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Critical point of a triangular Potts model with two- and three-site interactions†

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Received 2 June 1980, in final form 29 September 1980

Abstract. The q -state Potts model on the triangular lattice with nearest-neighbour interactions and three-site interactions in half of the triangular faces is considered. The exact duality relation is re-examined from the point of view of determining its critical point. Using the continuity and uniqueness arguments we determine the exact critical point in the ferromagnetic model. It is argued that a transition exists in an antiferromagnetic model only for $q=3$. A conjecture is then made on the phase diagram for the $q=3$ isotropic model. These results are used to determine the exact criticality of a dilute Potts model on the honeycomb lattice.

1. Introduction

The q -state Potts model on the triangular lattice has been of considerable recent interest. The model with nearest-neighbour ferromagnetic interactions is known to possess a unique transition (Baxter *et al* 1978, Hintermann *et al* 1978) similar to that of the square lattice (Baxter 1973). The $q=3$ model is of further importance because of its possible realisation in the adsorption of krypton atoms on graphite (Berker *et al* 1978), and because of the expected ordering at low temperatures for antiferromagnetic interactions.

As suggested by the lattice symmetry, investigation of the triangular Potts model is often facilitated by the inclusion of three-site interactions. Schick and Griffiths (1977) have carried out a renormalisation group analysis in this enlarged parameter space, which leads to a qualitative understanding of the $q=3$ ferromagnetic and antiferromagnetic transitions. Quantitative analysis of this model, especially for general q , appears to be difficult, and has been lacking up to now.

A model which differs slightly from that considered by Schick and Griffiths (1977) is one in which the three-site interactions are present in half of the triangular faces. This model is unique in that it possesses an exact duality relation (Baxter *et al* 1978, Wu and Lin 1980). However, the implications of this duality relation appear not to have been explored in detail. In particular, its relationship with the determination of the transition point has not been satisfactorily discussed. We consider this problem here. We shall re-examine the implications of the duality relation, making clear the necessary assumptions in determining the Potts critical point.

† Supported in part by National Science Foundation grant no DMR 78-18808.

2. Formulation

Consider a q -state Potts model on a triangular lattice of N sites with two-site interactions ϵ_1, ϵ_2 and ϵ_3 (in the respective directions), and three-site interaction ϵ surrounding every up-pointing (triangular) face. A drawing of the lattice can be found in figure 5 of Wu and Lin (1980). The Hamiltonian now reads

$$\mathcal{H} = \sum_{\Delta} E_{abc} \tag{1}$$

where the summation is taken over all up-pointing faces and

$$E_{abc} = -(\epsilon_1 \delta_{bc} + \epsilon_2 \delta_{ca} + \epsilon_3 \delta_{ab} + \epsilon \delta_{abc}). \tag{2}$$

Here a, b, c are the three sites surrounding an up-pointing triangle, $\delta_{ab} = \delta_{K_r}(\xi_a, \xi_b)$, $\delta_{abc} = \delta_{ab} \delta_{bc}$ and $\xi_a = 1, 2, \dots, q$ refers to the spin states at site a . For $q = 2$ this model is isomorphic to an Ising model (Wu and Lin 1980) and is exactly soluble. We shall therefore focus our attention on $q \geq 3$.

It has been shown both algebraically (Baxter *et al* 1978) and graphically (Wu and Lin 1980) that the partition function Z of the model (1) satisfies the following duality relation:

$$Z(q; f_1, f_2, f_3, y) = (y/q)^N Z(q; f'_1, f'_2, f'_3, y') \tag{3}$$

$$f'_i = qf_i/y, \quad y' = q^2/y \tag{4}$$

$$f_i = \exp(\beta \epsilon_i) - 1$$

$$y = \exp[\beta(\epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3)] - (f_1 + f_2 + f_3 + 1) \tag{5}$$

and $\beta = 1/kT$. The duality relation (3) and (4) maps, for all q , the partition function onto itself along the paths[†]

$$f_i^2/y = C_i; \quad C_i = \text{constants} \tag{6}$$

in the four-dimensional (f_i, y) space (the ω space). The sections $|y| \geq q$ of the path (6) map onto each other, while the sign of f_i remains unchanged for $y > 0$ and reverses for $y < 0$. It is then clear that the fixed points of the transformation (4) are the hyperplane

$$y = q, \quad \text{for } y > 0 \tag{7}$$

and the point

$$y = -q, \quad f_i = 0, \quad \text{for } y < 0. \tag{8}$$

It was conjectured (Baxter *et al* 1978, Wu and Lin 1980) that, if a unique transition exists in the Potts model (1), it occurs at (7). The conjecture is certainly verified by the exact $q = 2$ (Ising) and the $\epsilon = 0, \epsilon_i > 0$ (Hintermann *et al* 1978) critical points. However, since the self-dual path (6) does not describe a Potts model with fixed interactions, the validity of the above argument is at best dubious. We now examine the situation more closely.

