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Triangular Lattice Potts Models

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In this paper we study the 3-state Potts model on the triangular lattice which has two- and three-site interactions. Using a Peierls argument we obtain a rigorous bound on the transition temperature, thereby disproving a conjecture on the location of its critical point. Low-temperature series are generated and analyzed for three particular choices of the coupling constants; a phase diagram is then drawn on the basis of these considerations. Our analysis indicates that the antiferromagnetic transition and the transition along the coexistence line are of first order, implying the existence of a multicritical point in the ferromagnetic region. Relation of the triangular q-state Potts model with other lattice-statistical problems is also discussed. In particular, an Ashkin–Teller model and the hard-hexagon lattice gas solved by Baxter emerge as special cases in appropriate limits.

KEY WORDS: Potts model; triangular lattice; Peierls argument; low-temperature series; phase diagram; relations with other lattice models.

1. INTRODUCTION

The q-component Potts model[1] is a generalization of the Ising model (the $q = 2$ case) and it has recently been of particular theoretical interest.[3] The first comprehensive investigation of the $q > 2$ models was a study of the $q = 3$ case by Straley and Fisher[3] using series analysis. A large number of subsequent studies using both series analysis and renormalization group techniques failed to give consistent descriptions of the critical behavior. While Baxter[4] has shown that the transition in two dimensions is first order for $q > 4$ and is continuous for $q \leqslant 4$; neither series analysis[5] nor (prior to the work of Nienhuis *et al.*[6,7]) renormalization group techniques

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have consistently indicated the change from continuous to first-order behavior. Some progress has been made toward the understanding of the ferromagnetic $q = 3$ model, however. Baxter[8] has recently solved the hard-hexagon lattice gas, a system which is believed to be in the universality class of the $q = 3$ Potts model. Subsequently, Enting[9] has shown that the series for the $q = 3$ ferromagnetic model with pure two-site interactions appear to be consistent with the hard-hexagon's exponents, although the convergence is extremely slow.

In view of the difficulties encountered in studying the ferromagnetic Potts models, it is perhaps not really surprising that there have been very few studies of the antiferromagnetic Potts models. While evidences appear to indicate that the antiferromagnetic model exhibits no transition on the square lattice for all $q \geqslant 3$,[2,10,11] the $q = 3$ model on the triangular lattice is of particular interest which is worthy of further investigation. Schick and Griffiths[12] have studied such a Potts model with both two-site and three-site interactions, using renormalization group techniques. For appropriate negative values of the couplings, they found an antiferromagnetically ordered phase terminating with a line of critical points. They also found that the ferromagnetic and antiferromagnetic phases coexist at finite temperatures, with the coexistence line terminating at a bicritical point. (It should be pointed out that the system considered by Schick and Griffiths differs from the "loose-packed" system which has three-site interactions on only half the triangles and which has been studied by Baxter *et al.*,[13] Wu and Zia,[14] and Enting.[15,16])

In this paper we study in further details the "close-packed" $q = 3$ model of Schick and Griffiths,[12] with emphasis on its critical behavior along the coexistence line and in the antiferromagnetic region. Our study was motivated in part by a discrepancy between a recent conjecture by Wu[17] on the critical point of this close-packed system and the phase diagram obtained in Ref. 12. To clarify the situation we have used a generalized Peierls argument to obtain a rigorous bound on the location of the critical point. This bound clearly shows that Wu's conjecture is incorrect for $q = 3$. We further developed series expansions for three particular choices of the coupling strengths. Our series analysis provides numerical estimations which lend support to the general locations of the phase boundaries found by the renormalization group approach. However, there are a number of indications that some of the transitions are of first order, which is not obtained from the renormalization group analysis. We also discuss the connection of the general q-state model with other lattice-statistical problems. In particular, we show that the hard-hexagon lattice gas solved by Baxter[8] can be generated from the present model by taking a special limit.

The organization of this paper is as follows: In Section 2 we consider the symmetry of the 3-state model. The main results of our study are summarized in Section 3. In Section 4 we present a Peierls argument to derive a rigorous bound on the transition temperature which disproves the Wu conjecture. Section 5 describes the techniques used to derive the low-temperature series, and Section 6 discusses the series analysis; the series are tabulated in Section 5. Section 7 relates the general q system to other lattice-statistical problems.

2. GENERAL CONSIDERATIONS

Consider the 3-state Potts model on the triangular lattice in which each site can be in one of three spin states; 0, 1, or 2. In addition to the nearest-neighbor interactions, there is a three-site interaction in *each* of the triangular faces. The Hamiltonian $\mathcal{H}$ takes the form

$$-\beta\mathcal{H} = K\sum_{\langle ij\rangle}\delta_3(\sigma_i - \sigma_j) + L\sum_{\langle ijk\rangle}\delta_3(\sigma_i - \sigma_j)\delta_3(\sigma_j - \sigma_k) \tag{1}$$

where the first summation is over all edges (connecting sites i and j) of the lattice, and the second summation over all elementary triangles (surrounding sites i, j, and k). In (1), $\beta = 1/kT$, $\sigma_i = 0, 1, 2$ specifies the spin state at the ith site and $\delta_q(i-j)$ is 1, if $i - j = 0$ (mod. q), and is zero otherwise.

The symmetry properties of Hamiltonian (1) have been described by Schick and Griffiths.[12] It is convenient to follow their treatment and define the variable

$$M = 3K + 2L \tag{2}$$

Figure 1 shows the three distinct situations that can arise on an elementary triangle. Depending on which of these arrangements has the lowest energy, the system will have as its ground state one of the ferromagnetic orderings, one of the antiferromagnetic orderings, or will be in the paramagnetic regime with no ground-state ordering. We denote the three types of triangular configuration as F, A, or P accordingly. The energy E per

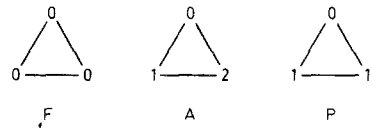

Fig. 1. The three distinct spin configurations that can arise on an elementary triangle. Ferromagnetic (F), antiferromagnetic (A), and paramagnetic (P).

