Monte Carlo renormalization-group study of the $d=3$ planar model

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The $d=3$ planar model is analyzed for the first time with the Monte Carlo renormalization-group (MCRG) method. To increase the efficiency of the calculation, an operator is introduced in analogy with the "vacancy" operator used in the MCRG analysis of the $q=4$ Potts model. This operator is shown to be important in understanding the effect of the renormalization transformation on the Hamiltonian, and in improving the convergence of the method.

I. INTRODUCTION

Monte Carlo (MC) computer simulations,[1,2] combined with a renormalization-group (RG) analysis,[3–6] have been shown to be useful for calculating properties of phase transitions in statistical models.[6–28] In principle, the MCRG methods that have been developed are extremely general and can be applied to any model of interest on a lattice in any number of dimensions. In practice, there are restrictions arising from limitations of computational power. These restrictions and other considerations have led to a concentration of most work to date on two-dimensional systems with discrete spin degrees of freedom.[29]

The main purpose of this work is to demonstrate the extension of the MCRG approach to systems with continuous degrees of freedom in three dimensions. Recent advances in MCRG methods now make it possible to attack such problems with available computers, and prepare the way for more accurate calculations with special-purpose machines.[6]

The most serious difficulty with the MCRG approach arises from the initial MC computer simulation. The restricted availability of computer time imposes a limit on the total number of MC steps that can be used for a given calculation. This must be divided by the number of sites in the system to be studied to determine the possible length of the MC simulation for a given problem. Increasing the size of the system necessarily reduces the number of Monte Carlo steps per site that can be used, and consequently reduces the accuracy to which the required correlation functions can be determined. The effect is naturally more pronounced in higher dimensions and further aggravated by the diverging relaxation times (critical slowing down) when the critical point is being studied. For a three-dimensional system, doubling the system's length L directly affects the length of the simulation by a factor of 8 and the relaxation times increase by roughly a factor of 4. The computer time required for a given accuracy therefore increases by a factor of 32. This generally produces a rather well-defined practical limit to the size of the lattice that can be treated.

On the other hand, for the MCRG analysis, it is desirable for the system to be as large as possible. Since each renormalization transformation reduces the linear dimensions by the scale factor b, the system rapidly becomes so small that finite-size effects dominate. For three dimensions, the maximum value of L for most computer facilities is about 32 and the simplest RG transformations have a scale factor $b=2$. Since finite-size effects are often noticeable when the renormalized lattice is reduced to $L=4$, there are at most three RG transformations from which useful information about the critical exponents can be obtained.

It is clear from these considerations that rapid convergence is extremely important. Two recent improvements in technique have made it possible to optimize the convergence.

The first essential improvement is a method of determining the critical temperature directly from the MCRG analysis for any model of interest, without having to rely on data obtained by another method, such as high-temperature series or duality relationships. This makes it possible to introduce more parameters into the initial Hamiltonian without loss of accuracy.[6,15,16,20–22]

The second improvement comes from the insight into the nature of the renormalized couplings that has been obtained from the study of the q-state Potts model in two dimensions.[30–42] In that problem, the existence of both first- and second-order transitions for different numbers of states highlighted the necessity of understanding the effect of block-spin RG transformations on renormalized Hamiltonians. The breakthrough for real-space methods using truncation approximations came with the introduc-

tion of vacancies (an additional state), which enabled a compact description of the renormalized couplings.[32–37] The recognition that "effective vacancies" could also be described by four-spin operators without introducing an extra state, enabled the borderline case of the $q=4$ Potts model to be handled directly by explicitly compensating for the renormalized interactions with an additional term in the original Hamiltonian.[22]

In Sec. II the essential equations of the MCRG method are summarized for completeness. The nearest-neighbor $d=3$ planar (or XY) model is introduced in Sec. III and the MCRG calculation of the critical exponents is presented, based on a simulation at its critical temperature. It is seen that the statistical errors are not unreasonably large, but that the convergence is slow. The model is generalized in Sec. IV to demonstrate the improvement of the convergence. The prospects for future work and applications to other three-dimensional models are discussed in Sec. V.

