PHYSICAL REVIEW B VOLUME 23, NUMBER 11 1 JUNE 1981

q-state Potts model in general dimension

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(Received 1 December 1980)

Critical properties of the q-state Potts and Potts-lattice-gas models are calculated by means of the Kadanoff variational renormalization group for dimensions 1.58, 2, and 2.32, and the Migdal approximation for arbitrary dimensions. Accurate results for the critical and tricritical exponents are obtained as well as for q_c, the largest value of q for which the Potts transition is continuous. It is concluded unambiguously that the three-state Potts model in three dimensions undergoes a first-order phase transition.

I. INTRODUCTION

One reason the q-state Potts model[1] has received much attention in recent years is the interesting dependence of its critical properties on the parameter q. Whereas Landau mean-field arguments[2] predict that the transition is first order for all $q > 2$ independent of dimension, Baxter[3] proved that, in two dimensions, this prediction is correct only for $q > q_c = 4$. For $q \leq q_c$, the transition is continuous. This result led to many attempts to calculate the critical exponents of the model for arbitrary q, but none reproduced the abrupt change in the nature of the transition at q_c.[4] In 1979, den Nijs[5] conjectured that for $q \leq q_c$ the thermal exponent of the Potts model, y_T, is related to that of the eight-vertex model, y_T^{8v},[6] according to

$$(y_T - 3)(y_T^{8v} - 2) = 3 \ , \tag{1}$$

where $y_T^{8v} = (2/\pi)\cos^{-1}(\sqrt{q}/2)$ taken along the branch $0 \leq y_T^{8v} \leq 1$. That such a relation might exist is plausible in light of the mapping between the Potts model and the Baxter line of the eight-vertex model.[3,5] Nienhuis, Berker, Riedel, and Schick[7] then showed how the change in the nature of the transition with q emerges readily in the context of a renormalization-group (RG) calculation when carried out on a generalization of the Potts model, the Potts-lattice gas.[8] This model has three fixed points, critical, tricritical, and discontinuity, when $q < q_c$, and a single discontinuity fixed point, when $q > q_c$, such that the phase transition of the pure Potts model is governed for $q < q_c$ by the critical fixed point and for $q > q_c$ by the discontinuity fixed point. As usual, the discontinuity fixed point describes first-order behavior.[9] At $q = q_c$, the critical and tricritical fixed points annihilate, which reflects the special properties of the four-state Potts model.[3] Once this mechanism for the change in the nature of the transition at q_c is established, analyticity of the RG equations implies that one analytical relation must yield the critical and tricritical exponents as functions of q. In particular, Nienhuis *et al.*[7] suggested that the extension of the den Nijs conjecture of Eq. (1) to the branch $-1 \leq y_T^{8v} < 0$ yields the tricritical thermal exponent of the Potts-lattice gas. An approximate calculation employing the Kadanoff variational RG method[10] yielded critical and tricritical exponents in very good agreement with these conjectures.[11] The same approximation was applied to obtain values for the magnetic exponents, y_H, and the results suggested the relationship[12,13]

$$(4y_H + y_T^{8v} - 6)(y_T^{8v} - 2) = -3 \ . \tag{2}$$

The other critical exponents follow from the usual scaling relations with $\nu = 1/y_T$ and $\delta = y_H/(d - y_H)$. The topology of smoothly merging lines of critical and tricritical fixed points[7] has been used to construct phenomenological scaling-field equations from which the singularity structure of the free energy has been extracted.[14,15] Recently, Black and Emery[16] have presented a microscopic derivation of the den Nijs conjecture (1).

The purpose of this paper is to study the critical properties of the Potts model for general dimension, d. In particular, the dependences of the critical exponents on q and d and of the critical value, q_c, on d are determined numerically. The calculation incorporates the same ideas that led to the successful evaluation of the properties of the two-dimensional Potts model. The techniques employed are the Kadanoff variational RG procedure,[10] for dimensions $d = 1.58$, 2, and 2.32, and the Migdal bond-shifting technique,[17] for general d. Both schemes are applied to the Potts and the Potts-lattice-gas models. Other recent work on the Potts model in d dimensions is discussed in Sec. IV.

The main results of this study are as follows.[18] First, q_c decreases rapidly as a function of d near two dimensions and is already less than three for $d = 2.32$. Therefore, the three-state Potts model in three dimensions exhibits a first-order transition.

