PHYSICAL REVIEW B VOLUME 24, NUMBER 11 1 DECEMBER 1981

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Critical exponents and marginality of the four-state Potts model: Monte Carlo renormalization group

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(Received 21 September 1981)

The thermal critical exponent of the four-state Potts model in two dimensions is evaluated as $\nu^{-1} = 1.49 \pm 0.01$, using the Monte Carlo renormalization-group method. The presence of a marginal scaling direction is also indicated. These results confirm previous conjectures, universality, and logarithmic corrections. A purely Potts Hamiltonian is considered. A four-point interaction is used to control the chemical potential of effective vacancies, without the introduction of explicit vacancy states.

Several years ago, Baxter[1] rigorously derived the latent heats of the two-dimensional Potts models,[2] showing that they go to zero as the number of states q is lowered to $q_c = 4$. This was interpreted as the occurrence of second-order phase transitions[3] for $q \leq q_c$, and of first-order transitions for $q > q_c$. The renormalization-group mechanism[4] for this changeover at q_c, obtained more recently, involves a line of fixed points [CMT in Fig. 1(a)] controlling all higher-order phase transitions. This fixed line, parametrized by q, turns over and reverses stability within the phase boundary surface, at q_c. Thus, phase boundary points with $q > q_c$ cannot attain this fixed line, and instead renormalize to first-order fixed points [ZF in Fig. 1(a)].

Previously to the renormalization-group solution mentioned above, den Nijs[5] had proposed a conjecture for the exact values of the critical exponents $y(q)$ for $0 \leq q \leq 4$:

$$[y(q) - 3][\hat{y}(q) - 2] = 3 \quad , \tag{1}$$

where

$$\cos[\tfrac{1}{2}\pi\hat{y}(q)] = \tfrac{1}{2}\sqrt{q} \quad .$$

This curve [$y_2^c(0)y_2(4)$ in Fig. 1(b)] passes, of course, through Onsager's[6] exact result $y_2^c(q=2) = 1$. In the renormalization-group treatment, it was noticed that the tricritical fixed points of these Potts models [TM in Fig. 1(a)] are a smooth continuation of the critical fixed points (CM), and that, on the other hand, the den Nijs formula (1) is multivalued. This led to the extension[4] of the conjecture, to include exact values for the tricritical exponents [$y_2^t(0)y_2(4)$ in Fig. 1(b)]. The entire curve is in general agreement with previous[7,8] and subsequent[9–16] calculations, most notably with the subsequent derivation of $y_2^c(3) = \frac{6}{5}$ by Baxter[15] (for the hard hexagon problem which has the ordering symmetry of the $q = 3$ Potts model), and of the entire critical branch $y_2^c(0)y_2(4)$ by Black and Emery.[16]

However, confirmation of the turnover point at $q = 4$ has not been satisfactory. This point should have the leading thermal exponent

$$\nu^{-1} = y_2(q=4) = \tfrac{3}{2} \quad , \tag{2a}$$

according to the den Nijs conjecture.[5] Furthermore, the renormalization-group description of the changeover from first- to second-order transitions indicates[4]

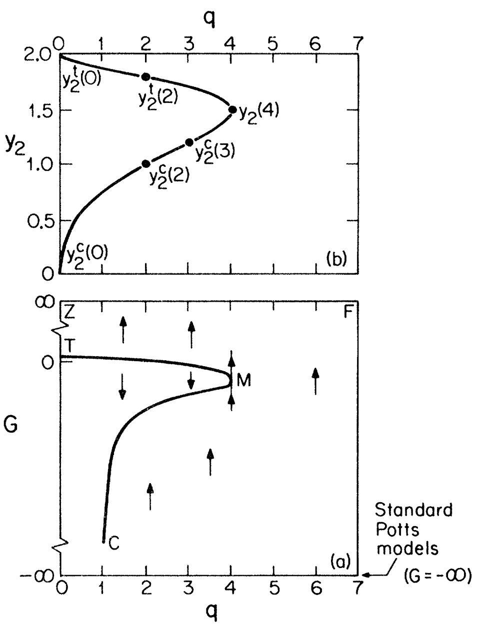

FIG. 1. (a) Schematic renormalization-group flows within the phase boundary surface. *CMT* and *ZF* are lines of fixed points controlling higher- and first-order transitions, respectively. *G* is a dilution chemical potential. See Refs. 4 and 23. (b) Extended den Nijs conjecture for the exact values of critical, $y_2^c(q)$, and tricritical, $y_2^t(q)$, exponents. At the turnover point, $y_2^c(q_c)=y_2^t(q_c)\equiv y_2(q_c=4)$.