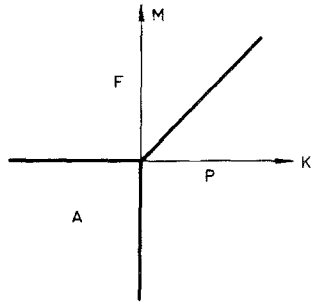

Fig. 2. Regions of the lowest energy for the three types of spin arrangements in Fig. 1.

triangle is given by

$$\begin{aligned} E(F) &= -M/2\beta \\ E(A) &= 0 \\ E(P) &= -K/2\beta \end{aligned} \tag{3}$$

The regions with the various ground states are thus

(i) Ferromagnetic if $M > K$, $M > 0$,
(ii) Antiferromagnetic if $0 > K$, $0 > M$,
(iii) Paramagnetic if $K > 0$, $K > M$.

These different regions are shown in Fig. 2.

Since the degeneracies of the ferromagnetic and antiferromagnetic ground states are finite and the degenerate states are related by definite symmetry operations of the Hamiltonian, it follows from a theorem due to Slawney[18] that a phase transition exists in the sense that, at sufficiently low temperatures, the free energy has a discontinuous derivative with respect to any symmetry-breaking field. In the paramagnetic regime the ground-state entropy is nonzero. Argument can then be made as in the case of the antiferromagnetic Ising model[19] that states of different long-range orders can be mixed without causing an energy increase. This then rules out the occurrence of a phase transition accompanying the onset of a long-range ordering.

The discussion of the model is simplified if we introduce a number of spin transformation operations. For single spins we define

$$\begin{aligned} &i\text{: identity (no change)} \\ &j\text{: } 0 \to 2 \to 1 \to 0 \\ &k\text{: } 0 \to 1 \to 2 \to 0 \end{aligned} \tag{4}$$

There are nine distinct global transformations defined by applying one of

the transformations (4) to *all* spins in one of the three (triangular) sublattices a, b, and c. They are

$$\begin{aligned} &I\colon (i,i,i) && \text{on} \quad (a,b,c) \\ &A\colon (j,j,j) && \text{on} \quad (a,b,c) \\ &B(=AA)\colon (k,k,k) && \text{on} \quad (a,b,c) \\ &X\colon (i,j,k) && \text{on} \quad (a,b,c) \\ &Y\colon (i,k,j) && \text{on} \quad (a,b,c) \end{aligned} \tag{5}$$

The remaining four transformations are AX, AY, BX, and BY. It may be verified directly that, while the transformations (5) mix the F and A triangles of Fig. 1, the P triangles remain invariant under all nine transformations.

3. THE PHASE DIAGRAM

For continuity in reading, we now summarize our main findings. Details of the analyses will be found in Sections 4–6.

Our first result is an application of the Peierls argument[20,21] leading to a bound on the boundaries of the region in which long-range order can exist. For $M = 0$, and $K < 0$, viz., the coexistence line between the ferromagnetic and antiferromagnetic ground states, we obtain the following rigorous bound on the critical point:

$$|K_c| < 11.39 \tag{6}$$

We then argue that the bound should persist to $M \neq 0$ to yield the bounds

$$M - K < 11.39 \tag{7}$$

in the ferromagnetic region, and

$$|K| < 11.39 \tag{8}$$

in the antiferromagnetic region. These bounds are shown in Fig. 3. We also plot in Fig. 3 Wu's conjecture (for $q = 3$) on the ferromagnetic phase boundary:[17]

$$e^M = 3e^K + q - 2 \tag{9}$$

It is seen that the conjectured boundary extends into the ordered region for small M and therefore must be incorrect. In particular, it yields the incorrect prediction of no transition ($K_c = -\infty$) for $M = 0$. Thus the rigorous bound (6) alone is sufficient to disprove the validity of (9) for $q = 3$.

In Fig. 4 we plot the same diagram in an enlarged scale so that the shaded regions of Fig. 3 are not seen. The circles I, II, III denote the three

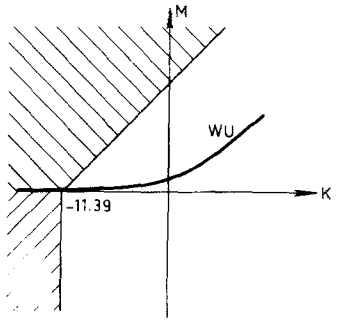

Fig. 3. Bounds on ordered regions as expected from the Peierls argument. The system is ordered in the shaded regions; the phase boundaries are confined in the unshaded region. The curve is a plot of the Wu conjecture (9) for $q = 3$.

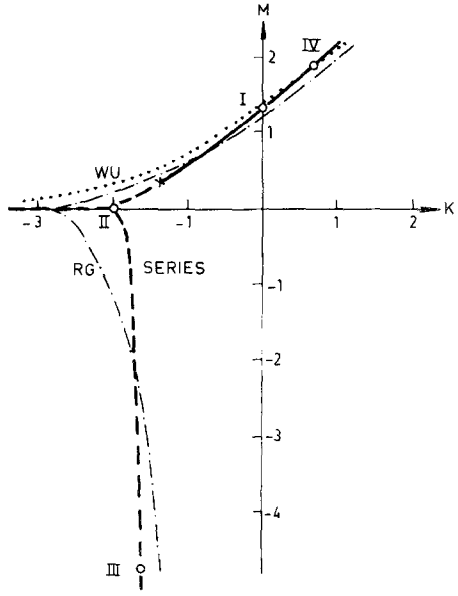

Fig. 4. Phase diagram in the (K, M) space. The circles I, II, III denote the three critical points determined from series analyses of this paper and the circle IV is the exact critical point of the ferromagnetic model with pure two-site interactions. The solid and broken lines are, respectively, the continuous transition and first-order transition phase boundaries obtained by connecting the four circles. The dotted curve is the ferromagnetic phase boundary predicted by the conjecture (9) for $q = 3$; the curve labeled RG is the phase boundaries determined by renormalization group (Ref. 12). The cross denotes the multicritical point expected to exist.

transition points determined from the series analysis of Section 5, and the circle IV denotes the exact critical point of the ferromagnetic model with pure two-site interactions.[22] Their locations and the apparent nature of transitions (see Section 5) are summarized as follows:

I. $K = 0$, $M_c \simeq 1.37$ (continuous, $\beta = 1/9$; $\gamma' = 13/9$)
II. $M = 0$, $K_c \lesssim -1.99$ (first order)
III. $M = 3K < 0$, $K_c \simeq -1.59$ (first order)
IV. $M = 3K > 0$, $K_c = \ln[2\cos(\pi/9)] = 0.63094\ldots$ (continuous, $\beta = 1/9$, $\gamma' = 13/9$)

Here the value of $\beta = 1/9$ for the exact critical point IV has been taken from Ref. 9. The solid and dashed lines in Fig. 4 are the phase boundaries obtained by connecting these four points. It must be noted, however, that the locations of the critical points I, II, and III are merely approximate, which are based on the best estimates deduced from the series analyses.

