided into three regions: a low-temperature region containing the q axis in which the system is in an ordered phase, a high-temperature region in which the system is disordered, and a two-phase region which arises only for $q > 4$. The two-phase region increases in size with q, and eventually prevails for all $p < 1$ in the $q \to \infty$ limit. This phase diagram is very similar to that of the *quenched* dilute Potts model obtained under the effective interaction approximation.[4] The intercepts of the phase boundary in Fig. 3 are the following:

$$p = \tfrac{1}{2}, \qquad q \leqslant 4, \quad T = 0$$

$$= \tfrac{1}{2}[1 \pm \Delta(q)], \qquad q \geqslant 4, \quad T = 0 \tag{25}$$

$$e^{K_c} = (2p)^{1/2}/[(2p)^{1/2} - 1], \qquad q = 1 \tag{26}$$

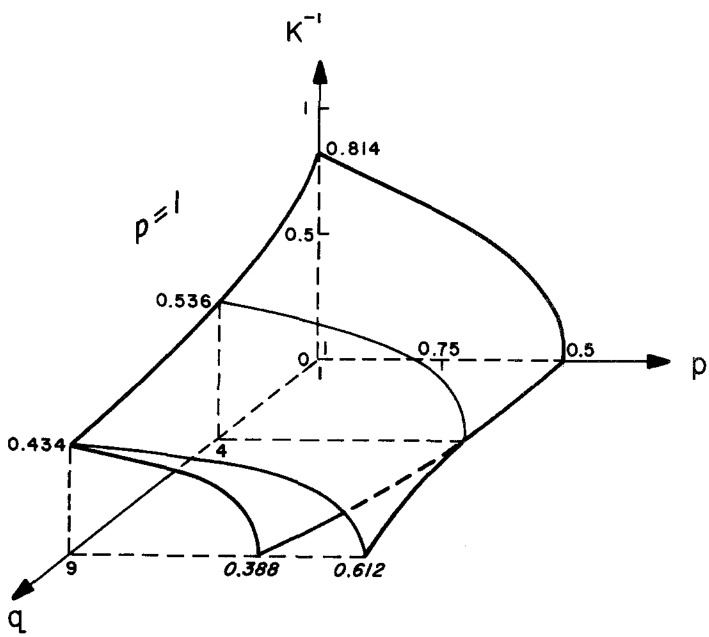

Fig. 3. Exact phase diagram for ferromagnetic ($K > 0$) interactions. A two-phase region arises for $q > 4$.

$$e^{K_c} = 1 + \sqrt{q} + \sqrt{q}(1 + \sqrt{q})^{1/2}, \qquad p = 1 \tag{27}$$

4.2. Antiferromagnetic Interactions

For $K < 0$ or $-1 \leqslant v_c \leqslant 0$, it can be seen that the two sides of (16) can never be made equal for $q \geqslant 4$. Hence there is no transition for $q \geqslant 4$.

For $q < 4$, (16) can be written more explicitly as

$$e^{-|K_c|} = 1 + \frac{\sqrt{q}}{2p - 1}\{1 - [1 + \sqrt{q}(2p - 1)]^{1/2}\} \tag{28}$$

Note that the right-hand side of (28) does not diverge at $p = 1/2$. The critical surface represented by (28) is constructed in Fig. 4. The phase space is divided into a low-temperature (ordered) region containing the origin and a high-temperature (disordered) region. We also find the following expression for the critical probability:

$$p_c(q) = \tfrac{1}{2}[1 + \sqrt{q}(q - 2)], \qquad q < \tfrac{1}{2}(3 + \sqrt{5}) = 2.618 \tag{29}$$

As a consequence, the antiferromagnetic model has a phase transition only for $q = 2$. This result is consistent with our expectation, since for $q \geqslant 3$ the ground state of the decorated model has a nonzero entropy. We also note that, for $q = 2$, the critical temperature (28) coincides with that of the ferromagnetic

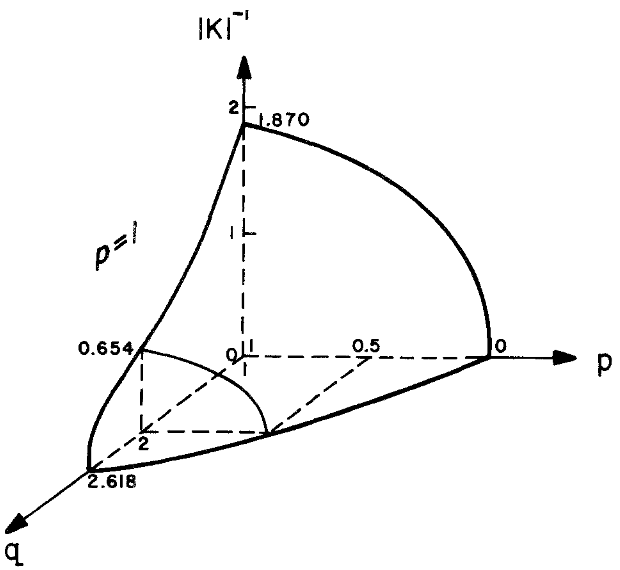

Fig. 4. Exact phase diagram for antiferromagnetic ($K < 0$) interactions.

