Critical behavior of the three-state Potts model: Monte Carlo renormalization group

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The critical behavior of the three-state Potts model in two dimensions is investigated with the use of the Monte Carlo renormalization group (MCRG), and the results are compared with conjectured values as well as with other methods. Recent advances in the MCRG enable greatly improved convergence, as well as greater insight into the structure of the renormalization transformation. The introduction of a four-point interaction is used to control the chemical potential of effective vacancies in a purely Potts Hamiltonian.

I. INTRODUCTION

A q-state Potts model[1] orders at low temperatures into one of q phases related by global q-fold permutation symmetry. The $q=3$ Potts model in two dimensions ($d=2$) attracted attention by the fact that its phase transition is second order,[2-6] in qualitative violation of classical theory, which dictates a first-order transition with the occurrence of a third-order term in the free-energy functional.[7] Subsequently, it was noted that inert gases epitaxially adsorbed onto basal graphite, undergoing critical and tricritical phenomena, are realizations of the $q=3,d=2$ Potts model[8] and of its extension by vacancies.[9] A precise specific-heat measurement[10] for helium on graphite yielded an unusually large specific-heat exponent α which was later confirmed by theory. This measurement, along with various other information, led to a conjecture for the exact critical exponents of q-state Potts models in two dimensions,[11] later extended to tricritical exponents,[12] and proven in the critical branch.[13,14] The exact solution[15] of the hard-hexagon problem, with the $q=3$ Potts-ordering symmetry, also confirmed the critical conjecture. Renormalization-group (RG) studies of the critical behavior of the $q=3,d=2$ Potts model have been carried out using finite-cluster truncation,[16] variational optimization,[17-19] and finite-size scaling.[20,21] The Monte Carlo renormalization group[22-42] (MCRG) provides an alternative approach, which is highly accurate and flexible, unambiguously yielding many of the critical properties.

Recent advances in MCRG methods have greatly increased the number of systems for which they can be successfully used to calculate critical properties. In particular, two new features have made it possible to optimize the convergence.

First, a method of determining the critical temperature directly from the MCRG analysis has been developed, without having to rely on any other method. This makes it possible to introduce more parameters into the initial Hamiltonian without loss of accuracy (Refs. 24, 25, 28, 36, 40, and 41).

The second improvement is more fundamental to the general theory of the RG and arises from an improved understanding of the effect of the renormalized transformation. It was obtained from calculations for the q-state Potts model in two dimensions,[12] in which the introduction of vacancies (an additional state, accounting for fluctuations in the amplitude of the order parameter) into the renormalized Hamiltonians enabled both first- and second-order transitions to be described by real-space truncation approximations. Later, it was recognized that "effective vacancies" could also be described by four-spin operators without introducing an extra state.[42] Explicit calculations for the $q=4$ Potts model showed that such terms were important in the renormalized Hamiltonian and could be exploited to obtain accurate estimates of the critical exponents despite the difficulties caused by the presence of a marginal operator.[43-50]

In the following section, the basic equations of the MCRG method will be summarized. The results for the $q=3$ Potts model will be presented in Sec. III and discussed in Sec. IV.

II. MCRG FORMALISM

The operator on lattice site i will be denoted by σ_i. For the q-state Potts model,[1] σ_i takes on integer values 1 through q and the Hamiltonian can be written as

$$H=\sum_{\alpha} K_{\alpha} S_{\alpha} , \tag{1}$$

where the S_{α}'s are the various combinations of the σ_i's. The nearest-neighbor (NN) Potts operator is simply

$$S_{\mathrm{NN}}=\sum_{\langle ij\rangle} \delta_{\sigma_i,\sigma_j} . \tag{2}$$

The block-spin renormalization transformation we have used for the $d=2$ Potts model divides the square lattice into 2×2 blocks (scale factor $b=2$) and gives the block spin σ_i' the value of a plurality of the spins in the block. Ties are assigned to each of the spin values in question with equal probability using a random-number generator.