For comparison we also plot in Fig. 4 the conjecture (9) for $q = 3$ (the dotted line) and the phase boundaries determined from the renormalization group RG.[12] It is rather remarkable that, in the range of $-1 \lesssim K \lesssim 1$ at least, the phase boundaries from both the series and the renormalization group analyses are well approximated by the expression (9).

The results on the nature of transition obtained from the series analysis appear to suggest the existence of a multicritical point, indicated by $\times$ in Fig. 4. Indeed, the existence of such a multicritical point is supported by recent Monte Carlo analysis.[23] The transition would be of first order for values of M below that of the multicritical point, as indicated by the phase boundary in broken lines, and continuous otherwise, as indicated by the phase boundary in a solid line. This would imply that the antiferromagnetic systems all have first-order transitions. However, since we have been unable to obtain definitive conclusions for the antiferromagnet with pure two-site interactions (point III), the possibility still exists that there may exist a second multicritical point at a point of sufficiently small negative M. Finally, the fact that $\beta = 1/9$, $\gamma' = 13/9$ for both points I and IV corroborates the picture that the critical points on the line of continuous transitions all belong to the hard-hexagons universality class. It should also be mentioned that our analyses of α' encountered difficulties similar to those found by Fisher and Straley.[3]

4. PEIERLS ARGUMENT

We now present a Peierls argument[20,21] to obtain bounds on the critical temperature.

The idea of Peierls argument is to establish that, with the boundary spins fixed at a given ordered configuration and at sufficiently low temperatures, the fraction of interior spins that are also in the same ordered state is arbitrarily close to unity. This serves to establish the existence of a transition as well as a bound on the critical point.

We shall consider first the crucial case of $M = 0$, $K < 0$ for which the conjecture (9) contradicts the renormalization group analysis of Ref. 12.

On the coexistence line $M = 0$, $K < 0$, the ground state is any one of the nine ferromagnetic and the antiferromagnetic states. For simplicity we can therefore choose a boundary condition in which all boundary sites are in the spin state 0. The goal is then to show that, at sufficiently low temperatures, the fraction of the interior sites that are also in the spin state 0 can be arbitrarily close to unity.

The energy of a spin configuration containing n P triangles is $n|K|/2\beta$. For each spin configuration S we can then construct a graph G by shading the P elementary triangles. A typical G constructed in this fashion is shown in Fig. 5. Note that not all graphs obtained by shading randomly chosen triangles correspond to a spin configuration. In fact, for a large triangular lattice of N sites, there are 3^N spin configurations generating a much lesser number of G, while there are $4^N = 2^{2N}$ ways that the 2^N triangles can be independently shaded.

Generally, a graph G consists of disjoint clusters of shaded triangles, and more than one S can produce the same G. The spin configuration(s) associated with a given G can be reconstructed by working inward from the boundary. Putting all boundary spins in the spin state 0 and working toward the center, a possible ambiguity in assigning spin states to the interior sites arises only for the P triangles (*a property unique to the* 3*-state model*). Let g_c be the number of ways of assigning distinct spin states to a cluster of t_c triangles, once the states of the sites surrounding its perimeter are fixed. We can then convert the spin sum into a sum over the graphs by

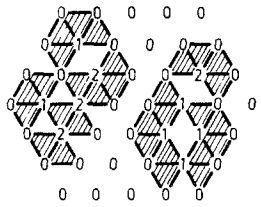

Fig. 5. Typical spin configuration S on a lattice of 44 sites. The boundary spins are fixed in the spin state 0, and the associated graph G is obtained by shading the P triangles. For clarity borders of the F and A triangles are not drawn.

writing

$$\sum_S e^{-\beta E} = \sum_G \prod_c \left[g_c e^{-t_c|K|/2} \right] \tag{10}$$

where the product is over all clusters of G.

It is now a simple matter to proceed as usual[4] to construct a Peierls argument. Let there be $\nu(t)$ ways of embedding a connected cluster of t shaded triangles on the lattice. Number these embeddings from 1 to $\nu(t)$. For a given spin configuration we define the variable

$$\begin{aligned} X_t^{(j)} &= 1 \quad \text{if the } j\text{th embedding of a cluster of } t \text{ shaded triangles is in the graph} \\ &= 0 \quad \text{otherwise} \end{aligned} \tag{11}$$

Then the number N_w of spins that are in the wrong states, viz., 1 or 2, is bounded by the inequality

$$N_w \leqslant \sum_{t=6,8,\ldots} \left(\frac{t}{6} \right)^2 \sum_{j=1}^{\nu(t)} X_t^{(j)} \tag{12}$$

where we have used the fact that the number of sites interior to a cluster of t triangles is at most $(t/6)^2$.

The inequality (12) remains valid upon taking the thermal average. After introducing (10), we find

$$\langle N_w \rangle \leqslant \sum_{t=6,8,\ldots} \left(\frac{t}{6} \right)^2 \sum_{j=1}^{\nu(t)} \langle X_t^{(j)} \rangle \tag{13}$$

where

$$\begin{aligned} \langle X_t^{(j)} \rangle &= \sum_S{}' e^{-\beta E} \Big/ \sum_S e^{-\beta E} \\ &= \sum_G{}' \prod_c \left[g_c e^{-t_c|K|/2} \right] \Big/ \sum_G \prod_c \left[g_c e^{-t_c|K|/2} \right] \end{aligned} \tag{14}$$

Here the summations $\sum'$ are over those S or G for which the jth cluster of t shaded triangles, T_j, is present.