II. MCRG FORMALISM

We shall denote the operator on lattice site i by σ_i and write the Hamiltonian in the general form

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

where the S_{α}'s are combinations of the σ_i's

For the RG analysis transformations will be considered in which the spin variables on neighboring sites are grouped into "blocks" and values for each "block spin" are assigned on the basis of the values of the spins in each block. The probability distribution of the new configurations is then described by a Hamiltonian of the form of Eq. (1) but with different (renormalized) coupling constants.

Starting with a MC simulation at criticality, the RG trajectory moves the renormalized Hamiltonian towards a fixed point. The renormalization-group transformation can then be linearized about the fixed point,

$$K_{\alpha}^{(n+1)}-K_{\alpha}^{*}=\sum_{\beta} T_{\alpha\beta}(K_{\beta}^{(n)}-K_{\beta}^{*}) , \tag{2}$$

and characterized by the matrix

$$T_{\alpha\beta}=\frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}} . \tag{3}$$

The asymptotic behavior and the critical exponents are calculated from the eigenvalues of this matrix, which is found by solving the set of chain-rule equations

$$\frac{\partial\langle S_{\gamma}^{(n+1)}\rangle}{\partial K_{\beta}^{(n)}}=\sum_{\alpha}\frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}}\frac{\partial\langle S_{\gamma}^{(n+1)}\rangle}{\partial K_{\alpha}^{(n+1)}} , \tag{4}$$

with derivatives obtained from MC correlation functions,

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

The expectation values of certain operators vanish by symmetry, so that some of the subtractions in Eq. (5) can be eliminated, improving the accuracy.

To calculate the critical temperature, it is necessary to compensate the size effect by simulating lattices of two different sizes. For systems differing by the scale factor b, one RG transformation of the large system will match the size of the smaller system. Differences in the correlation functions are then entirely due to differences in the Hamiltonians.[6] If these differences are not too large, we can calculate the effect of changing the coupling constants by making the linear approximation

$$\delta\langle S_{\alpha}^{(n)}\rangle=\sum_{\beta}\frac{\partial\langle S_{\alpha}^{(n)}\rangle_{L}}{\partial K_{\beta}^{(0)}}\delta K_{\beta}^{(0)} , \tag{6}$$

where L (S) refers to the large (small) lattices. The derivatives are calculated in analogy to Eq. (5).

A particularly effective alogrithm for calculating an approximate fixed point or locating the critical temperature uses differences in the correlation functions to calculate deviations of the coupling constants in $H^{(n)}$ from the fixed-point Hamiltonian,[43]

$$\langle S_{\alpha}^{(n)}\rangle_{L}-\langle S_{\alpha}^{(n-1)}\rangle_{S}=\sum_{\beta}\left[\frac{\partial\langle S_{\alpha}^{(n)}\rangle_{L}}{\partial K_{\beta}^{(0)}}-\frac{\partial\langle S_{\alpha}^{(n-1)}\rangle_{S}}{\partial K_{\beta}^{(0)}}\right]\delta K_{\beta}^{(0)} . \tag{7}$$

Since deviations from the fixed point in relevant directions are amplified by RG transformations, this method is extremely sensitive to the location of the critical point. A least-squares fit to a single coupling constant can be made and the consistency of the predicted change in the critical coupling compared with the measured differences in the correlation functions.[15,16,20,21]

III. THE NEAREST-NEIGHBOR MODEL

I shall first present an MCRG analysis of the nearest-neighbor three-dimensional planar model, defined on a simple cubic lattice by the Hamiltonian

$$H=K\sum_{\langle i,j\rangle}\sigma_i\sigma_j . \tag{8}$$

The renormalization transformation consists of

dividing the lattice into $2\times2\times2$ blocks, adding the two-dimensional vectors associated with each of the eight sites in the block, and renormalizing the sum to obtain a block spin of unit length. This RG transformation will be used throughout.