The renormalized coupling constants are assumed to be

analytic functions of the original coupling constants. Linearizing, we write the RG transformation as

$$(K_\alpha^{(n+1)}-K_\alpha^*)=\sum_\beta T_{\alpha\beta}(K_\beta^{(n)}-K_\beta^*)\ , \tag{3}$$

where

$$T_{\alpha\beta}=\frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} \tag{4}$$

is found numerically by solving the set of chain rule equations

$$\frac{\partial\langle S_\gamma^{(n+1)}\rangle}{\partial K_\beta^{(n)}}=\sum_\alpha \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}}\frac{\partial\langle S_\gamma^{(n+1)}\rangle}{\partial K_\alpha^{(n+1)}}\ , \tag{5}$$

and the derivatives in Eq. (5) are obtained from Monte Carlo correlation functions, using equations of the form

$$\frac{\partial\langle S_\gamma^{(n+1)}\rangle}{\partial K_\beta^{(n)}}=\langle S_\gamma^{(n+1)}S_\beta^{(n)}\rangle-\langle S_\gamma^{(n+1)}\rangle\langle S_\beta^{(n)}\rangle\ . \tag{6}$$

The techniques for determining the critical point of a general model developed from an approach introduced by Wilson[28] for the study of lattice gauge theories (Refs. 24, 25, 36, 40, and 41). The size effect is compensated by simulating lattices differing by the scale factor b and using the RG transformation to obtain different renormalized Hamiltonians on the same-size lattice. A particularly efficient procedure for calculating the differences in coupling constants from differences in correlation functions is to solve the set of linear equations

$$\langle S_\alpha^{(n)}\rangle_L-\langle S_\alpha^{(n-1)}\rangle_S=\sum_\beta\left[\frac{\partial\langle S_\alpha^{(n)}\rangle_L}{\partial K_\beta^{(0)}}-\frac{\partial\langle S_\alpha^{(n-1)}\rangle_S}{\partial K_\beta^{(0)}}\right]\delta K_\beta^{(0)}\ , \tag{7}$$

where L and S refer to the large and small systems and the derivatives are calculated in analogy with Eq. (6). To find the condition of criticality, we used Eq. (7) to minimize the differences in the correlation functions while varying a single coupling constant.

III. GENERALIZED POTTS MODEL

We consider a general two-dimensional, three-state, nearest-neighbor Potts model of the form

$$H=KS_{\rm NN}+FS_v\ , \tag{8}$$

where the operator for nearest-neighbor coupling is defined in Eq. (2) and the "vacancy" operator by sums over plaquettes (plaq)

$$S_v=\sum_{\rm plaq}(1-\delta_{i,j})(1-\delta_{j,k})(1-\delta_{k,l})(1-\delta_{l,j})\ . \tag{9}$$

Preliminary work on this model used MCRG methods to map out the phase diagram.[41] Fairly small lattices were used for the MC simulations, the largest being 16×16. Comparisons were made with 8×8 and 4×4 lattices using Eq. (7) to calculate the critical value of K for various fixed values of F. It was shown that all simulations were consistent with the critical exponents conjectured, but that the convergence for $F=0.4$ was particularly rapid.

In the light of these results, we also concentrated our effort on $F=0.4$. An improved value for the nearest-neighbor coupling, $K=-1.0307$, was taken from the results of the previous simulations at $K=-1.032$, comparing 16×16 and 8×8 lattices.

Table I contains data for the MC simulations of three different lattices, with linear dimensions $L=16$, 32, and 64. In each case, the data were stored in about 100 separate groups and all aspects of the analysis were repeated for each of several subsets of the data to obtain estimates of the statistical errors. The operators used in the RG analysis of the MC data are given in Table II.

The correlation functions of the renormalized systems are affected by both the change in the coupling constants through renormalization and the change in system size. If the generalized Hamiltonian we have used is really close to the fixed point of the RG transformation, then the Hamiltonian will remain nearly unchanged by the transformation and the major effect on the correlation functions comes from the change in lattice size. This implies that systems reaching the same size after different numbers of RG steps should show equal correlation functions. Data testing this assumption are given in Table III. Nearest-neighbor and vacancy correlation functions are shown for each of the three lattices simulated after vari-

TABLE I. MC simulation data for MCRG calculations. $d=2,q=3$ Potts model $K=-1.0307$, $F=0.4$. Data taken for correlation functions every 10 MC steps per site.