For each graph G in the numerator of (14) we construct a graph G^* derived from G by eliminating the cluster T_j entirely. We now show that G^* can indeed be generated from a spin configuration S^* obtained as follows: Starting from any one of the spin configurations S which generates G, we derive S^* by (i) keeping the states of all sites exterior to T_j unchanged, (ii) assigning all sites in T_j the same (ground) spin state as those sites immediate exterior to T_j, and (iii) applying one of the nine transformations (5) to

[4] See, e.g., Ref. 21.

sites interior to T_j, if any, such that the graph interior to T_j remains unchanged. Note that the last step is possible because the transformations (5) leave the P triangles invariant, and the last step will not change the overall energy interior to T_j (*a property unique to* $M = 0$).

Now for each G in the numerator of (14) we keep only the term G^* in the denominator, thus obtaining a bound. Also, since g_c cannot be larger than 2^t, we obtain

$$\langle X_t^{(j)} \rangle < 2^t e^{-t|K|/2} \tag{15}$$

Now the contour of a cluster of t triangles forms a Hamiltonian circuit. It follows that the number $\nu(t)/N$ is bounded by 5^{3t}, the number of a random walk of $3t$ steps on an N-site triangular lattice without immediate reversals. Putting these bounds together, we obtain from (13)

$$\frac{1}{N}\langle N_w \rangle < \sum_{t=6,8,\ldots} \left(\frac{t}{6}\right)^2 5^{3t} 2^t e^{-t|K|/2} \tag{16}$$

Now the right-hand side of (16) converges and can be made arbitrarily small at low enough temperatures. We have thus completed the proof that the fraction of interior sites in the spin state 0 can be arbitrarily close to unity. In fact, a bound on the critical temperature $|K_c|$ can be obtained by setting $(1/N)\langle N_w \rangle = 2/3$. This leads to (6) after carrying out the summation. Needless to say, this bound is very generous, as seen obviously from the steps used in reaching (16). [To complete the formal proof of the existence of a transition, the bound (16) is to be used in conjunction with the usual convexity argument[21] to establish a discontinuity of the free energy in the field derivative at sufficiently low temperatures.]

We consider next bounds in the ferromagnetic and antiferromagnetic regimes. For $M > 0$ and $M > K$ the energies (3) can be written as

$$\begin{aligned} E(F) &= 0 \\ E(A) &= M/2\beta > 0 \\ E(P) &= (M - K)/2\beta > 0 \end{aligned} \tag{17}$$

while for $M < 0$ and $K < 0$ they are

$$\begin{aligned} E(F) &= |M|/2\beta \\ E(A) &= 0 \\ E(P) &= |K|/2\beta \end{aligned} \tag{18}$$

The two cases can be viewed as raising $E(A)$ and $E(F)$, respectively, from $E(F) = E(A) = 0$, $E(P) > 0$. Intuitively we expect the transition temperature of a spin system to be nondecreasing when the energies of the excited states are increased. It follows then that the bound (6) is still valid,

provided that the appropriate new values of $E(P)$ are used. This consideration then leads to the bounds (7) and (8).

5. SERIES DERIVATION

In this section the finite-lattice method of series expansions[24–26] is used to obtain low-temperature expansions for the three-state Potts model (1) for three choices of the coupling constants:

I. Pure three-site interactions ($K = 0$, $L > 0$) with the expansions parameter $w = e^{-L}$. The series are obtained through w^{33}.
II. The coexistence line ($M = 0$, $K < 0$) with the expansion parameter $v = e^{K/2} = e^{-L/3}$. The series are obtained through v^{21}.
III. The antiferromagnet with pure two-site interactions ($L = 0$, $K < 0$) with the expansion parameter $u = e^{K}$. The series are obtained through u^{11}.

Series for the partition function, the order parameter, and the zero-field susceptibility in each of the three cases are tabulated in Tables I–III. It should be noted that series of a fourth special case, viz., the ferromagnet with pure two-site interactions ($L = 0$, $K > 0$), has been previously obtained and analyzed.[15]

The low-temperature series are obtained through the approximants of the form

$$Z = \prod_{m,n} Z(m,n)^{a(m,n)} \tag{19}$$

with

$$\begin{aligned} a(m,n) &= 1, && m+n = 2W+1 \\ &= -3, && m+n = 2W \\ &= 3, && m+n = 2W-1 \\ &= -1, && m+n = 2W-2 \\ &= 0, && \text{otherwise} \end{aligned}$$

The parameter W is the maximum width of the rectangle that need be treated so long as the symmetry $Z(m,n) = Z(n,m)$ is fully exploited. The function $Z(m,n)$ is the partition function of a finite $m \times n$ rectangle surrounded by sites which are in the appropriate ground state. For our purposes the triangular lattice is treated as a square lattice with second-neighbor interactions in one diagonal direction.

It was found that for series I, the use of width W gave terms through w^{4W+5} while in series III width W gave terms through u^n with $n = \text{Int}[(4W+7)/3]$. In series II the coefficients were given correctly through v^{2W+5} and the coefficient of v^{2W+7} was also given correctly.