a reversal of fixed-point stability at $q_c=4$. It was pointed out[10,17] that this picture directly implies a next-leading thermal exponent which is marginal,

$$y_4(q=4)=0 \quad , \tag{2b}$$

and logarithmic corrections in the critical properties of the $q=4$ Potts model. However, the predicted values (2) have not been firmly established by direct calculation, as discussed below. Moreover, although the exact value of $y_2=\frac{3}{2}$ was previously obtained[18] for the triplet Ising (Baxter-Wu) model, which has the ordering symmetry of the $q=4$ Potts model and is therefore related by universality, logarithmic corrections were rigorously absent.[18]

Monte Carlo renormalization-group[8,19] studies of the Potts models have given good agreement with the above conjectures, both for the critical exponents[8,10] $y_2^c(2)$ and $y_2^c(3)$, and for the tricritical exponent[12] $y_2^t(2)$. However, the method failed to converge for $q=4$, successive renormalization-group iterations giving[10,11] estimates for $y_2(4)$ of 1.21, 1.27, 1.30, and 1.33. This slow convergence was surprising in the light of the corresponding Monte Carlo renormalization-group calculation[20] for the triplet Ising model, which showed very rapid convergence.

The $q=4$ Monte Carlo renormalization-group results were interpreted by Rebbi and Swendsen[10] as arising from slow convergence to the fixed point due to the marginal operator. They were able to say that the data were consistent with the existence of a marginal operator and $y_2(4)=\frac{3}{2}$, but could not explicitly confirm the predictions of Eqs. (2). On the other hand, Eschbach, Stauffer, and Herrmann[11] argued that the sequence of estimates could be extrapolated to obtain $y_2(4)=1.34$. Variational position-space renormalization-group calculations[9] and a recent finite-size scaling calculation[14] did give good agreement with the conjectured $y_2(4)$.

In this paper, we present the results of a new Monte Carlo renormalization-group calculation, which accurately reproduces Eq. (2a). Specifically, we find

$$y_2(4)=1.49\pm0.01 \quad , \tag{3}$$

as well as indication of the marginality of the next thermal exponent $y_4(4)$. The four-state Potts model is studied on the square lattice, with the Hamiltonian:

$$-\beta\mathcal{H}=J\sum_{\langle ij\rangle}\delta_{s_is_j} + F\sum_{\langle ijkl\rangle}(1-\delta_{s_is_j})(1-\delta_{s_js_k})(1-\delta_{s_ks_l})(1-\delta_{s_ls_i}) \quad , \tag{4}$$

where $s_i=a$, b, c, or d, and $\delta_{s_is_j}=1(0)$ for $s_i=s_j$ $(s_i\neq s_j)$. The first term is the usual nearest-neighbor coupling. The second term is a four-point coupling which assigns an energy F to any elementary square $\langle ijkl\rangle$ with all four bonds broken. Thus, this term controls local disorder, which in the renormalization-group solution[4] was shown to be important. The changeover in the order of the phase transitions in Potts models has been studied in terms of somewhat different four-point interactions in two other works.[21,22]

A comparison, in this respect, may be useful. The renormalization-group treatment of Ref. 4 projects the locally disordered, entropically important regions as effective vacancies, which appear in the renormalized Hamiltonian.[23] The fixed point is then located in the Hamiltonian space of this extended (Potts-lattice-gas[24]) model. In the present Monte Carlo renormalization-group calculation, vacancy projection is never introduced. Each site is always in one of the four permutation-symmetric states of the $q=4$ model. Nevertheless, the effective vacancies still exist, inherently but not manifestly. They could be thought of as elementary excitations of the system. They have a non-negligible presence at the fixed point.

The control over the effective vacancies provided by the four-point coupling is used to circumvent the difficulty of approaching the fixed point along the marginal direction, under renormalization-group transformations. By adjusting F, we were able to analyze a system that approaches the fixed point

TABLE I. Values for the leading thermal eigenvalue exponent, $y_2(4)$, calculated with a 48×48 lattice. Data were taken from a run of 4.25×10^5 MC step/site at intervals of 10 MC step/site, after discarding 4.5×10^4 MC step/site to establish thermodynamic equilibrium. Using eight interaction parameters, the Monte Carlo renormalization-group analysis was performed for scale factors 2^m. The number of the renormalization-group iteration is denoted by n. Estimates of the statistical uncertainty of the last digits are given in parentheses. The conjectured values is $y_2(4)=1.5$.

n	$m=1$	2	3	4
1	1.512(3)	1.503(3)	1.50(1)	1.50(4)
2	1.490(5)	1.49(1)	1.49(4)	
3	1.49(2)	1.49(5)		
4	1.49(7)			

along a direction essentially orthogonal to the marginal one. Such a $q=4$ Potts model has no logarithmic corrections to scaling, and thus is very much like the triplet Ising model. Convergence in the Monte Carlo renormalization group is very rapid.