It is convenient to regard f_i and y as the variables at this point and consider the per-site free energy $F(q; f_1, f_2, f_3, y)$. Besides an additive term which is analytic, F is again invariant under the transformation (4). Generally, the free energy F will be

[†] The duality relation also maps the partition function onto itself along the q -dependent paths $af_i^n = y^n + q^n$ for all real a and n .

singular along some ‘critical’ trajectory Σ in the ω space. We now postulate the continuity assumption:

The critical trajectory Σ in the ω space is continuous.

The assumption that the singularities of a thermodynamic free energy lie on a continuous locus in the parameter space appears to have been stated clearly first by Thibaudier and Villain (1972). In the present model this assumption is reasonable in view of the explicit expressions (5) of the variables f_i and y .

In a given model (1) with fixed ϵ_i and ϵ , and as the temperature rises from 0 to ∞ , the variables f_i and y as given by (5) trace a continuous thermodynamic path Γ in the (f_i, y) space. If the path Γ happens to intersect Σ , we say that a transition occurs in this Potts model at the point(s) of intersection. There is no transition if Γ does not intersect Σ .

To proceed further, we now examine the locus of Γ more closely. For this purpose it is convenient to name the $q \geq 3$ model according to its ground-state configuration.

The ground state can be the repetition of any one of the five configurations (around an up-pointing triangle) shown in figure 1. Specifically the system is

(a) ferromagnetic if

$$\epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3 < \{0, \epsilon_i\} \tag{9}$$

(b) antiferromagnetic if

$$0 > \{\epsilon_i, \epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3\} \tag{10}$$

(c) paramagnetic if

$$\epsilon_i < \{0, \epsilon_i, \epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3\}. \tag{11}$$

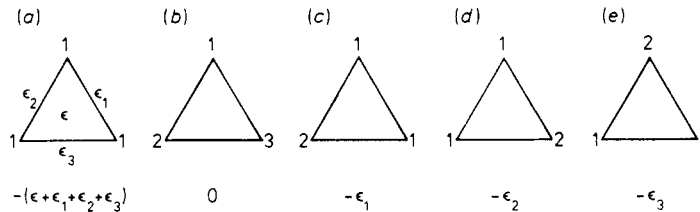


Figure 1. The five possible ground state spin arrangements with the associated energies: (a) Ferromagnetic. (b) Antiferromagnetic. (c)–(e) Paramagnetic.

As the temperature is lowered from ∞ , the thermodynamic path Γ starts out from the origin initially tangent to the vector (ϵ_i, ϵ) in ω space. The subsequent behaviour of Γ depends on the nature of the ground state:

(a) Ferromagnetic. Γ eventually reaches, as $\beta \rightarrow \infty$, the hyperplane $y = \infty$. It is easily verified that, for $y \geq 2$ at least, y is a monotonically increasing function of β .

(b) Antiferromagnetic. Γ starts out from the origin and terminates at the point $(f_i, y) = (-1, 2)$.

(c) Paramagnetic. Γ starts out from the origin and reaches, as $T \rightarrow 0$, $f_i \sim -y_i = \infty$. Note that the paths Γ do not intersect, and that every point in the physical region of real ϵ_i and ϵ , or

$$f_i \geq -1, y + f_1 + f_2 + f_3 \geq -1, \tag{12}$$

is traversed by one and only one Γ .

With these considerations, we can divide ω space into four regions:

(a) Ferromagnetic region:

$$\begin{aligned} y + f_j + f_k &\geq 0 && \text{for } f_i \geq \{0, f_j, f_k\} \\ y + f_1 + f_2 + f_3 &\geq 0 && \forall f_i \leq 0 \end{aligned} \quad (13)$$

(b) Antiferromagnetic region:

$$\begin{aligned} -1 &\leq y + f_1 + f_2 + f_3 \leq 0 \\ -1 &\leq f_i \leq 0 \end{aligned} \quad (14)$$

(c) Paramagnetic region:

$$\begin{aligned} f_i &\geq 0 && i \neq j, k \\ -(f_i + 1) &\leq y + f_j + f_k \leq 0 \end{aligned} \quad (15)$$

(d) Unphysical region: complement of the above three.

The different regions for isotropic interactions $f_1 = f_2 = f_3 = f$ are shown in figure 2.