Table I. Series expansions for ferromagnet with pure three-site interactions ($K = 0$, $L > 0$, $w = e^{-L}$)

$$Z_0 = 1 + \sum_{n=6}^{\infty} a_n w^n, \qquad R = 1 + \sum_{n=6}^{\infty} b_n w^n, \qquad \chi = \sum_{n=6}^{\infty} c_n w^n$$

n	a_n	b_n	c_n
6	2	− 3	2
7	0	0	0
8	0	0	0
9	0	0	0
10	12	− 36	48
11	0	0	0
12	− 8	24	− 20
13	12	− 54	108
14	78	− 360	744
15	12	− 72	192
16	− 126	522	− 612
17	168	− 1 044	2 904
18	672	− 4 212	11 836
19	72	− 882	4 452
20	− 1 506	7 983	− 12 018
21	1 936	− 15 822	59 052
22	7 098	− 55 503	194 958
23	− 948	− 1 458	60 804
24	− 16 582	105 021	− 171 670
25	21 936	− 223 344	1 056 696
26	81 474	− 760 662	3 213 204
27	− 29 248	118 254	726 652
28	− 191 832	1 406 079	− 2 342 142
29	272 664	− 3 265 668	18 433 320
30	960 054	− 10 453 170	52 139 564
31	− 524 940	3 241 152	7 779 528
32	− 2 340 372	19 445 643	− 31 967 142
33	3 668 236	− 49 620 678	320 364 444

Comparison of approximations using $W = 1$ to 7 showed that the coefficients of v^{2W+6} were too small by 2 in the partition function series, too large by $3(W + 1)$ in the order parameter series, and too small by $2(W + 1)^2$ in the susceptibility series. All of these regularities were confirmed for $W = 1$ to 6. The series given in Tables I–III are based on the assumption that these regularities persist, or equivalently that the class of graphs giving the lowest-order corrections have been correctly identified. For series I and II these limiting graphs are chains of $W + 1$ perturbed sites connected by a line of diagonal bonds on the square lattice. For series III the limiting graphs correspond to perturbations of the type shown in Fig. 6.

The partition functions $Z(m, n)$ were calculated using a transfer-matrix formalism based on building up finite rectangles one site at a time. For width $W = 1, 2, \ldots, 7$ it was necessary to consider $n_W = 2, 5, 14, 41, 122,$

Table II. Series expansions along the coexistence line ($M = 0$, $K < 0$, $v = e^{K/2} = e^{-L/3}$)

$$Z_0 = 1 + \sum_{n=6}^{\infty} a_n v^n, \qquad R = 1 + \sum_{n=6}^{\infty} b_n v^n, \qquad \chi = \sum_{n=6}^{\infty} c_n v^n$$

n	a_n	b_n	c_n
6	2	− 3	2
7	0	0	0
8	6	− 18	24
9	0	0	0
10	24	− 99	186
11	12	− 54	108
12	94	− 540	1 400
13	84	− 504	1 344
14	396	− 2 880	9 468
15	604	− 4 500	15 072
16	1 830	− 16 443	66 630
17	3 612	− 32 508	131 400
18	9 232	− 98 328	472 352
19	21 480	− 228 654	1 095 876
20	50 484	− 620 304	3 439 044
21	124 536	− 1 541 526	8 594 908

365, 1094 components, respectively, in the vectors involved. In general $n_W = 3n_{W-1} - 1$ and is less than 3^W because we can make use of the equivalence of states 1 and 2 (assuming a ground state of state 0). For series III the equivalence is site dependent and it is simplest to work with 3^W components in the vectors.

Table III. Series expansions for antiferromagnet with pure two-site interactions ($L = 0$, $K < 0$, $u = e^K$, $x = u/(1 + u)$)

$$Z_0 = 1 + \sum_{n=3}^{\infty} a_n u^n = 1 + \sum_{n=3}^{\infty} a'_n x^n$$

$$R = 1 + \sum_{n=3}^{\infty} b_n u^n = 1 + \sum_{n=3}^{\infty} b'_n x^n$$

$$\chi = \sum_{n=3}^{\infty} c_n u^n = \sum_{n=3}^{\infty} c'_n x^n$$

n	a_n	a'_n	b_n	b'_n	c_n	c'_n
3	2	2	− 3	− 3	2	2
4	3	9	− 9	− 18	12	18
5	12	36	− 45	− 99	78	138
6	25	135	− 150	− 495	402	932
7	105	525	− 711	− 2 511	2 280	6 132
8	297	2 124	− 2 754	− 12 834	11 574	39 168
9	1 213	8 993	− 12 681	− 66 759	61 994	247 126
10	4 140	39 555	− 53 613	− 352 044	315 774	1 543 464
11	16 725	179 760	− 243 450	− 1 878 480	1 635 708	9 570 072

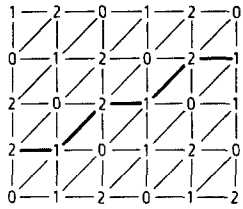

Fig. 6. The limiting graph for the series III showing a chain of perturbation (the heavy lines) from the ground state.

For the antiferromagnet (series II) a spin transformation given by (5) is needed to map the antiferromagnetic ground state into the "all-zero" state. This, of course, changes the Hamiltonian (1). In fact, the transformation $\sigma_i \to \sigma_i' = \sigma_i - c_i$ induces the following change in (1):

$$K\delta_3(\sigma_i - \sigma_j) \to K\delta_3(\sigma_i - \sigma_j - c_i + c_j) \tag{20}$$

We choose a particular ground state and set the constants c_i to be the ground-state values of σ_i. While the interaction formally depends on the position through the variables c_i, in fact the quantity $c_i - c_j$ does not depend on the position but only on the orientation of the edge connecting sites i and j. Thus the transformation has mapped a system which has a staggered (antiferromagnetic) ground state onto one which has a uniform ground state with a translationally invariant (albeit anisotropic) interaction. Consequently, no special modifications are required when applying the finite lattice method.

For each series calculation a field was applied such that each site not in the ground state has a weight z. As described by Enting[26] the coefficients of the temperature variable are polynomials in z. They can equally well be written as polynomials in $x = 1 - z$ with the expansion truncated at x^2 giving

$$Z = Z_0 + xZ_1 + x^2Z_2 + \cdots \tag{21}$$

This enables us to find the zero-field partition function Z_0, the order parameter

$$R = 1 - 3Z_1/2Z_0 \tag{22}$$

and the zero-field susceptibility

$$X = (2Z_0Z_2 - Z_0Z_1 + Z_1^2)/Z_0^2 \tag{23}$$

On the coexistence line, $M = 0$, we could use M as an alternative ordering field by putting $x = 1 - e^{-M}$. If the bicritical point exists then the scaling power associated with this field would determine the shape of the

two incident critical lines. Since we believe that the transition is actually of first order, we have not pursued this calculation.

