Monte Carlo calculation of renormalized coupling parameters. II. $d=3$ Ising model

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The majority-rule, block-spin, renormalization-group transformation for the $d=3$ Ising model is studied, with the use of a recently developed technique for calculating renormalized coupling parameters from a single Monte Carlo simulation. Renormalization-group trajectories and the approximate fixed point are calculated. Improvements in the convergence of the Monte Carlo renormalization-group calculations of critical exponents are discussed.

I. INTRODUCTION

In a previous paper[1] a new technique for calculating renormalized coupling constants from a single Monte Carlo (MC) computer simulation[2] was applied to various renormalization-group (RG) transformations of the $d=2$ Ising model. The purpose was to establish the validity of the method and investigate the differences in the effects of different RG transformations on a model with known properties.

In this paper I apply the method to the three-dimensional Ising model. The discussion will deal with the $2\times2\times2$ majority-rule block-spin transformation, with the goal of justifying the assumptions of the RG formalism concerning short-range interactions and the existence of a fixed point,[3,4] as well as improving methods for the numerical calculation of critical properties.[5]

Since the original paper by Ma,[6] Monte Carlo renormalization-group (MCRG) methods for the calculation of critical properties have been developed[6–21] and applied to a variety of models in both statistical mechanics[7–16] and lattice gauge theories.[17,18] Just as the two-dimensional Ising model has always been essential for testing any new improvement, the three-dimensional model has played a central role as the most important application. Since the $d=3$ Ising model is physically important, conceptually simple, and unsolved, it has traditionally been the object of the most strenuous efforts.

Although early work[19,20] served primarily to demonstrate the feasibility of MCRG for the study of three-dimensional models, improvements in both method and computer hardware have been such that the most recent efforts have attained an accuracy comparable to that of the best competing calculations.[21] Further improvement of the MCRG results will come from both the continuing development of fast computational facilities and the development of new methods of calculation. A major object of the current study is to provide information on the effects of the RG transformation used in the most accurate MCRG calculations to lay the groundwork for future developments, such as the use of optimized transformations.[22]

A brief introduction to real-space RG formalism and calculational methods is given in Sec. II, along with a description of the numerical extrapolation to the fixed point. The calculations using the majority-rule RG transformation with $b=2$ is discussed in Sec. III, and results are summarized in Sec. IV.

II. CALCULATION OF EFFECTIVE RENORMALIZED COUPLING CONSTANTS

The following discussion is included for completeness. Details are found in Refs. 1–3, 14, and 15.

The Ising Hamiltonian is written in the form

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

where the S_{α}'s are the various combinations of the "spins" σ_i, which take on the values $+1$ or -1. The nearest-neighbor (NN) coupling for the Ising model is written as

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

where the sum is taken over nearest-neighbor pairs. Factors of the inverse temperature times the Boltzmann constant are included implicitly in the definition of the set of coupling constants $\{K_{\alpha}\}$.

The RG transformation we shall consider consists of dividing the system into $2\times2\times2$ blocks and assigning a block spin of $+1$ or -1 depending on whether the sum of the spins in the block is positive or negative (ties being awarded equally). The probability distribution for the new spin configurations can then be interpreted in terms of an effective renormalized Hamiltonian, parametrized in terms of a new set of coupling constants $\{K'_{\alpha}\}$.

The renormalized Hamiltonian is generally quite complicated and requires an infinite number of coupling constants to describe it completely. Fortunately, only a small number of renormalized coupling constants is generally important.

The new calculational method is based on a comparison of two different expressions for the correlation functions, one of which depends explicitly on knowledge of the effective renormalized coupling constants.[1,2] The first expression is the usual direct summation, using Eq. (2). The

TABLE I. Coupling constants used for the MCRG calculation of renormalized Hamiltonians for the $d=3$ Ising model in the order used for presentation of data for trajectories and fixed points.