Second, when dimension one is approached from above, q_c behaves like $\exp[2/(d-1)]$. Third, the small-q behavior of the exponents predicted by Eqs. (1) and (2), $y_T \propto q^{1/2}$ and $d - y_H \propto q^{1/2}$, is peculiar to two dimensions. For all other dimensions, y_T and y_H linearly approach finite values between zero and d as $q \to 0$. Fourth, for d greater than two the degree of instability of the fixed points along the "tricritical" line changes from two to three, with decreasing q, at a value $q_m(d)$. This may indicate that the tricritical behavior is classical for q less than $q_m(d)$.

II. METHODS

Central to the success of the computational approach to the Potts model,[7,11,12] which yields first *as well as* second-order phase transitions, is the idea of enlarging the Hamiltonian space to that of the Potts-lattice gas. Some remarks motivating this method are in order. Any RG describing a phase transition must preserve the symmetries that relate the phases involved.[19] For the q-state Potts model, the q equivalent ordered phases transform into each other under the elements of the permutation group of q objects, while the disordered phase is invariant under this group of transformations. In a first-order transition the symmetry must be preserved at a discontinuity fixed point, which occurs at zero temperature.[9] Since one is limited, in approximate RG calculations, to finite systems one faces the difficulty that no zero-temperature cluster of Potts spins is both disordered and invariant under the permutation group. An easy way around this difficulty is to introduce a new spin state to be associated with the disordered phase in analogy to the q states of the original Potts spin associated with the q ordered phases.[7] The new state referred to as the vacancy state must be chosen such that it is invariant under permutation of the other q states. In practice, this procedure is implemented by mapping disordered clusters of Potts spins onto the vacancy state rather than onto a Potts spin. Under repeated iteration the disordered phase is mapped by this RG transformation onto a state in which all sites are vacant. The symmetries of this state are easily preserved at zero temperature along with those of the ordered states which guarantees the existence of a discontinuity fixed point. This procedure describes the Potts model as embedded in the more general space of Potts-lattice-gas Hamiltonians. The nearest-neighbor Hamiltonian for a Potts-lattice gas is

$$-\beta\mathcal{H} = \sum_{<i,j>} t_i t_j (K + J\delta_{s_i,s_j}) - \Delta \sum_i t_i \ , \tag{3a}$$

with the symmetry-breaking term

$$-\beta\mathcal{H}' = \sum_i t_i \delta_{1,s_i} + \sum_{<i,j>} t_i t_j [L(\delta_{1,s_i} + \delta_{1,s_j}) + M\delta_{1,s_i}\delta_{1,s_j}] \ . \tag{3b}$$

The lattice-gas variable t_i equals unity if a Potts spin $s_i = 1, 2, \ldots, q$ occupies lattice site i and is zero otherwise. The chemical potential Δ governs the concentration of vacancies. Throughout the calculation, q enters as a continuously variable parameter. The topology of the lines of critical and tricritical fixed points associated with this model was briefly reviewed in the Introduction.[7]

The above ideas are easily incorporated into standard RG approximation methods. Here we employ the Kadanoff variational method[10] and the Migdal bond-moving scheme.[17] Consider the model (3) on a hypercubic lattice of d dimensions. In the variational approach, this Potts-lattice-gas Hamiltonian can be written as a sum over local Hamiltonians, each representing 2^d sites of an elementary hypercube, $-\beta\mathcal{H} = \sum \mathcal{H}_{hc}$. The RG transformation maps each block of spins onto a single site. The dimension of the lattice enters solely through the number of sites of the elementary hypercube, and the transformation is well defined whenever 2^d is an integer. However, the computation time needed to solve the variational equations grows rapidly with d. Therefore, only the cases $2^d = 3$, 4, and 5, or $d = 1.58$, 2, and 2.32, were investigated for general q. The pure Potts subspace is considered for comparison since, in two dimensions, it had been found to yield superior critical exponents when $q \ll q_c$. Details of the computational method are found elsewhere.[10,11,20,21]

Migdal recursion relations can be easily formulated for general d.[17] We used the approach to obtain qualitatively the critical behavior of the Potts model for general q and d. There is an ambiguity in the procedure as to what fraction, p, of the on-site chemical potential, Δ, is to be shifted with the nearest-neighbor bonds. Results of the Migdal method depend in general on this parameter, p, and also on the value of the rescaling factor, l. In certain limits universal, i.e., parameter independent results are found that appear to be more reliable. For example, Migdal[17] observed that the method yields for the n-vector model with $n > 2$, $d \gtrsim 2$, critical exponents that to leading order are independent of l and in agreement with exact results. For the Potts model we find that in the limit $d \to 1+$ the value for q_c becomes independent of p and l.