Lattice size (L)	64	32	16
10^5 MC steps per site used	14	50	83
10^4 MC steps per site discarded	14	5	9

TABLE II. Coupling constants used in the RG analysis of MC simulations of the $d=2,q=3$ Potts model.

N_c	Description
	Even couplings
1	Nearest neighbor (10)
2	"Vacancy" operator on elementary plaquette
3	Next-nearest neighbor (11)
4	"Crossed-product" operator
5	Third neighbor (20)
6	"Vacancy" operator on sublattice plaquette
7	Three-spin "vacancy" operator
	Odd couplings
1	Magnetic field
2	Three spins on a plaquette (00)-(10)-(11)
3	Three spins in a row (00)-(10)-(20)
4	Three spins at an angle (00)-(10)-(12)

TABLE III. Nearest-neighbor and "vacancy" correlation functions for the $d=2,q=3$ Potts model as a function of the renormalized lattice size and the linear dimension of the original lattice (L). $K=-1.0307$, $F=0.4$.

Renormalized lattice	N_c	Original lattice size (L) 64	32	16
64×64	1	0.412(1)		
	2	0.0159(1)		
32×32	1	0.407(2)	0.403(6)	
	2	0.0165(1)	0.0153(1)	
16×16	1	0.383(3)	0.389(2)	0.383(1)
	2	0.0155(2)	0.0156(1)	0.0143(1)
8×8	1	0.339(4)	0.351(2)	0.354(1)
	2	0.0133(3)	0.0139(1)	0.0139(1)
4×4	1	0.270(6)	0.283(4)	0.288(2)
	2	0.0104(5)	0.0110(2)	0.0114(1)
2×2	1		0.166(4)	0.171(2)
	2		0.0065(3)	0.068(1)

ous numbers of renormalization steps. The data are presented in such a way that all numbers in a given row correspond to the same-size renormalized lattice and would be equal if the original system were exactly at the fixed point and there were no statistical errors. It can be seen that the agreement is quite good, although there seems to be a slight trend for the correlations to be weaker as the number of RG steps increases. This effect is very small in terms of the change implied in the initial value of the critical coupling as shown in Table IV. On the basis of this data, our best estimate for the critical value of K would be -1.0313, although this change of less than 0.1% is within the statistical uncertainty and does not affect our results.

Table V presents our MCRG data for the leading thermal eigenvalue exponent y_T. It should be remembered that the RG analysis should give the correct critical exponents in the limit of many coupling constants (to describe the eigenvectors correctly) and many RG iterations (to get close to the fixed point). From the data it is very easy to include sufficient coupling constants, and there are no significant changes after taking first- and second-neighbor coupling and the vacancy operator into account. The size effect is also small. It only amounts to about 1% between renormalized lattice sizes of 8×8 and 16×16. Between 16×16 and 32×32 it is smaller than

TABLE IV. Estimates of the deviation of the simulated coupling constant from the true critical value for K when $K=-1.0307$ with the value of F fixed at 0.4. $d=2,q=3$ Potts model. Data obtained by a least-squares fit to the differences in seven calculated correlation functions. 2×2 RG block transformation.

N_r	Lattice sizes being compared 64–32	32–16
2	0.0005(3)	0.0005(5)
3	0.0007(4)	0.0005(5)
4	0.0006(5)	

TABLE V. Critical eigenvalue exponent y_T (exact value is 1.200) for the $d=2,q=3$ Potts model as a function of the number of RG iterations (N_r), the number of coupling constants in the RG analysis (N_c), and the linear dimension of the lattice (L). 2×2 block transformation.