α	Description
1	(100) neighbor
2	(110) neighbor
3	(111) neighbor
4	(200) neighbor
5	(210) neighbor
6	(211) neighbor
7	(220) neighbor
8	(221) neighbor
9	(222) neighbor
10	(300) neighbor
11	4-spin: (000), (100), (010), (110)
12	4-spin: (000), (100), (011), (111)
13	4-spin: (000), (100), (010), (001)
14	4-spin: (000), (020), (100), (120)
15	4-spin: (000), (110), (101), (011)
16	6-spin: (000), (010), (020), (100), (110), (120)
17	8-spin: All corners of a cube

other expression was first suggested by Callen,[23] and recently applied to lattice gauge theories by Parisi, Petronzio, and Rapuano[24] in another context. Differences in the results of using the two expressions indicate differences between the assumed values of the renormalized coupling constants and the true values. A minimization of these differences then leads to the true values.[1,2]

The second expression for the correlation functions requires definition of operators $S_{\alpha,l}$ as the sum of all terms in S_α that include σ_l. Then S_α is given by

$$S_\alpha = m_\alpha^{-1} \sum_l S_{\alpha,l} , \tag{3}$$

where m_α is 2 for two-spin operators, 4 for four-spin operators, etc. If we also define the operators $\hat{S}_{\alpha,l}$,

$$\sigma_l \hat{S}_{\alpha,l} = S_{\alpha,l} , \tag{4}$$

Callen's representation of the correlation functions can be written as

$$\langle \tilde{S}_\alpha \rangle = m_\alpha^{-1} \sum_l \left\langle \hat{S}_{\alpha,l} \tanh \left[\sum_\beta \tilde{K}_\beta \hat{S}_{\beta,l} \right] \right\rangle , \tag{5}$$

where I have introduced a second set of coupling constants, $\{\tilde{K}_\alpha\}$, for convenience.[1,2] The brackets still indicate averages with respect to the "true" coupling constants, $\{K_\alpha\}$.

The equality $\langle \tilde{S}_\alpha \rangle = \langle S_\alpha \rangle$ is valid *if and only if* $\tilde{K}_\alpha = K_\alpha$ for all α. If the two sets of coupling constants differ, this equality will not hold.

The derivative matrix can also be easily calculated from the MC configurations:

$$\frac{\partial \langle \tilde{S}_\alpha \rangle}{\partial \tilde{K}_\beta} = m_\alpha^{-1} \sum_l \left\langle \hat{S}_{\alpha,1} \hat{S}_{\beta,1} \operatorname{sech}^2 \left[\sum_\delta \tilde{K}_\delta \hat{S}_{\delta,l} \right] \right\rangle . \tag{6}$$

TABLE II. Estimates of effective renormalized coupling constants from an MC simulation of a $32\times32\times32$ lattice at the critical point ($K=0.221\,66$) (Ref. 21) with a $2\times2\times2$ majority-rule RG transformation. The MC simulation used 2.17×10^5 MC steps per site (MCS/S), starting from the last configuration of an old simulation, with data taken every 10 MCS/S. Relaxation times for the energy on the unrenormalized lattice were typically 120 MC steps per site (MCS/S). The first column gives the number of iterations of the RG transformation, while the second column gives the number of the coupling constant in accordance with Table I.