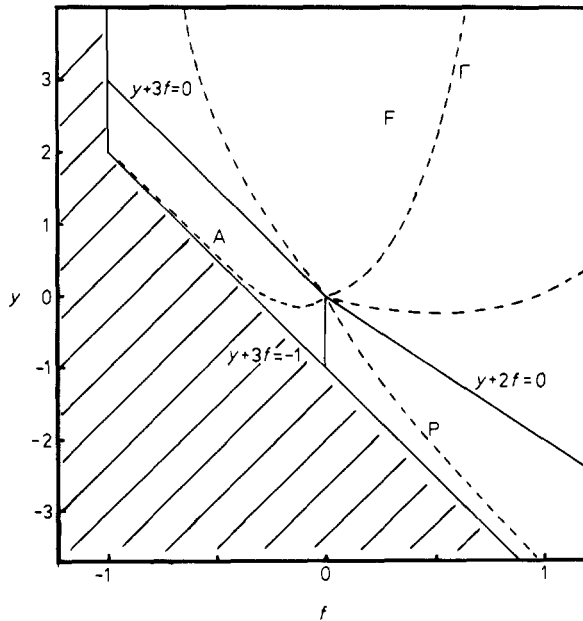


Figure 2. Regions in ω space for the $q \geq 3$ isotropic model. The ferromagnetic (F), antiferromagnetic (A) and paramagnetic (P) regions are described by (13)–(15). The shaded region is unphysical. Broken curves are examples of thermodynamic paths Γ .

3. Ferromagnetic model

For interactions subject to condition (9) favouring a ferromagnetic ground state, we expect a transition to exist, and shall assume that the transition is unique. We now proceed to show that, with our assumptions, the critical surface Σ is indeed the hyperplane (7) or $y = q$.

First, due to the monotonic nature of y (for $y > 2$) in β , Γ intersects $y = q$ only once. Now, the proof follows essentially from the continuity and uniqueness assumptions. To make the situation clearer, however, we start from the known result of $\epsilon = 0$ (Hintermann *et al* 1978) that this particular Γ intersects Σ at $y = q$. Consider now the model with an infinitesimal but non-zero ϵ . The two assumptions quoted above now dictate that the new Γ would again intersect Σ at $y = q$. Continuing in this fashion by varying ϵ , we eventually reach all points in $y = q$ in the physical region, and establish $y = q$ to be the only critical surface in the entire ferromagnetic region (13). It follows that, in a given Potts model of fixed ϵ_i and ϵ subject to (9), a transition occurs at the conjectured point of $y = q$.

4. Antiferromagnetic and paramagnetic models

The duality relation (4) generally maps the antiferromagnetic and paramagnetic regions (14) and (15) into unphysical regions outside (12) and is therefore not very useful for extracting information. However, we do know that, for $q \geq 4$, the antiferromagnetic ground state (figure (1b)) has a non-zero entropy. Argument can then be made as in Wannier (1950) that the states of *different* long-range orders can be mixed such that a fixed long-range order is no longer energetically favourable. Consequently, we expect no transition to occur[†]. For the $q = 3$ antiferromagnetic model, however, the ground state is six-fold degenerate. It is then expected that a critical temperature exists such that below it there is a long-range ordering.

The situation with the paramagnetic model is the following: In the isotropic model ($\epsilon_1 = \epsilon_2 = \epsilon_3$) the ground state has a non-zero entropy (valid for all $q \geq 2$). As argued above, this fact alone is sufficient to rule out the occurrence of a transition. But the ground state degeneracy in the anisotropic model is of the order of $(q - 1)^{N^{1/2}}$. It is conceivable that one (or more) transitions may exist for $q \geq 3$.

5. Isotropic model

We now consider the isotropic model $\epsilon_1 = \epsilon_2 = \epsilon_3$ for which definite conclusions can be drawn. For $q \geq 4$, our discussion has led to the conclusion that a transition exists only in the ferromagnetic model. This has the consequence that $y = q$ is the only critical trajectory Σ in the physical region (12). For $q = 3$, however, both the ferromagnetic and antiferromagnetic models are expected to order at low temperatures; an additional branch of Σ will appear in the antiferromagnetic region.

For the $q = 3$ isotropic model we have seen that the critical trajectory Σ is $y = 3$ in the ferromagnetic region, and does not extend into the paramagnetic region. To determine the trajectory of the branch of Σ in the antiferromagnetic region, we argue that it must pass through the two points $(f, y) = (-1, 2)$ and $(0, -1)$. To see this, write the energies of an antiferromagnetic model as

$$-\Delta \equiv \epsilon + 3\epsilon_1 < 0, \quad \epsilon_1 < 0 \quad (16)$$

for which the thermodynamic path Γ is a curve connecting $(0, 0)$ and $(-1, 2)$. However,

[†] Berker and Kadanoff (1980) have recently suggested the existence of an algebraic order in a state of non-zero entropy. We shall not consider such possibilities.