As is usual in MCRG calculations, the positions of the blocks on every level of renormalization were shifted every time correlation functions were evaluated to maximize the independence of the contributions of successive configurations.[13,19–21]

The operators used to analyze the results of the RG transformations for the nearest-neighbor model are given in Table I. Four separate MC simulations of this model were performed for lattices of various sizes ranging from $4\times4\times4$ to $32\times32\times32$. Table II contains technical data to aid in evaluating the statistical accuracy. For this part of the work, the simulations were performed at the critical coupling strength of $K_1=0.453\,93$, obtained from series expansions.[44] The confirmation of this value of the critical coupling by MCRG is discussed below.

Table III contains MCRG data for the leading thermal eigenvalue exponent $y_T=1/\nu$. The finite-size effect for the smallest lattice ($L=4$) is large and the entries in Table III for the first iteration of the RG transformation differ considerably from those obtained from the system with $L=8$. This is not surprising, since the renormalized lattice is only $2\times2\times2$ and imposes a substantial truncation on the renormalized Hamiltonian. Unfortunately, even the entries for $L=8$ are about 10% less than those of larger lattices. It is only when we compare the results of $L=16$ with $L=32$ that we find agreement, so that the finite-size effect can be regarded as negligible. Therefore, only the first two iterations of the RG transformation for the $L=32$ lattice (and the first RG transformation for the $L=16$ lattice) are characteristic of the infinite lattice. Since the first two iterations give different estimates of y_T, the renormalized Hamiltonians are not close enough to the fixed point for the sequence of estimates to have converged. This internal evidence is also confirmed by comparison with the value of 1.49, obtained from other methods,[44–47] which differs considerably from the values of 1.0 and 1.3 obtained from the first two RG transformations.

Table IV gives estimates of the magnetic eigenvalue exponent y_H, obtained from the same simulations. The situation here is somewhat better, in that the finite-size effect is only evident for an RG transformation which reduces a $4\times4\times4$ lattice to a $2\times2\times2$ lattice. Even for these extremely small lattices, the finite-size effect is less than 3%. The statistical accuracy of the results is also substantially better than for the thermal eigenvalues. This is a common effect due to the vanishing of all odd correlation functions, which makes it unnecessary to perform the subtractions in Eq. (5).

However, the convergence of the magnetic eigenvalues is also rather slow. The three available RG iterations give values for y_H of 2.27, 2.39, and 2.44. These are all below the expected value of 2.48.[44–48] Although they are consistent with a smooth convergence from below, the convergence is too slow to make clear predictions.

Another method of extracting critical exponents from the same MC data is illustrated in Table V. This table shows estimates of the critical exponent η obtained from the calculated values of the magnetic susceptibility at the critical point, using finite-size scaling on the renormalized systems. Both a strong lattice dependence and and a strong dependence on

TABLE I. Coupling constants used in the analysis of the nearest-neighbor $d=3$ planar model.

	Even couplings
N_c	Description
1	Nearest neighbor (100)
2	Next-nearest neighbor (110)
3	Bi-quadratic nearest neighbor (100)
4	Third-nearest neighbor (111)
5	Fourth-nearest neighbor (200)
6	Sixth-nearest neighbor (211)
7	Seventh-nearest neighbor (221)
8	Eighth-nearest neighbor (222)
	Odd couplings
N_c	Description
1	Magnetic field: $(h*\sigma_i)$
2	$(h*\sigma_i)*(\sigma_i*\sigma_i)$
3	$(h*\sigma_i)*(\sigma_i*\sigma_j)$ nearest neighbor
4	$(h*\sigma_i)*(\sigma_i*\sigma_j)$ (110) neighbor
5	$(h*\sigma_i)*(\sigma_i*\sigma_j)$ (111) neighbor

TABLE II. MC simulation data for MCRG calculations for the $d=3$ planar model. Nearest-neighbor interaction $K_1=0.453\,93$. Data taken for correlation functions every 10 MC steps per site.

Lattice size (L)	32	16	8	4
10^3 MC steps per site used	55	336	1536	240
10^3 MC steps per site discarded	12	36	64	10

TABLE III. Critical eigenvalue exponent y_T for the $d=3$ planar 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). $K_1=0.453\,93$.