The series for Z_0, R, χ are listed in Tables I–III. We remark that, in principle, the finite lattice method can be applied whenever the ratio K/L involves small integers. Between the M axis and the negative K axis (i.e., $-2/3$), the appropriate ratios are $-1/1$, $-1/2$, $-1/3$. One remaining practical difficulty in deriving such series is the correct identification of the limiting graphs.

6. SERIES ANALYSIS

The three groups of series I, II, and III are each analyzed in the light of the conjectured phase diagram.

6.1. Pure Three-Site Interactions ($K = 0$, $L > 0$, $w = e^{-L}$)

During the course of this investigation it was these series that provided our first indication that the conjecture (9) might be incorrect.

The analysis consisted of constructing Padé approximants to the logarithmic derivatives of R, χ/w^6, and c/w^6, where c is the zero-field specific heat. To obtain any consistent description it was necessary to examine the trends in the Padé tables:

(i) R: The higher-order approximants indicated $w_c = 0.5038 \pm .0005$, $\beta = 0.106 \pm .001$. The estimates of both w_c and β tended to increase as the order of the approximant increased. (A similar trend is found for the $q = 3$ square lattice Potts model[9] and the $q = 3$ loose-packed pure three-site model on the triangluar lattice.[16]) This means that, overall, increasing w_c is correlated with increased β estimates due to the "length" effect, but the estimates showed an additional correlation between increases in w_c and β for approximants of similar order.

(ii) χ: Both w_c and γ' estimates tended to decrease as the order of the approximants increased (as in Ref. 16) and again there was additional correlation between w_c and γ' for approximants of similar order. The higher-order approximants gave $w_c = 0.504 \pm .001$, $\gamma' = 1.40 \pm .02$.

(iii) c: The results were very irregular and did not show any systematic changes in w_c and α' as the order of the approximant increased. The approximants indicated $w_c = 0.508 \pm .005$, $\alpha' = 0.65 \pm .10$ with higher w_c estimates generally associated with higher α' estimates. (It should be noted that it has proved difficult to analyze Potts model specific heats in other cases and that one of the more successful techniques—analyzing $E - E_c$ for $1 - \alpha'$ with the critical energy E_c obtained from a duality relation—cannot be used here.)

There are at least two ways of combining these results into a consistent description:

(a) The system has the hard-hexagons exponents, $\alpha' = 1/3$, $\beta = 1/9$, $\gamma' = 13/9$ with $w_c = 0.5048 \pm .0005$ (this value for w_c is obtained from Padé approximants to R^{-9}). Evaluating Padé approximants to $(w_c - w)(d/dw)\ln(\chi/w^6)$ at w_c gives $\gamma' = 1.445 \pm .002$. The inconsistency on the α' estimates is attributed to the series being too short, as indicated by the irregularities mentioned above and by the absence of any systematic trend as the number of terms is increased.

(b) Alternatively it could be suggested that the hard-hexagons exponents are being masked by the nearby multicritical point and that the series are revealing the values of a set of effective exponents with $\delta' \approx 1.35$, $\beta \approx 0.105$, $\alpha' \approx 0.44$ obeying an effective scaling relation and having $w_c \approx 0.5038 \pm .0005$. This set of values would be obtained by taking the approximants of $(d/dw)\ln R$ at face value; the γ' value is obtained from approximants to $(w_c - w)(d/dw)\ln(\chi/w^6)$. Approximants to $(w - w_c)(d/dw)\ln(c/w^6)$ give $\alpha' = 0.55 \pm .15$ which includes the effective "scaling" value $\alpha' = .44$.

The two explanations are somewhat similar in that they both can be interpreted as being due to a singularity that is more complicated than a simple power law so that there may be a systematic bias in the estimates. (Our "error" limits are, as always, merely measures of consistency.) Nevertheless we believe that the deviation of our estimate on w_c from the value $w_c = 1/2$ dictated by (9) (for $q = 3$) is significant.

It is noteworthy that the $q = 1$ limit of the Hamiltonian (1) for general q spin states generates a percolation on the honeycomb lattice (see Section 7 below).[27,28] Using this equivalence and a finite-size Monte Carlo estimation of the critical threshold for the site percolation ($K = 0$, $w_c = e^{-L}$), Vicsek and Kertêsz[29] have found that at $q = 1$ the conjecture (9) gives a value of $w_c = 1/\sqrt{2}$ slightly larger than their numerical estimate. Note, however, that the conjecture is correct at $q = 2$, giving the exact critical point for the Ising model.[17]

6.2. The Coexistence Line ($M = 0$, $K < 0$, $v = e^{K/2} = e^{-L/3}$)

The series were analyzed by constructing Padé approximants to the following functions:

(i) $(d/dv)\ln R$. The higher-order approximants yielded the estimates $v_c = 0.370 \pm .001$, $\beta = 0.028 \pm .001$.

(ii) $(d/dv)\ln(\chi/v^6)$. The higher-order estimates were $v_c = 0.377 \pm .005$, $\gamma' = 1.5 \pm .2$.

(iii) $(d/dv)\ln(c/v^6)$. This yielded highly irregular estimates, with many approximants having no positive real poles.

(iv) $(d/dv)\ln[(dR/dv)/v^5]$. The approximants yielded the estimates $v_c = 0.365 \pm .004$, $1 - \beta = 1.15 \pm .06$.

The discrepancies in the first three estimates tend to indicate that the implicit assumption of a continuous transition with power-law singularities might be incorrect. The result from the fourth estimate giving a negative value of β clearly indicates that the singularity seen is not a physical transition.

We interpret these results as indicating a first-order transition occurring at $v_c \lesssim 0.37$, rather than being a bicritical point as predicated by Schick and Griffiths[12] from the renormalization group. For comparison they found $v_c = 0.257$; the Monte Carlo study[23] yields a first-order transition occurring at $v_c = 0.369$.

6.3. Antiferromagnet with Pure Two-Site Interactions ($L = 0$, $K < 0$, $u = e^K$)

The shortness of these series seriously limits the possibilities for useful analysis. We began by constructing Padé approximants to the following functions:

(i) $(d/du)\ln R$. The estimates for the critical parameters were $u_c = 0.203 \pm .002$, $\beta = 0.070 \pm .005$.