The Monte Carlo renormalization-group method has been described in detail in several other places.[8,19] In this calculation, square cells and a majority rule with a random tie breaker were used. We have located the criticality condition at $J_c=1.20463$, for $F/J=0.85$. Self-consistent checks[19] within the Monte Carlo renormalization-group method indicate an accuracy for J_c of 1 part in 10^3. Our numerical results are summarized in Tables I–IV, as obtained from simulating a 48×48 lattice. The finite-size effect was found to be negligible, from comparison with simulations of 24×24 and 12×12 lattices.

Table I shows the immediate convergence of $y_2(4)$ to the conjectured[5] value of 1.5. This rapid convergence is comparable to that obtained in a Monte Carlo renormalization-group study[20] of the triplet Ising model, which also has no logarithmic corrections, and contrasts strongly with the slow convergence obtained in direct simulations,[10,11] of the nearest-neighbor $q=4$ Potts model, which does have logarithmic corrections. The consistency of the analyses with different scale factors 2^m indicates that the eigenvector is well represented.

Tables II and III show our results for the leading, $y_1(4)$, and the next-leading, $y_3(4)$, magnetic eigenvalue exponents in good agreement with the conjectured[25] exact values of 1.875 and 0.875. The very small rise in y_1 at the higher iterations n must be due to a slight residual error in the determination of the critical point.

Table IV contains the results for a more difficult part of the computation—the confirmation of the presence of a marginal eigenvalue, $y_4(4)=0$. Superimposed on the larger statistical errors in determining a nonleading eigenvalue, a clear systematic trend is seen towards smaller values of $|y_4|$ as the scale factor is increased. This is characteristic of having included an insufficient number of interactions into the analysis. Since the renormalization-group transformations with larger scale factors include many more interactions in the implicit calculation of higher powers of the recursion matrix, we have a strong indication of a marginal eigenvalue with a complicated eigenvector.

Finally, the use of Hamiltonian (4) provides the possibility of exploring a new direction. By making F

TABLE III. Values for the next-leading magnetic eigenvalue exponent, $y_3(4)$. The conjectured value is 0.875.

n	$m=1$	2	3	4
1	0.890	0.882	0.885	0.876
2	0.876	0.878	0.868	
3	0.881	0.863		
4	0.859			

TABLE II. Values for the leading magnetic eigenvalue exponent, $y_1(4)$, calculated under the conditions described in Table I. The conjectured value is 1.875.

n	$m=1$	2	3	4
1	1.868	1.872	1.877	1.886
2	1.875	1.881	1.892	
3	1.887	1.899		
4	1.911			

TABLE IV. Values for the next-leading thermal eigenvalue exponent, $y_4(4)$. This is expected to be marginal, $y_4(4)=0$.

n	$m=1$	2	3	4
1	−0.08	−0.09	−0.15	−0.10
2	−0.38	−0.25	−0.15	
3	−0.36	−0.26		
4	−0.45			

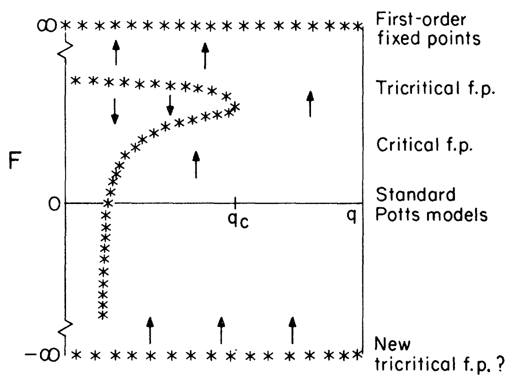

FIG. 2. Speculative flow diagram within the phase boundary surface, in a space where the effective vacancies can be suppressed (by $F < 0$). Asterisks (*) represent renormalization-group fixed points, whose natures are indicated on the right-hand side.

negative, the effective vacancies of the usual Potts models are removed. For $q = 20$, and $F/J = -1$, we see from Monte Carlo analysis that the latent heat of the first-order transition is reduced by a least 50%. (The transition temperature, J^{-1}, is increased by only 15%.) Thus, the first-order character of Potts transitions can be considerably weakened by this suppression of local disorder, although not completely removed as vacancies occur at a larger length scale. (Long-range interactions suppressing effective vacancies at all length scales should restore the second-order transitions, with corresponding novel universality classes, at $q > q_c$.) Accordingly, one could speculate in terms of the flow diagram shown in Fig. 2.

ACKNOWLEDGMENTS

A.N.B. would like to thank the Physics Group at the IBM Zürich Laboratory for their warm hospitality. Work at MIT was supported by NSF Grant No. DMR-79-26405.

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