III. RESULTS

The calculational techniques can be tested for the two-dimensional Potts model against the presumably exact results (1) and (2) for the thermal and magnetic exponents. Figures 1(a) and 1(b) summarize results obtained by the Kadanoff variational method as well as the conjecture.[11,12] Critical and tricritical data are shown as lower and upper branches. Applied to the Potts-lattice gas, the method yields, in

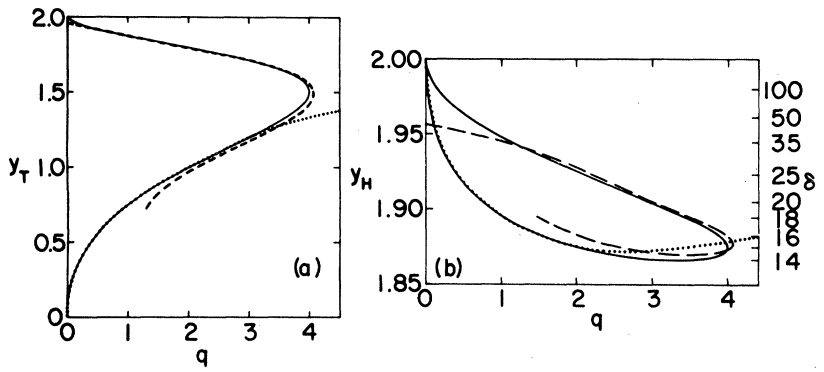

FIG. 1. Thermal exponent y_T (a) and magnetic exponent y_H (b) as functions of q for the critical and tricritical Potts transitions in two dimensions (lower and upper branch, respectively) from variational renormalization-group calculation for pure and dilute Potts systems (dotted and broken curves, respectively). The solid curves represent the conjectured data that are presumably exact.

the vicinity of q_c and along the tricritical branch, exponents in excellent agreement with the conjectures. For smaller q on the critical branch, the calculation for the pure Potts model gives more accurate exponent values. In fact, no dilute critical fixed point was found for the Potts-lattice gas when $q < 1$. Of course, only the lattice-gas calculation reveals the changeover to first-order behavior. The critical value $q_c \approx 4.08$ compares well with the exact one,[3] $q_c = 4$. Burkhardt[20] has independently carried out the variational calculation for $d = 2$ and finds full agreement with our results. Finally, in the limit of small q, the Migdal method yields excellent critical exponents as shown in the inset of Fig. 2.

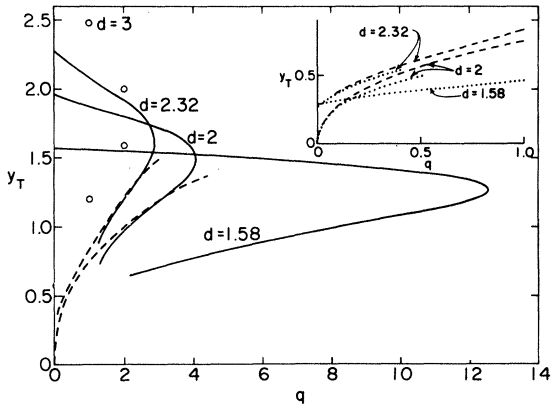

FIG. 2. Thermal exponent y_T vs q for the q-state Potts model of dimensions $d = 1.58$, 2, and 2.32 from variational renormalization-group calculation (dashed and solid curves for pure and dilute Potts systems, respectively) and Migdal approximation (dotted curves in the inset of the figure). The results for $d = 2$ are identical with those in Fig. 1(a). Circles denote exponent values for the one- and two-state Potts models in three dimensions.

Figures 2–5 present data for the leading and next-to-leading thermal and magnetic exponents as obtained from variational RG calculations for the Potts-lattice gas (solid curve) and the pure Potts model (dashed curve) for dimensions $d = 1.58$, 2, and 2.32. Lower and upper branches refer again to critical and tricritical transitions and, for $q > q_c(d)$, the transitions are first order. The circles in Fig. 2 denote values for the critical and tricritical thermal exponents of the three-dimensional Potts model for $q = 1$ and 2 obtained by other techniques.[22] The points can be connected smoothly by a curve of a shape similar to those depicted for $d < 3$. This yields $q_c(d = 3) \approx 2.2$. Figure 3 shows that the tips of the curves coincide very closely with the point at which the second thermal exponent, $y_{T,2}$, changes sign. This provides a criterion for the quality of the approximation and internal consistency of the calculation. Figures 4 and 5 exhibit results for the first and second magnetic eigenvalues, y_H and $y_{H,2}$, respective-