(ii) $(d/du)\ln[(dR/du)/u^2]$. This yielded the estimates $u_c = 0.204 \pm .003$, $1 - \beta = 0.94 \pm .05$.

(iii) $(d/du)\ln(\chi/u^3)$. The estimates were $u_c = 0.204 \pm .003$, $\gamma' = 1.4 \pm .1$.

These estimates are all based on a small number of low-order approximants. (For comparison, Schick and Griffiths[12] found $u_c = 0.210$ and Monte Carlo data[23] yield $u_c = 0.205$.) We have also attempted to use the ratio method by changing variables to $x = u/(1 + u)$ so that $u_c = 0.204 \pm .003$ corresponds to $x_c^{-1} = 5.90 \pm .07$. The ratio analyses for the $R(x)$ and $\chi(x)$ series are consistent with the existence of a singularity in this range of x values, and this estimate was used to find the following exponent estimates:

$$\beta = 0.05 \pm .10, \qquad \gamma' = 1.55 \pm .15.$$

Direct application of the ratio method to the order parameter series R

indicates $x_c^{-1} = 5.9$, while the susceptibility series χ indicates $x_c^{-1} = 5.8$. It should be noted that it is this lower value of x_c^{-1} which corresponds to the negative end of the range of β estimates quoted above.

As in series II, the negative β estimates are the most obvious indication of a first-order transition. The positive β estimates correspond to values smaller than those normally found in two-dimensional systems, but there are special cases in which such small values are known to occur. (Most notably the polarization exponent in the 8-vertex model[30] can take on any positive value.)

Given the difficulties which many workers have encountered in trying to determine the nature of the transition in the $q = 3$ three-dimensional Potts ferromagnets, it is not surprising that our 11 terms series do not give a definite answer. One possible way of determining the nature of transition in this case would be to compare the results with an analysis of the high-temperature series, but again experience with the three-state three-dimensional ferromagnets suggests that the results might still be inconclusive. It should be mentioned that Monte Carlo simulations[23,31] of the model (with pure two-site antiferromagnetic interaction) have also indicated evidence of a first-order transition.

7. RELATION TO OTHER PROBLEMS

In this section we discuss the connection of the system described by the Hamiltonian (1) with other lattice-statistical problems. For this purpose we shall consider more generally the Hamiltonian (1) for general q, for which the only change involved is the replacement of δ_3 by δ_q in (1). Namely, we now consider the q-state triangular Potts model (1).

Our first result is a "duality" relation which relates the Potts model (1) to a Potts model on the Kagomé lattice shown in Fig. 7. Denoting the

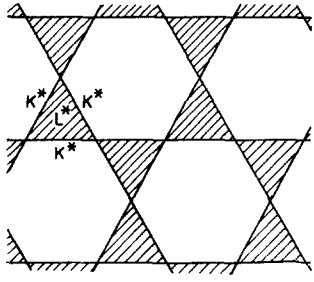

Fig. 7. The Kagomé model with two- and three-site interactions K^* and L^* equivalent to the q-state triangular model (1). The equivalence is given by (24).

respective partition functions by Z_Δ and Z_K, the exact relation between the two models reads

$$Z_\Delta(K, L) = (y/q)^N Z_K(K^*, L^*) \tag{24}$$

with

$$\begin{aligned} e^{K^*} - 1 &= q(e^{K/2} - 1)/y \\ y^* &= e^{L^*+3K^*} - 3e^{K^*} + 2 \end{aligned} \tag{25}$$

where

$$\begin{aligned} y &= e^{L+3K/2} - 3e^{K/2} + 2 \\ y^* &= e^{L^*+3K^*} - 3e^{K^*} + 2 \end{aligned} \tag{26}$$

and N is the number of sites of the triangular lattice. The Kagomé lattice can be considered as the covering lattice[32] of the triangular lattice. In fact, the derivation of the duality (24) makes use of this same geometry and relies on a duality transformation due to Burkhardt.[33] Although Burkhardt considered only the square lattice, his method is more general and applicable to any planar lattice whose dual is bipartite. A straightforward application of his transformation to the Kagomé lattice in the present case then leads to (24). We refer to Ref. 33 for details which are straightforward and will not be repeated here. We remark that the duality relation (24) can also be generalized to anisotropic interactions.

Next we state an equivalence which is obtained from an application of a general theorem[28] that a Potts model of the type (1) is related to a dilute Potts model. For the present problem this leads to the equivalence of (1) with a dilute Potts model[6,7] on the honeycomb lattice whose Hamiltonian is

$$-\beta\mathcal{H} = \sum_{ij} t_i t_j \left[K' + K^* \delta_q(\sigma_i - \sigma_j) \right] + \Delta \sum_i t_i \tag{27}$$

with

$$\begin{aligned} e^{K^*} &= (e^K + q - 1)/(e^K - 1) \\ e^{K'} &= 1 - e^K \\ e^{-\Delta} &= q(e^L - 1) \end{aligned} \tag{28}$$

Here $t_i = 0, 1$ and $\sigma_i = 1, \ldots, q$ for $t_i = 1$ only.

The Potts models (1) or (27) also generate a site-bond percolation. Consider the honecomb lattice for which each site is occupied with a probability s and each bond a probability p, then the critical threshold of this percolation process is[27,28]

$$f(1, -\ln p, -\ln s) = 0 \tag{29}$$

where $f(q, K, L) = 0$ is the ferromagnetic critical point of the system (1). However, the general expression of $f(q, K, L)$ is not known except in the cases of pure two-site interactions for which[22]

$$f(q, K, 0) = e^{3K} - 3e^{K} - q + 2 \tag{30}$$

and the Ising case for which[34]

$$f(2, K, L) = e^{K+L} - 3 \tag{31}$$

Consider next the limit of

$$e^{-(M-K)/2} = y = \text{finite}, \qquad M \to \infty, \quad K \to \infty \tag{32}$$

From (3) we see that the A (antiferromagnetic) triangles have zero weights. It follows that if we draw bonds on the dual (honeycomb) lattice to separate spins in different states, the resulting graphs G are always *closed* polygons. In fact, the mapping between the spin configurations and the polygonal graphs G is $q(q-1)^p$ to 1, where p is the number of polygons in G. Furthermore, since each bond carries a weight y, we obtain the following identity in the limit (32):

$$q^{-1}e^{-2NM}Z(q, L, K) \to F(q, y) \equiv \sum_{G} (q-1)^p y^b \tag{33}$$

Here, as before, N is the number of sites of the triangular lattice, $Z(q, L, K)$ is the partition function of (1), and b is the number of bonds in G. A typical G in the expansion of $F(q, y)$ is shown in Fig. 8.