N_r	N_c	Lattice size (L) 64	32	16
1	1	1.143(3)	1.137(1)	1.129(1)
	2	1.149(2)	1.144(1)	1.136(1)
	3	1.175(2)	1.174(1)	1.172(1)
	4	1.175(2)	1.174(1)	1.172(1)
	5	1.176(2)	1.174(2)	1.173(1)
	6	1.176(2)	1.174(2)	1.173(1)
	7	1.176(2)	1.175(2)	1.173(1)
2	1	1.168(3)	1.159(1)	1.144(2)
	2	1.173(3)	1.166(1)	1.152(2)
	3	1.188(3)	1.189(1)	1.185(2)
	4	1.188(3)	1.189(1)	1.184(2)
	5	1.189(3)	1.190(1)	1.183(1)
	6	1.189(3)	1.189(1)	1.180(1)
	7	1.189(3)	1.188(1)	1.179(1)
3	1	1.167(4)	1.151(2)	1.139(2)
	2	1.174(4)	1.158(2)	1.147(2)
	3	1.195(4)	1.190(2)	1.213(2)
	4	1.194(4)	1.188(2)	1.211(2)
	5	1.194(4)	1.187(2)	
	6	1.193(5)	1.184(3)	
	7	1.193(5)	1.183(3)	
4	1	1.171(8)	1.142(4)	
	2	1.177(8)	1.149(4)	
	3	1.211(8)	1.216(4)	
	4	1.210(9)	1.214(4)	
	5	1.203(16)		
	6	1.198(16)		
	7	1.197(16)		

TABLE VI. Critical eigenvalue exponent y_H (exact value is 1.866 67) for the $d=2,q=3$ Potts model as a function of the number of RG iterations (N_r), the number of coupling constants in the RG analysis (N_c), and the linear dimension of the lattice (L). 2×2 RG block transformation.

		Lattice size (L)		
N_r	N_c	64	32	16
1	1	1.8699(2)	1.8701(1)	1.8705(2)
	2	1.8697(1)	1.8694(1)	1.8689(2)
	3	1.8694(1)	1.8690(1)	1.8683(2)
	4	1.8694(1)	1.8690(1)	1.8683(2)
2	1	1.8679(4)	1.8683(3)	1.8684(3)
	2	1.8665(3)	1.8658(2)	1.8643(3)
	3	1.8663(3)	1.8654(2)	1.8636(3)
	4	1.8663(3)	1.8654(2)	1.8636(2)
3	1	1.8690(4)	1.8700(6)	1.8696(6)
	2	1.8664(3)	1.8651(4)	1.8626(7)
	3	1.8661(3)	1.8645(4)	1.8613(7)
	4	1.8660(4)	1.8645(4)	
4	1	1.8735(10)	1.872(2)	
	2	1.8695(5)	1.865(2)	
	3	1.8699(5)	1.864(2)	
	4	1.8688(8)		

TABLE VIII. Critical eigenvalue exponent y_{H2} (exact value is 0.667) for the $d=2,q=3$ Potts model as a function of the number of RG iterations (N_r), the number of coupling constants in the RG analysis (N_c), and the linear dimension of the lattice (L). 2×2 RG block transformation.

		Lattice size (L)		
N_r	N_c	64	32	16
1	2	0.60(1)	0.598(4)	0.595(1)
	3	0.68(1)	0.683(4)	0.682(1)
	4	0.68(1)	0.684(6)	0.682(2)
2	2	0.61(1)	0.613(4)	0.606(4)
	3	0.68(2)	0.688(3)	0.684(4)
	4	0.68(2)	0.685(3)	0.675(5)
3	2	0.59(2)	0.592(4)	0.583(6)
	3	0.66(2)	0.671(4)	0.697(5)
	4	0.66(2)	0.660(5)	
4	2	0.57(2)	0.591(9)	
	3	0.66(3)	0.703(9)	
	4	0.65(3)		

the statistical errors. This means that the systematic error due to the size effect is negligible for the first two RG transformations of the 32×32 lattice and the first three transformations of the 64×64 lattice. Even the first transformation is only 2% below the conjectured value of $y_T=1.2$ and the third iteration is within 0.6%. This is a substantial improvement over the convergence from the nearest-neighbor Hamiltonian, where the first three RG iterations gave values of 1.11, 1.14, and 1.17 for y_T.[33]

The convergence of the leading magnetic eigenvalue is even better, as shown in Table VI. The statistical errors are much smaller than for y_T for the usual reason that the expectation value of the magnetization vanishes on finite lattices, so that the second term in Eq. (6) can be ignored.