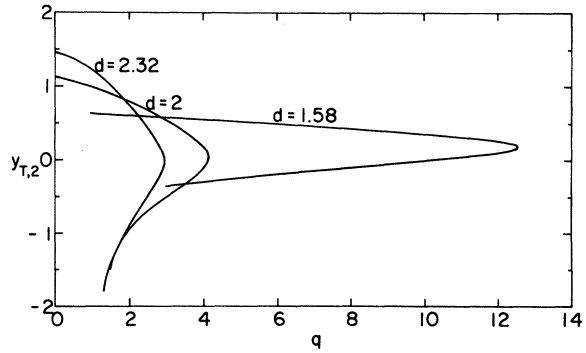

FIG. 3. Second thermal exponent $y_{T,2}$ vs q for the q-state Potts-lattice-gas model in dimensions $d = 1.58$, 2, and 2.32 from variational renormalization-group calculation. The exponents change sign at $q = q_c(d)$ to good approximation.

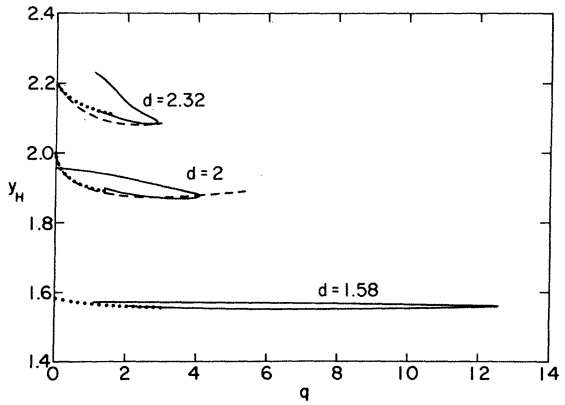

FIG. 4. Magnetic exponent y_H vs q for the q-state Potts-lattice gas in dimensions $d=1.58$, 2, and 2.32 from variational renormalization-group calculation (dashed and solid curves) and Migdal approximation (dotted curves). The results for $d=2$ are identical with those in Fig. 1(b).

ly, which are relevant for both the critical and tricritical transitions. We expect that $y_{H,2}$ is also approximated well by the variational method since, for $d=2$ and $q=q_c$, it yields $y_{H,2}\approx\frac{7}{8}$ in agreement with a conjecture by Barber.[23]

In comparing the results for different dimensions one makes the following observations.

(i) The shapes of the curves close to the tips, i.e., for $q \lesssim q_c$, are very similar. This indicates that in this range of dimensions the same mechanism is responsible for the changeover from continuous to first-order behavior and that the exponents are analytic functions of q near q_c. This property is likely to change at $d=4$, when q_c becomes equal to 2. As is apparent from Figs. 2 and 3, the eigenvalues y_T and $y_{T,2}$ for $d=2.32$ on the tricritical branch exceed their classical values two and one, respectively, for all $q \lesssim q_m \simeq 1.46$. For these values of q, we find three relevant thermal exponents indicating that the fixed points no longer describe tricritical phenomena.[24] We infer that the tricritical line of fixed points intersects with the Gaussian fixed line at $q=q_m$ and that the actual tricritical behavior for all $q<q_m$ is classical. If so, $q_m(d)$ should approach two as d approaches four, the upper tricritical dimensionality of the Potts model.[25]

(ii) Much attention has been paid to the question of how the critical value q_c, at which the Potts transition changes from continuous to first order, depends on the dimension d of the system. There are one exact result, $q_c(d=2)=4$,[3] and two conjectures, $q_c(d\geq 4)=2$ (Ref. 26) and $q_c(d\to 1+)\propto\exp[2/(d-1)]$. The data points in Fig. 6 summarize the results for $q_c(d)$ obtained from the variational RG approach to the Potts-lattice gas as well as, for $d=3$, from the interpolation through the data points in Fig. 2. The smooth curve in Fig. 6 is a guide to the eye. In dimensions $d=1.58$, 2, and 2.32 we find the sequence for q_c of 12.6, 4.08, and 2.85. Therefore, near two dimensions, q_c decreases rapidly as a function of d and is less than three at $d=2.32$. Hence we conclude that the three-state Potts model in three dimensions undergoes a first-order phase transition. In the limit $d\to 1+$, we find from numerical work employing the Migdal method that q_c assumes the asymptotic form $q_c\propto\exp[2/(d-1)]$, independent of the RG parameters p and l (compare Sec. II). Berker and collaborators[27] have obtained this result independently, but did not consider the p dependence.