		Lattice size (L)			
N_r	N_c	32	16	8	4
1	1	1.08(2)	1.10(1)	1.16(1)	1.48(1)
	2	1.06(2)	1.08(1)	1.15(1)	1.53(1)
	3	1.01(3)	1.03(1)	1.06(1)	1.28(1)
	4	0.99(3)	1.00(1)	1.04(1)	1.28(1)
	5	0.98(3)	0.99(1)	0.96(1)	
	6	0.96(5)	0.97(1)	0.89(2)	
	7	0.97(5)	0.98(1)	0.89(2)	
	8	0.97(5)	0.98(1)	0.89(2)	
2	1	1.41(2)	1.50(1)	1.89(1)	
	2	1.39(3)	1.48(1)	1.92(1)	
	3	1.36(3)	1.41(1)	1.65(1)	
	4	1.34(3)	1.40(1)	1.65(1)	
	5	1.31(3)	1.29(2)		
	6	1.30(5)	1.22(5)		
	7	1.30(5)	1.22(6)		
	8	1.30(6)	1.22(6)		
3	1	1.59(4)	2.03(2)		
	2	1.56(5)	2.06(2)		
	3	1.50(5)	1.78(1)		
	4	1.49(5)	1.78(1)		
	5	1.36(6)			
	6	1.19(9)			
	7	1.24(7)			
	8	1.25(8)			
4	1	1.97(10)			
	2	1.99(10)			
	3	1.72(9)			
	4	1.72(10)			

the number of RG iterations (distance from the fixed point) is seen. Although this method has been shown to be effective in some systems, it does not produce useful results here.

A clear success of the MCRG analysis, despite the slow convergence for the critical exponents, is the confirmation of the critical temperature obtained from series expansions. Table VI shows the results of comparing pairs of lattices and performing a least-squares fit of the deviation of the coupling constant used for the simulation from the true critical coupling. The comparison of the $L=8$ and $L=4$ systems shows a systematic deviation of less than 3%, while the larger lattices show no deviation within the statistical errors.

It should, however, be noted that only on the second iteration do the deviations predicted by the small changes in the coupling constant really correspond to small differences in all measured correlation functions. Before this, the irrelevant deviations from the fixed point are still important and result in both positive and negative discrepancies. These discrepancies are very important in providing a hint as to the nature of the effect of the RG transformation on the Hamiltonian, leading to the modified MC simulations described in the following section.

Table VII shows raw data for the first- and second-nearest-neighbor correlation functions from the MC simulations both before and after RG transformations. The table is constructed with data for each correlation function for all lattices of a given size *after renormalization* shown on the same line. Therefore, by moving to the left on a given line, we can see the effect of renormalizing the Hamiltonian *without* changing the lattice size. The most striking feature is that both correlation func-

TABLE IV. Critical eigenvalue exponent y_H for the $d=3$ planar 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). $K_1=0.453\,93$.

		Lattice size (L)			
N_r	N_c	32	16	8	4
1	1	2.314(1)	2.318(1)	2.333(1)	2.385(1)
	2	2.314(1)	2.318(1)	2.333(1)	2.385(1)
	3	2.273(2)	2.274(1)	2.273(1)	2.243(2)
	4	2.273(2)	2.274(1)	2.273(1)	2.242(2)
	5	2.273(2)	2.274(1)	2.273(1)	2.242(2)
2	1	2.418(2)	2.440(2)	2.507(1)	
	2	2.418(2)	2.440(2)	2.507(1)	
	3	2.393(2)	2.393(1)	2.347(2)	
	4	2.393(2)	2.393(1)	2.343(2)	
	5	2.393(2)	2.393(1)	2.343(2)	
3	1	2.480(7)	2.558(4)		
	2	2.479(6)	2.558(4)		
	3	2.446(4)	2.395(4)		
	4	2.444(4)	2.392(4)		
	5	2.444(4)	2.392(4)		
4	1	2.556(2)			
	2	2.555(2)			
	3	2.386(2)			
	4	2.378(3)			
	5	2.379(3)			

tions increase as the renormalized Hamiltonians move towards the fixed point. The most plausible explanation seems to be that the nearest-neighbor coupling constant becomes stronger under renormalization. However, since we remain at criticality, additional interactions must be generated that compensate for this effect. This could be simply longer-range antiferromagnetic exchange, but attempts in this and other systems to compensate for the effect by introducing antiferromagnetic interactions between more distant neighbors have not been successful in improving the MCRG convergence. The alternative assumption that the important interactions in the renormalized Hamiltonians are relatively compact, many-spin terms is the basis for the investigation of a generalized model in the following section.