for $\Delta \equiv 0$, Γ becomes the line segment connecting $(0, 0)$ and $(-1, 3)$, while for $\epsilon_1 \equiv 0$, Γ is the segment of y axis between $(0, 0)$ and $(0, -1)$. Now there is no transition when either $\Delta = 0$ or $\epsilon_1 = 0$. For small Δ or ϵ_1 we argue that kT_c , while small, is still 'large' such that $\Delta/kT_c(\Delta) \rightarrow 0$ or $\epsilon_1/T_c(\epsilon_1) \rightarrow 0$. This appears to be a generally valid statement when one of the two or more interactions is vanishingly small, and is verified by the known critical points of the Ising model and the Baxter model. In the present model this implies that Σ is continuous in the limits $\Delta \rightarrow 0^+$ and $\epsilon_1 \rightarrow 0^-$. It follows that Σ must pass through the two points $(-1, 2)$ and $(0, -1)$. A schematic plot of this branch of Σ is now shown in figure 3. Note that the duality relation (4) maps this locus outside the physical region. A consequence of our conjectured Σ is that a unique transition exists in *all* isotropic $q = 3$ antiferromagnetic models.

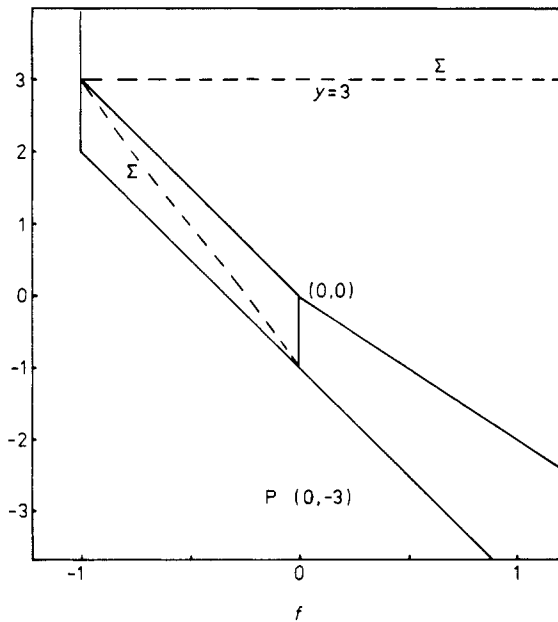


Figure 3. Critical trajectory Σ (the broken lines) in the $q = 3$ isotropic model. The line $y = 3$ and the point P at $(0, -3)$ are the fixed points.

6. Dilute Potts model on the honeycomb lattice

Results of this paper can be used to determine the exact critical point of a dilute Potts model on the honeycomb lattice.

In a dilute Potts model the sites of a regular lattice can be either occupied by atoms or be vacant, with two atoms occupying neighbouring sites interacting with a Potts interaction $-E\delta_{ij}$. While not much is known about this dilute model in its most general form, the critical point has been determined for a decorated lattice where the annealed vacancies are confined to the decorating sites (Wu 1980). To remove the more stringent restriction of decorating vacancies, we now consider a honeycomb lattice for which vacancies can occur on one of the two sublattices. The situation is shown in figure 4.

We consider again an annealed model and attach a fugacity z to each vacancy. Summing over the sites (black circles) where vacancies may occur, we find the resultant

to be precisely the isotropic model discussed in the previous section. This equivalence is shown in figure 5. The relations between $(\beta E, z)$ and (f, y) are

$$f = v^2(3v + q + z)^{-1}, \quad y = vf \tag{17}$$

where

$$v = \exp(\beta E) - 1.$$

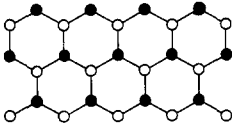


Figure 4. A dilute Potts model on the honeycomb lattice. The open circles are always occupied by atoms while the black circles can either be occupied or vacant.



Figure 5. Equivalent two- and three-site Potts interactions.

For real $E, z \geq 0$ and $q \geq 3$, it is clear that $f > 0$ and $y \geq -f$. Thus we are always in the ferromagnetic region. Criticality then occurs exactly at $y = q$

$$v^3 = q(z + q + 3v). \tag{18}$$

Thus we have at least one dilute Potts model on a regular lattice for which the exact criticality is known. The result (18) can be used to check the accuracy of other approaches, such as the renormalisation group (Nienhuis *et al* 1979, 1980).

7. Conclusion

The q -state Potts model on the triangular lattice with two- and three-site interactions (in every other triangle) has been considered. In the ferromagnetic region the exact critical point is determined under the assumptions that the transition is unique and that the singularity is continuous in the parameter space. In the antiferromagnetic model a transition exists only for $q=3$, regardless of the isotropy of the interactions. This contrasts with the Ising ($q=2$) result for which a transition exists only for anisotropic interactions. Finally, we expect no transition in the isotropic paramagnetic model.

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