TABLE VII. Estimates of the exponent for the $d=2,q=3$ Potts model from finite-size scaling on renormalized lattices. The exact value is $\eta=0.266\,67$. Values of η obtained by comparison of renormalized lattices (n) and ($n-1$) from a single MC simulation as a function of the size of the original lattice (L). 2×2 RG block transformation.

	Lattice size (L)		
n	64	32	16
1	0.260	0.258	0.254
2	0.263	0.259	0.249
3	0.257	0.247	0.223
4	0.239	0.218	

Since the statistical errors are about 0.0003, an apparent size effect of about 0.0007 or 0.0009 between renormalized lattice sizes of 8×8 and 16×16 might be real (compare the first transformations starting from the 32×32 and 16×16 lattices and compare the second transformations between the 64×64 and 32×32 lattices). The 64×64 lattice then gives the sequence 1.8694(1), 1.8663(3), and 1.8660(4), where the last number might have been depressed by 0.0007 due to the size effect. Not only do the second and third iterations agree, indicating convergence, but the deviation from the conjectured[45,46] then proven[51] value of $y_H=\frac{28}{15}=1.866\,67$ is less than 0.04% (even without correcting for a finite-size effect in the third iteration). The distinction between the value of $\frac{28}{15}$ for the $q=3$ Potts model and the value of $\frac{15}{8}=1.875$ for the $q=2$ Potts model (Ising model) is therefore clearly demonstrated, even though it is only 0.45%.

The accuracy for y_H is actually about the same as that achieved by the finite-size scale method, working with infinite strips of finite width.[20,21] In this context, it is interesting to check the results of a finite-size scaling calculation using the same MC data, as shown in Table VII. These results for the exponent $\eta=d+2-2y_H$ are less satisfactory than either the MCRG or finite-strip results, although still consistent with the conjectured $\eta=0.266\,67$. The dependence on lattice size is too strong to produce highly accurate values.

An advantage of the MCRG method is that it produces estimates automatically for several eigenvalues from the same MC simulation. In particular, a second relevant magnetic eigenvalue appeared in these calculations, as it had previously in the data of Rebbi and Swendsen.[33] The two sets of values are consistent, although our convergence is much better and our statistical errors are much

TABLE IX. Critical eigenvalue exponent y_{T2} for the $d=2,q=3$ Potts model as a function of the number of RG iterations (N_r), the number of coupling constants in the RG analysis (N_c), and the linear dimension of the lattice (L). 2×2 RG block transformation.

		Lattice size (L)		
N_r	N_c	64	32	16
1	2	−2.11(4)	−2.09(2)	−2.13(2)
	3	−2.04(6)	−2.00(2)	1.97(2)
	4	−1.46(2)	−1.47(2)	−1.46(1)
	5	−1.00(5)	−1.03(2)	−1.04(2)
	6	−1.15(5)	−1.17(2)	−1.15(1)
	7	−0.87(3)	−0.84(1)	−0.83(1)
2	2	−2.13(3)	−2.16(2)	−2.11(4)
	3	−2.32(4)	−2.32(3)	−2.20(4)
	4	−1.50(3)	−1.49(3)	−1.41(2)
	5	−1.08(4)	−1.11(3)	−1.37(2)
	6	−1.19(3)	−1.18(2)	−1.22(1)
	7	−0.86(2)	−0.88(1)	−0.87(1)
3	2	−2.14(8)	−2.13(4)	
	3	−2.30(12)	−2.23(4)	
	4	−1.56(4)	−1.42(3)	
	5	−1.13(4)	−1.37(3)	
	6	−1.17(2)	−1.22(2)	
	7	−0.93(3)	−0.89(2)	
4	2	−2.11(8)		
	3	−2.22(9)		
	4	−1.42(6)		
	5	−1.31(7)		
	6	−1.17(5)		
	7	−0.86(5)		

smaller, as shown in Table VIII. The size effect seems to be negligible within the statistical errors and all the data are consistent with a value of y_{H2} of about 0.68, in very satisfactory agreement with the conjectured[46] and recently derived[51] value of $\frac{2}{3}$. Since we only used four interactions with odd symmetry in our analysis, we checked the results by reanalyzing the data using repeated RG transformations as single transformations with scale factor 2^m. No systematic changes were found.