TABLE V. Estimates of the exponent η for the $d=3$ planar model from finite scaling on renormalized lattices. 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). $K_1=0.453\,93$.

	Lattice size (L)		
n	32	16	8
1	0.372	0.362	0.325
2	0.162	0.113	−0.043
3	0.033	−0.143	
4	−0.139		

IV. THE GENERALIZED MODEL

The speed of convergence of the MCRG method is determined by the magnitude and direction of the deviation of the original model from the fixed point of the RG transformation. To improve conver-

TABLE VI. Estimates of the deviation of the simulated coupling constant from the critical value for the $d=3$ planar model. $K_1=0.453\,93$.

		Lattice sizes being compared		
N_r	N_c	32–16	16–8	8–4
1	8	0.0028	0.0050	0.0127
2	8	0.0002	0.0022	0.0100
3	8	−0.0005	0.0015	
4	8	−0.0006		

TABLE VII. First- and second-nearest-neighbor correlation functions for the $d=3$ planar model as a function of the renormalized lattice size and the linear dimension of the original lattice (L). $K_1=0.453\,93$.

Renormalized lattice	N_c	Original lattice size (L) 32	16	8	4
32×32	1	0.994(2)			
	2	1.265(3)			
16×16	1	1.172(5)	1.015(1)		
	2	1.66(2)	1.322(3)		
8×8	1	1.33(2)	1.253(4)	1.066(1)	
	2	1.99(4)	1.85(1)	1.461(2)	
4×4	1	1.55(5)	1.58(1)	1.452(2)	1.213(2)
	2	2.6(2)	2.64(3)	2.384(5)	1.842(5)
2×2	1	2.21(7)	2.28(2)	2.213(3)	2.051(5)
	2	4.2(2)	4.22(4)	4.073(8)	3.69(2)

gence, we need information concerning the location of the fixed point, or, in other words, the effect of the RG transformation on the Hamiltonian. This information is difficult to obtain, but recent work on two models of interest in two dimensions has provided the hints that led to the calculation in this section.

The most important insights have come from the study of q-state Potts models in two dimensions.[13,22,27,30–42] These models exhibit second-order phase transitions for $q \leq 4$, and first-order phase transitions for $q > 4$.[31] The borderline case of $q=4$ is particularly difficult (and interesting), due to the presence of a marginal operator. This peculiarity leads to logarithmic corrections for the critical singularities,[13,35,36] differing in this respect from the Baxter-Wu model,[42] which is in the same universality class. It also leads to extremely slow convergence of the MCRG estimates for the critical exponents, since the rate at which the fixed point is approached in the marginal direction goes to zero close to the fixed point.[13,22]

Real-space renormalization-group calculations using truncation approximations showed that the artificial introduction of "vacancies" into the renormalized configurations allowed a compact description of the effects of renormalization and a qualitatively correct distinction between first-order transitions for large-q-values and second-order transitions for small-q values. Based on this success, Berker suggested that the effect of vacancies in the renormalized Hamiltonian could be imitated without introducing an extra state by using terms such as

$$S_F = \sum_{\text{plaq}} (1-\delta_{i,j})(1-\delta_{j,k})(1-\delta_{k,l})(1-\delta_{l,i}) , \tag{9}$$

where i, j, k, and l label the corners of a plaquette (plaq) or elementary square of the lattice, and $\delta_{i,j}$ is unity if the operators on sites i and j have the same value and zero otherwise. Explicit calculations then demonstrated that the convergence of the MCRG method was improved dramatically by proper choice of the coupling constant multiplying the additional term in the Hamiltonian being simulated; excellent agreement with the expected value of $y_T=1.5$ was obtained.[22]