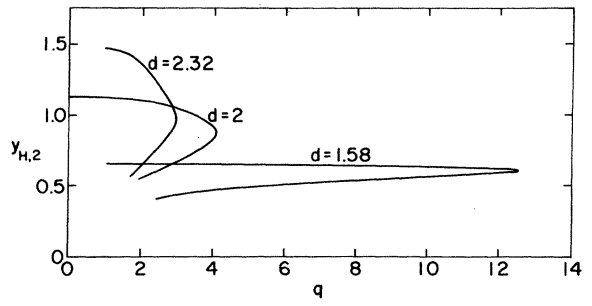

FIG. 5. Second magnetic exponent $y_{H,2}$ vs q for the q-state Potts-lattice gas in dimensions $d=1.58$, 2, and 2.32 from variational renormalization-group calculation. In two dimensions at q_c, the exponent assumes to within 0.2% the value $\frac{7}{8}$ conjectured by Barber.

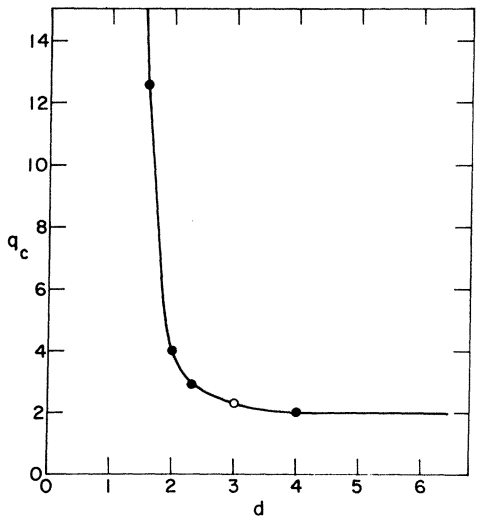

FIG. 6. Critical value q_c as function of d from variational renormalization-group calculation for $d=1.58$, 2, and 2.32, respectively, smooth interpolation of series expansion data for $d=3$, and conjecture for $d\geq 4$.

(iii) The small-q behavior of the exponents predicted by Eqs. (1) and (2), $y_T \propto q^{1/2}$ and $y_H - d \propto q^{1/2}$, is peculiar to two dimensions. For all other dimensions, y_T and y_H linearly approach finite values between zero and d. Specifically, Fig. 2 shows that the thermal critical exponent y_T equals zero at $q=0$ only when $d=2$. The inset of that figure compares the results of the variational RG (dashed curve) with those of the Migdal bond-moving scheme (dotted curve). The agreement for q close to zero is striking and may indicate the reliability of these calculations for small q. Furthermore, we find that within the Migdal approximation the tricritical thermal and magnetic exponents approach d for all dimensions. The variational RG calculation does not show that, probably for the following reason. The probability for the presence of a spin, $\langle t \rangle$, is proportional to the number of spin states q. When q approaches zero the system will be depleted of all spins unless the chemical potential diverges like $\ln q$. At the tricritical fixed point generated by an approximate RG this is not normally the case. The ambiguity in the Migdal bond-moving scheme (compare Sec. II) allows one to cure this problem by setting $\Delta = \tilde{\Delta} - \ln q$ and shifting only $\tilde{\Delta}$. This yields magnetic and thermal exponents that approach d when q vanishes.

(iv) The special role that dimension $d=2$ plays is apparent from Figs. 7 and 8, which show the thermal and magnetic exponents as functions of d for some values of q. The results are for the pure Potts model by means of the Migdal method. Although the Migdal results are incorrect for large d (for example, as $d \to 6$ the exponent y_T approaches one rather than two) they show the proper behavior for small q and d. The exceptional behavior at $d=2$ is due to the fact that this is the lower critical dimensionality of the zero-state Potts model.[28] It has been stated that this implies that the Migdal recursion relations become

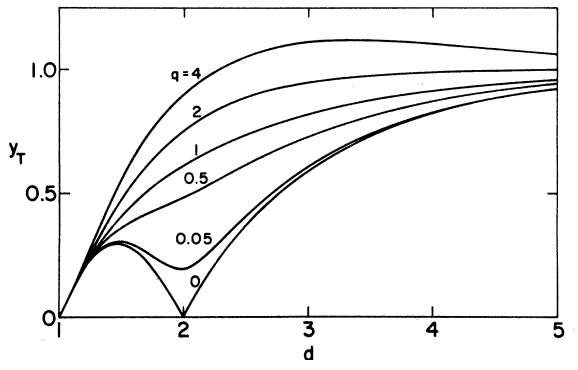

FIG. 7. Thermal exponent y_T as function of d for the critical Potts transition from Migdal recursion relations. The lower critical dimension of the zero-state Potts model is presumably two.