We have also investigated the second thermal eigenvalue,[52] with somewhat disappointing results. Although both the statistical errors and the size dependence are fairly small, there is a very strong dependence on the number of interactions used in the RG analysis, as shown in Table IX. Repetition of the analysis, treating two, three, and four iterations of the RG transformation as a single transformation confirmed the view that additional interactions played an important role, as demonstrated in Table X for data for the 64×64 lattice. The values for the repeated transformation are systematically smaller than the average of those for the single transformations, which is the typical warning signal that more couplings are needed. It is possible that a good determination of this eigenvalue could be made from any analysis of an extended Potts model, including vacancy states explicitly in the simulation. Such a simulation should also be able to investigate "tricritical" behavior.[36]

IV. CONCLUSIONS

Rebbi and Swendsen[33] have considered the nearest-neighbor $q=3$ Potts model as part of a general study of the q-state models. They performed fairly long simulations (5×10^4 MC steps per site) on large (96×128) lattices at the exact critical temperature, which is known from duality. The results were not inconsistent with the expected thermal eigenvalue exponent, $y_T=1.2$, but the convergence was very slow. The magnetic eigenvalue exponent also came rather close to the currently accepted value of 1.8667, even though a value of 1.875 had been expected at the time.

The present calculation dramatically improves MCRG convergence. This is because the fixed-point Hamiltonian is readily approached by varying the field coupling to the

TABLE X. Critical eigenvalue exponent y_{T2} for the $d=2, q=3$ Potts model as a function of the number of RG iterations (N_r), the number of coupling constants in the RG analysis (N_c), and the power of the scale factor m. 2×2 RG block transformation on a 64×64 lattice.

		m (scale factor, 2^m)			
N_r	N_c	1	2	3	4
1	2	−2.11(4)	−1.70(13)	−1.76(19)	−1.87(15)
	3	−2.04(6)	−1.75(10)	−1.50(18)	−1.19(11)
	4	−1.46(2)	−1.22(5)	−1.53(10)	−1.03(9)
	5	−1.00(5)	−1.06(5)	−1.16(13)	−1.06(14)
	6	−1.15(5)	−1.00(8)	−0.99(7)	−0.97(5)
	7	−0.87(3)	−0.83(3)	−0.71(6)	−0.66(7)
2	2	−2.13(3)	−1.94(25)	−1.70(20)	
	3	−2.32(4)	−2.09(13)	−1.67(16)	
	4	−1.50(3)	−1.22(6)	−1.00(12)	
	5	−1.08(4)	−1.10(6)	−0.89(11)	
	6	−1.19(3)	−1.05(7)	−0.82(9)	
	7	−0.86(2)	−0.84(4)	−0.81(9)	
3	2	−2.14(8)	−1.71(5)		
	3	−2.30(12)	−1.68(12)		
	4	−1.46(4)	−1.14(7)		
	5	−1.13(4)	−1.18(9)		
	6	−1.17(2)	−1.12(9)		
	7	−0.93(3)	−0.85(7)		
4	2	−2.11(8)			
	3	−2.22(9)			
	4	−1.42(6)			
	5	−1.31(7)			
	6	−1.17(5)			
	7	−0.86(5)			

vacancy operator. Thus the presence of effective vacancies—fluctuations in the amplitude of the order parameter—is indicated in the asymptotic critical behavior.[53] For $q=3$ here, these effective vacancies affect the quantitative critical properties. For higher q ($q>4$), they qualitatively affect the transition by changing it to first order. Our present calculation, in addition to yielding very accurate critical exponents for the $q=3, d=2$ Potts model, illustrates the essential symbiosis between the quantitatively powerful MCRG procedure and the qualitative physical understanding of phase-transition mechanisms.

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