The natural generalization of Eq. (9) to a planar model is

$$S_4 = \sum_{\text{plaq}} (1-\sigma_i\sigma_j)(1-\sigma_j\sigma_k)(1-\sigma_k\sigma_l)(1-\sigma_l\sigma_i), \tag{10}$$

where scalar products have replaced the δ functions. In the interest of simplicity, the same idea of a local, multispin interaction can lead to a term of the form

$$S_x = \sum_{\text{plaq}} (1-\sigma_i\sigma_k)(1-\sigma_j\sigma_l) . \tag{11}$$

The idea behind using these terms is that the RG transformations in Potts models and planar models show a certain similarity in the form of the blocks and the dominance of a majority of the spins in determining the value of the renormalized block spin. These formal considerations are strengthened by looking at the effect of such operators on the two-dimensional planar model. Kosterlitz and Thouless have shown the importance of the topological excitations known as vortices in determining the properties of the phase transitions.[49–51] Below the critical temperature, an RG transformation such as we have been using causes vortex-antivortex pairs to annihilate (this is rather easy to demonstrate numerically). The reduction of the number of vortices in the renormalized configurations requires a term in

the renormalized Hamiltonian that increases the vortex core energy, without affecting the Gaussian terms. The interactions in Eqs. (10) and (11) can be seen to have the desired properties, with S_x affecting the vortex core energy in a particularly direct manner, which can be exploited to improve our understanding of how first-order transitions can arise in models with planar symmetry.[52]

Since S_x is simpler than S_4, I have used S_x to explore the possibility of improving the convergence in the MCRG analysis of the three-dimensional planar model. Short preliminary runs were performed with $L=4$ and $L=8$ to find a reasonable value for the coupling constant K_x. I found that $K_x=0.10$ showed the effects quite clearly, so I fixed it at this value and varied K_1 to find the critical temperature. The operators used for the calculations with the generalized model reflected the new Hamiltonian, as specified in Table VIII. Data for the new MC simulations are given in Table IX.

The data in the preceding section have shown that the finite-size effect is important when the renormalized lattice is as small as $L=4$, but not when $L=8$. For a fully optimized calculation, it would be appropriate to investigate this point more carefully and determine more precisely for what lattices the finite-size effect becomes negligible. I have chosen not to do that, in order to make it easier to evaluate the results of the changes in the model parameters.

With the use of the procedures described in Sec. II, I determined the critical value of the nearest-neighbor coupling to be $K_1=0.6744$, when $K_x=0.10$. Table X shows that the MCRG estimates for the deviation of the true critical value of nearest-neighbor coupling constants are below the statistical uncertainties of about 0.2%.

The improvement of this starting point can be immediately seen in the behavior of the correlation functions, as shown in Table XI. The change in correlation strength upon renormalization is much less pronounced than it was for pure nearest-neighbor coupling in Table VII. The improvement has occurred as expected, with an increase in the nearest-neighbor correlations for the original simulation and only very small changes in the correlation functions after three RG transformations.

The most important test is the prediction of the thermal and magnetic critical exponents, which are shown in Tables XII and XIII. A comparison of Table XII with Table III shows that even the first RG transformation is closer to the expected value of 1.49.[44–47] The second iteration of the RG transformation, which was shown in the preceding section to be the closest to the fixed point without having a significant finite-size effect, is in complete agreement within statistical error.

As usual, the best convergence and smallest statistical errors are found for the magnetic eigenvalues, as seen in Table XIII. The size effect is again negligible down to a $4\times4\times4$ renormalized lattice, and both the second and third iterations starting with $L=32$ give values for y_4 in agreement with the expected 2.48 (Refs. 44—48) within statistical error.

In principle the MCRG method can also be used to investigate nonleading exponents. The necessary eigenvalues are delivered automatically by the computer analysis, but usually have much larger statisti-

TABLE VIII. Coupling constants used in the analysis of the $d=3$ planar model with the crossed-product operator. Odd couplings are the same as given in Table I.