Before we consider a further limit of (33), we pause here to consider the graph generating function $F(q, y)$.

Domany *et al.*[35] have shown that $F(q, y)$ is related to the partition function of a spin model with a $O(q-1)$ symmetry. It follows that the critical properties of a $O(N)$ model will show a change at $N = 3$ (corresponding to the $q = 4$ change of the Potts model).

Of particular interest is the function $F(3, y)$ which can be interpreted as generating physical models in a number of ways. First, consider an Ashkin–Teller model on the triangular lattice[36] and its graphical representation as follows: To each spin configuration draw bonds on the dual, the

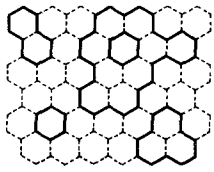

Fig. 8. Typical configuration of a term in the expansion (33) of the graph-generating function $F(q, y)$. Each bond has a weight y and each polygon has a weight $q - 1$.

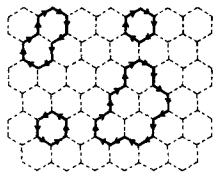

Fig. 9. Representation of the graph-generating function $F(3, y)$ as generating directed polygons. Each polygon can be directed independently in the clockwise or the counterclockwise direction. These graphs also generate a continuous XY-type model, and a special triangular spin model of s (> 3) states in which the states of two neighboring sites can differ by 0 or 1 (mod. s) only.

honeycomb lattice, to separate spins in different states. If, in the notations of Ref. 36, we take $\omega_1 = \omega_2 = y$, $\omega_3 = 0$, then only the configurations of closed polygons will survive, and the partition function is given precisely by $4F(3, y)$. Results of Ref. 36 then lead to the conclusion that $F(3, y)$ is critical at $y_c = 1/2$.

The function $F(3, y)$ can also be regarded as generating a triangular spin model of s (> 3) states in which, if the spin states are numbered from 1 to s, the states of two neighboring sites can differ by 1 and 0 (mod. s) only. The simplest way to see this equivalence is to direct the polygons, once in the clockwise and once in the counterclockwise direction. This takes care of the factor of 2^p in (33). A typical configuration of directed polygons is shown in Fig. 9. Going around a vertex of the honeycomb lattice, one makes the rule of an outgoing (ingoing) arrow increases (decreases) the spin states by 1. There then exists an exact one-to-one correspondence between the directed polygonal configurations and the spin configurations. By the same reasoning as indicated above the critical point of this spin model is determined at $y_c = 1/2$ for *all* $s > 3$.

The function $F(3, y)$ can also be regarded as the partition function of a continuous XY type model on the honeycomb lattice with the nearest-neighbor Boltzmann factor $1 + 2y\cos\theta_{ij}$. By writing $2\cos\theta = e^{i\theta} + e^{-i\theta}$ and representing the terms $e^{i\theta_{ij}}$ by a directed edge running from site i to site j, we see that the partition function is again represented by directed polygons, and hence by (33). Thus, the above consideration relates this XY model to the special spin model of s (> 3) states mentioned in the above. In fact, the last equivalence is more general and can be extended to all planar lattices. Following our considerations it is immediately seen that this special s-state spin model on any planar lattice is equivalent to an XY model on the dual, provided that $s > \gamma =$ the coordination number of the dual. For example, the $s > 4$ spin model on the square lattice [with the restriction that the spin states of neighboring sites can differ by only 0 or 1 (mod. s)] is equivalent to a square XY model. This last result has been established by Domany *et al.*[37] from a much more elaborate consideration.

Now we consider (33) further by making use of another observation due to Domany *et al.*[35] Taking $y = [z/(q-1)]^{1/6}$ and then the limit $q \to \infty$, the right-hand side of (33) generates precisely the hard-hexagon lattice gas configurations for which Baxter[8] has obtained the exact solution. In particular the critical point is found to be

$$z_c = \tfrac{1}{2}(11 + 5\sqrt{5}) = 11.09017\ldots \tag{34}$$

From the elaborate amount of analysis that led to Baxter's solution, it is perhaps safe to conclude that it will take a major breakthrough to solve the general q-state Potts model (1).

8. SUMMARY AND CONCLUSIONS

The main new conclusion of this paper for the three-state Potts model on the triangular lattice is the first-order transition found to exist on the coexistence line. This is compared to the continuous transition occurring at a bicritical point predicted by the renormalization-group analysis of Schick and Griffiths.[12] It is not surprising that they have failed to find a first-order transition since, prior to the introduction of transformations which include dilute variables,[6,7] virtually all real-space renormalization group studies had failed to find the known first-order transitions in the $q > 4$ ferromagnets. This may well be more than just an analogy, because one way of looking at our model is as a system of interacting triangles. Each triangle can take on one of 27 states, but the critical behavior should be dominated by interactions between clusters of the 6 (for $M \ll 0$) or 9 (for $M = 0$) types with the largest weights, so that the system can be regarded as a 6-state or 9-state Potts ferromagnet with additional anisotropic interactions. If these anisotropic interactions are irrelevant (in the sense of introducing no new fixed points), then the $M < 0$ and $M = 0$ systems would exhibit first-order transitions since they are equivalent to, respectively, the 6-state and 9-state Potts ferromagnets. A less radical assumption is to suppose merely that the anisotropic interactions are irrelevant only in models with sufficiently large q, so that for $q = 3$ we might allow the possibility of some new type of continuous transition for $M \ll 0$.

Finally, we have also demonstrated interesting connections of the q-state Potts model (1) on the triangular lattice with other lattice-statistical problems.

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