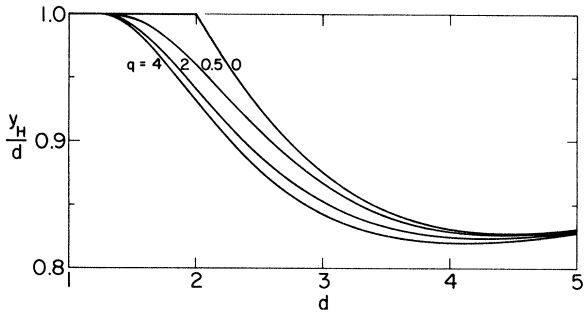

FIG. 8. Magnetic exponent y_H/d as a function of d for the critical Potts transition from Migdal recursion relations.

exact to first order in $(d-2)$, but we are not aware of a proof. If correct one would expect that at $d=2$ the exponents and critical temperature can be obtained exactly to first order in $\sqrt{q}$. The critical temperature is obtained correctly, $T_c = 1/\ln(\sqrt{q}+1)$. However, if the conjectures (1) and (2) for the exponents are exact then the Migdal results are off by a factor $3/\pi$ to first order in $\sqrt{q}$. We note that the situation is reverse for the n-vector model in the $(2-d)$ expansion, where the Migdal method yields the exact critical exponents but a critical temperature off by a factor $3/\pi$.[17]

IV. DISCUSSION

The results presented above are numerical in nature and contribute to the phenomenology of the critical properties of the Potts model. The thermal and magnetic exponents, for the critical and tricritical transitions, have been obtained as functions of q and d, and the critical value q_c as a function of d. The calculational method developed previously for the two-dimensional Potts model is of conceptual interest. In the remainder of this section we review other recent work on the Potts model and compare with our results.

Aharony and Pytte[26] have obtained near four dimensions,

$$q_c(d=4-\epsilon) = 2 + \epsilon + O(\epsilon^2) \ , \tag{4}$$

expanding about the Ising limit in terms of $q-2$. The upper critical dimension of the Potts model is six for $q \neq 2$. One observes that the curve in Fig. 6 does not follow the result (4) for $d \lesssim 4$. A similar expansion for the thermal and magnetic exponents, y_T and y_H, would be instructive since it could decide whether the exponents depend analytically on q near q_c for all $d < 4$.

With regard to the three-state Potts model in three dimensions, our calculation predicts that the transition is first order and explains why theoretical calcula-

tions[29] and experiments may have difficulty determining the order of the transition. The topology of the RG phase diagram is such that for q not much larger than q_c, the RG flows towards the discontinuity fixed points are strongly influenced by the operator that is marginal at q_c. As a result the latent heat is small {$L \propto \exp[-C/(q-4)^{1/2}]$ in two dimensions[3]} while the specific heat and susceptibility are large so that the transition almost appears to be second order. However, computer simulations,[30] a $1/q$ expansion,[31] the present study, as well as early momentum-space RG calculations[32] and an experiment[33] leave no doubt as to the first-order nature of the transition.

There is a large body of evidence supporting the validity of the conjectures (1) and (2) for the exponents of the two-dimensional Potts model. The first direct proof of (1) on the critical branch is a derivation by Black and Emery.[16] The analyticity arguments of Sec. I imply that (1) is also exact for the tricritical values. Evidence for (2) includes agreement with the new exact results for the hard hexagon model by Baxter,[34] which imply $y_H(q=3)=\frac{28}{15}$, as well as numerical results by the variational RG[11] and a transfer matrix calculation.[35] In the absence of such conjectures for $d \neq 2$, calculations such as those described herein must suffice to predict critical behavior of the Potts model in general dimension.

ACKNOWLEDGMENTS

This research was supported in part by the NSF under Grants No. DMR77-12676 A02 and No. DMR79-20785.

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