	Even couplings
N_c	Description
1	Nearest neighbor (100)
2	Next-nearest neighbor (110)
3	Cross-product operator
4	"Vacancy" operator
5	Biquadratic nearest neighbor (100)
6	Third-nearest neighbor (111)
7	Fourth-nearest neighbor (200)
8	Sixth-nearest neighbor (211)
9	Seventh-nearest neighbor (221)
10	Eighth-nearest neighbor (222)

TABLE IX. MC simulation data for MCRG calculations for the $d=3$ planar model. Data taken for correlation functions every 10 MC steps per site. $K_1=0.6744$, $K_x=0.10$.

Lattice size (L)	32	16	8
10^4 MC steps per site used	5	17	50
10^3 MC steps per site discarded	1	26	36

TABLE X. Estimates of the deviation of the simulated coupling constant from the critical value of the nearest-neighbor coupling for the $d=3$ planar model, with the crossed-product coupling held fixed. $K_1=0.6744$, $K_x=0.10$.

		Lattice sizes being compared	
N_r	N_c	32—16	16—8
1	10	0.0010(4)	0.0009(10)
2	10	0.0003(4)	0.0000(12)
3	10	0.0002(4)	−0.0002(14)
4	10	0.0002(5)	

TABLE XI. First- and second-nearest-neighbor correlation functions for the $d=3$ planar model as a function of the renormalized lattice size and the linear dimension of the original lattice (L). $K_1=0.6744$, $K_x=0.10$. This table should be compared with Table VII for the nearest-neighbor model.

		Original lattice size (L)		
RG lattice	N_c	32	16	8
32×32	1	1.246(3)		
	2	1.580(8)		
16×16	1	1.29(1)	1.270(5)	
	2	1.83(3)	1.65(2)	
8×8	1	1.39(3)	1.37(2)	1.348(2)
	2	2.13(7)	2.04(5)	1.877(3)
4×4	1	1.64(6)	1.61(5)	1.617(3)
	2	2.7(2)	2.7(1)	2.673(8)
2×2	1	2.3(1)	2.26(6)	2.282(4)
	2	4.2(3)	4.2(2)	4.21(1)

cal errors and a stronger dependence on the size of the system and the number of interactions used in the analysis.[21] For the current calculation, the second-largest magnetic eigenvalue seems to suffer mostly from finite-size effects as shown in Table XIV. The size clearly dominates when the renormalized lattice is $4\times4\times4$, but it remains a question as to how strongly the second iteration of the $L=32$ system is affected and whether the data can be interpreted as a second relevant eigenvalue, which might give rise to an important confluent singularity in the magnetic susceptibility. It is difficult to make a prediction on the basis of the data available, but it seems likely that the simulation of an $L=64$ system would be able to shed light on the problem.

To demonstrate from internal consistency of the MCRG calculation that the second iteration has already converged to the asymptotic value, at least one additional RG step would be needed. If the same sequence were followed, this would require simulating a system with $L=64$. This is by no means impossible with a special-purpose machine, but additional investigations should be made to see whether the finite-size effect can be neglected for lattices smaller than $8\times8\times8$, to see whether the required computer time could be reduced.

It should be noted that additional effort to find the optimal value of K_x would probably be rewarded by better convergence. It is also possible that Eq. (10), which is closer to the operator suggested by Berker and used in the MCRG analysis of the $d=2,q=4$ Potts model,[22] might be even more efficient in improving the convergence properties of the MCRG analysis.

TABLE XII. Critical eigenvalue exponent y_T for the $d=3$ planar 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). $K_1=0.6744$, $K_x=0.10$.