model. This is again consistent with our expectation, for the $q = 2$ Ising model is invariant under the change of $K \to -K$. The intercepts in Fig. 4 are

$$e^{-|K_c|} = (2p)^{1/2}/[(2p)^{1/2} + 1], \qquad q = 1 \tag{30}$$

$$e^{-|K_c|} = 1 + \sqrt{q} - \sqrt{q}(1 + \sqrt{q})^{1/2}, \qquad p = 1 \tag{31}$$

Finally, we remark that it is also possible to construct for both $K > 0$ and $K < 0$ the (p, q, Δ) phase diagram. The phase boundary is obtained directly from (11) as

$$\frac{1 + e^{\Delta}(e^{2K_c} + q - 1)}{1 + e^{\Delta}(2e^{K_c} + q - 2)} = \sqrt{q} - 1 \tag{32}$$

and the construction confirms the general correctness of the phase diagram obtained from the renormalization-group consideration.[3]

5. OTHER PROPERTIES AND DISCUSSIONS

The specific heat of the decorated dilute model is computed by substituting (15) into (7) and using (14) to relate v^* to v. The most direct way to see this latter relation is to expand (14) about the critical point $v = v_c$ and $v^* = \sqrt{q}$. Using the fact that

$$E(v^*) - E(\sqrt{q}) \sim (v^* - \sqrt{q})^{1-\alpha'}, \qquad T \approx T_{c-} \tag{33}$$

where $\alpha' < 1$ is the temperature exponent of the regular Potts model, we obtain the desired relation

$$(v^* - \sqrt{q})^{1-\alpha'} \sim v - v_c \tag{34}$$

for $0 \leqslant \alpha' < 1$. The expressions (33) and (34) now dictate that $\partial E(v^*)/\partial v$ is finite at the critical point, even though $E'(\sqrt{q})$ may diverge. It follows that the specific heat $c(p, K)$ will generally be finite at $K = K_c$. Detailed calculation shows explicitly that

$$c(p, K_c) \sim (2p - 1)/(1 - p), \qquad q \leqslant 4 \tag{35}$$

whence the specific heat diverges only for $p = 1$.

To study the behavior of $c(p, K)$ near K_c, it is again most convenient to directly expand (14) and (15). However, it is necessary here to keep the two leading terms in the expansions. As a result, we find after taking a temperature derivative,

$$\begin{aligned} c(p, K) = {} & c(p, K_c) + A(v - v_c) \\ & + B(v - v_c)^{\alpha'/(1-\alpha')} + C(v - v_c)^{1/(1-\alpha')} + \cdots, \qquad T \approx T_{c-} \end{aligned} \tag{36}$$

where A, B, and C are constants. A similar expression holds with α in place of α' for $T \approx T_c+$.

For $1/2 < \alpha' \leqslant 1$ the leading term in (36) is linear in $v - v_c$ and the specific heat has a cusp with finite slope at T_c. For $0 \leqslant \alpha' \leqslant 1/2$, however, the leading term is $(v - v_c)^{\alpha'/(1-\alpha')}$ and the specific heat cusp has an infinite slope at T_c. The occurrence of this infinite slope has been confirmed in the case of the dilute Ising model ($q = 2$), for which $\alpha = \alpha' = 0$.[6] We remark that, in a similar analysis of the specific heat for the dilute Ising model, Essam and Garelick[11,12] have reached essentially the expression (36), but with the omission of the term linear in $v - v_c$. This omission results in an incorrect prediction for $1/2 < \alpha' \leqslant 1$.

Using the conjectured value[13] of

$$\alpha = \alpha' = \frac{2}{3}\left[1 + \frac{2}{\pi}\cos^{-1}\left(\frac{\sqrt{q}}{2} - \frac{1}{2}\right)^{-1}\right], \qquad q \leqslant 4 \tag{37}$$

or $\alpha = \alpha' = 1/3$ for $q = 3$ and $\alpha = \alpha' = 2/3$ for $q = 4$, we see that the cusp in the specific heat has a finite slope for $q = 4$ and an infinite slope for $q = 2$ and 3.

To discuss the magnetic properties of the dilute model it is necessary to include an external field in the Hamiltonian(1). Unfortunately, the transformation (8) does not go through for $q \geqslant 3$. One possible remedy of this difficulty is to include two external fields. Further assuming that the magnetic exponents for these two fields are identical, one then obtains the renormalized exponents $\beta_d = \beta/(1 - \alpha')$, $\gamma_d = \gamma/(1 - \alpha')$, etc., where β_d and γ_d are the magnetic exponents for the decorated lattice. For the $q = 3$ models, for example, the best estimation[14] of $\beta = 1/9$ leads to the value $\beta_d = 1/6$ for the decorated dilute system.

Finally, we mention that analyses can also be carried out for the decorated models on the triangular and honeycomb lattices. Using the exact critical properties of the regular Potts model on these lattices,[15] similar exact results can be derived. Again, one finds a two-phase region in the phase diagram for $q > 4$. The critical probability $p_c(q)$ is found to be q dependent for all q.

To summarize, we have obtained the exact phase diagram for the decorated dilute Potts model on a square lattice. The phase boundary (16)–(18) leads to the exact transition temperatures as well as the exact critical probability $p_c(q)$. One novel feature of this dilute model is the existence of a two-phase region for $q > 4$. The specific heat is generally finite and has a cusp at the critical point. The slope of the cusp is finite for $q = 4$ and infinite for $q = 2$ and 3.

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