		Lattice size (L)		
N_r	N_c	32	16	8
1	1	1.33(1)	1.37(2)	1.44(1)
	2	1.31(1)	1.36(2)	1.42(1)
	3	1.25(1)	1.29(3)	1.25(1)
	4	1.25(2)	1.28(3)	1.26(1)
	5	1.22(2)	1.26(3)	1.24(1)
	6	1.19(4)	1.23(3)	1.22(1)
	7	1.20(4)	1.25(4)	1.13(2)
	8	1.18(5)	1.24(6)	1.04(4)
	9	1.18(5)	1.24(7)	1.04(4)
	10	1.18(5)	1.24(5)	1.04(4)
2	1	1.56(2)	1.66(2)	2.07(1)
	2	1.55(2)	1.66(2)	2.09(1)
	3	1.54(2)	1.55(2)	1.85(1)
	4	1.54(2)	1.55(2)	1.77(1)
	5	1.53(2)	1.55(2)	1.69(1)
	6	1.52(2)	1.54(2)	1.69(1)
	7	1.50(2)	1.46(3)	
	8	1.48(2)	1.43(5)	
	9	1.48(3)	1.45(5)	
	10	1.48(3)	1.45(6)	
3	1	1.66(3)	2.15(7)	
	2	1.66(3)	2.17(7)	
	3	1.60(5)	1.92(6)	
	4	1.59(6)	1.79(7)	
	5	1.60(5)	1.73(7)	
	6	1.60(5)	1.74(10)	
	7	1.53(5)		
	8	1.44(16)		
	9	1.45(16)		
	10	1.45(17)		
4	1	2.07(4)		
	2	2.10(5)		
	3	1.94(12)		
	4	1.91(30)		
	5	1.83(30)		
	6	1.83(30)		

V. FUTURE WORK

The purpose of this paper has been to demonstrate the power and flexibility of the MCRG method as a tool for investigating difficult systems in three dimensions. Although the accuracy of the method for the calculation of critical exponents is still far from that of some older methods,[4,5,44–48] it is surprisingly good. Furthermore, the prospects for further im-

TABLE XIII. Critical eigenvalue exponent y_H for the $d=3$ planar 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). $K_1=0.6744$, $K_x=0.10$.

		Lattice size (L)		
N_r	N_c	32	16	8
1	1	2.427(1)	2.434(2)	2.459(1)
	2	2.427(1)	2.434(2)	2.459(1)
	3	2.394(1)	2.393(1)	2.393(1)
	4	2.394(2)	2.392(2)	2.392(1)
	5	2.394(2)	2.392(2)	2.392(1)
2	1	2.469(3)	2.492(6)	2.570(2)
	2	2.469(3)	2.492(6)	2.570(2)
	3	2.458(2)	2.456(3)	2.402(3)
	4	2.457(2)	2.455(3)	2.397(3)
	5	2.457(2)	2.455(3)	2.397(3)
3	1	2.506(7)	2.573(2)	
	2	2.506(7)	2.573(2)	
	3	2.474(4)	2.391(2)	
	4	2.473(4)	2.380(2)	
	5	2.473(4)	2.380(2)	
4	1	2.58(2)		
	2	2.58(2)		
	3	2.42(2)		
	4	2.42(2)		
	5	2.42(2)		

TABLE XIV. Critical eigenvalue exponent y_{H2} for the $d=3$ planar 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). $K_1=0.6744$, $K_x=0.10$.

		Lattice size (L)		
N_r	N_c	32	16	8
1	2	−0.09(7)	−0.06(4)	0.09(1)
	3	−0.06(4)	−0.06(5)	0.08(2)
	4	−0.01(8)	0.11(3)	0.17(3)
	5	−0.01(9)	0.09(4)	0.16(3)
2	2	0.60(5)	0.70(5)	0.95(1)
	3	0.60(5)	0.70(6)	0.95(1)
	4	0.61(4)	0.71(5)	0.97(2)
	5	0.61(4)	0.72(5)	0.97(2)
3	2	0.74(8)	1.03(7)	
	3	0.74(7)	1.03(9)	
	4	0.74(7)	1.08(9)	
	5	0.74(7)	1.09(9)	
4	2	0.93(11)		
	3	0.93(11)		
	4	0.93(9)		
	5	0.93(9)		

provement are very bright. Aside from the rapid current progress in the construction of special-purpose machines that could reduce the costs of such calculations by orders of magnitude, insights into the nature of RG transformations should improve our understanding of phase transitions and provide practical techniques for optimizing calculations.

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