n	α	Rough estimate $K_\alpha^{(n)}$	First approximation $K_\alpha^{(n)}$	Second approximation $K_\alpha^{(n)}$
1	1	0.167	0.168 60(8)	0.168 53(6)
	2	0.027	0.026 13(3)	0.026 10(5)
	3	0.006	0.005 77(6)	0.005 83(5)
	4	−0.005	−0.005 90(1)	−0.005 88(3)
	5	−0.002	−0.001 99(4)	−0.001 95(1)
	6	−0.001	−0.000 77(1)	−0.000 84(2)
	7	0.000	−0.000 51(2)	−0.000 44(2)
	8	0.000	−0.000 10(2)	−0.000 17(1)
	9	0.000	−0.000 12(5)	0.000 00(1)
	10	0.000	0.000 46(13)	0.000 44(1)
	11	−0.001	−0.001 61(14)	−0.001 49(1)
	12	0.000	−0.000 00(1)	0.000 09(5)
	13	0.002	0.001 86(2)	0.001 82(3)
	14	0.000	0.000 20(4)	0.000 24(4)
	15	0.000	0.000 07(6)	−0.000 06(4)
	16	0.000	0.000 75(5)	0.000 77(3)
	17	0.000	0.000 13(14)	0.000 06(4)
2	1	0.164	0.1616(6)	0.1624(4)
	2	0.030	0.0306(2)	0.0305(1)
	3	0.005	0.0075(2)	0.0076(2)
	4	0.000	−0.0081(2)	−0.0080(2)
	5	0.000	−0.0031(1)	−0.0028(1)
	6	0.000	−0.0011(2)	−0.0013(1)
	7	0.000	−0.0002(1)	−0.0003(1)
	8	0.000	−0.0003(2)	−0.0001(1)
	9	0.000	0.0003(4)	0.0000(1)
	10	0.000	0.0006(1)	0.0008(1)
	11	−0.001	−0.0019(3)	−0.0015(4)
	12	0.000	0.0004(1)	0.0004(2)
	13	0.000	0.0030(1)	0.0026(1)
	14	0.000	0.0004(3)	0.0004(1)
	15	0.000	0.0003(2)	0.0002(2)
	16	0.000	0.0013(2)	0.0010(1)
	17	0.000	0.0004(1)	0.0004(3)
3	1	0.164	0.1603(12)	0.1610(5)
	2	0.030	0.0297(6)	0.0324(2)
	3	0.005	0.0091(13)	0.0081(2)
	4	0.000	−0.0099(7)	−0.0085(3)
	5	0.000	−0.0032(3)	−0.0035(1)
	6	0.000	−0.0011(4)	−0.0015(2)
	7	0.000	−0.0004(3)	−0.0006(2)
	8	0.000	−0.0004(2)	−0.0001(3)
	9	0.000	0.0006(6)	0.0000(3)
	10			
	11	−0.001	−0.0022(5)	−0.0001(6)
	12	0.000	0.0017(3)	0.0013(3)
	13	0.000	0.0041(1)	0.0029(2)

TABLE II. (*Continued*).

n	α	Rough estimate $K_\alpha^{(n)}$	First approximation $K_\alpha^{(n)}$	Second approximation $K_\alpha^{(n)}$
3	14	0.000	0.0017(3)	0.0005(2)
	15			
	16	0.000	0.0013(3)	0.0015(1)
	17	0.000	−0.0017(3)	0.0002(5)

By choosing the set $\{\tilde{K}_\alpha^{(n)}\}$ to make $\langle \tilde{S}_\alpha - S_\alpha \rangle = 0$, these equations allow calculation of the effective renormalized coupling constants $\{K_\alpha^{(n)}\}$ after n iterations of the RG transformation. To locate the fixed point by extrapolating the RG trajectories, the matrix of derivatives

$$T_{\alpha\beta} = \partial K_\alpha^{(n+1)} / \partial K_\beta^{(n)} \tag{7}$$

is first calculated by standard MCRG methods.[7,14,15] In an obvious notation, the fixed point is given by

$$\underline{K}^* = \underline{K}^{(n)} + (\underline{I} - \underline{T})^{-1} (\underline{K}^{(n+1)} - \underline{K}^{(n)}) \tag{8}$$

and $\underline{I}$ is the identity matrix. This equation can be rewritten to involve only a single matrix inversion and simplifying computer programming. The statistical errors involved in extrapolating to the fixed point are naturally larger than those for the renormalized coupling constants.

For technical reasons, it is often useful to be able to come close to the fixed point, within a limitation to certain operators that can be included in an MC simulation on a special purpose computer. Since the behavior of the RG transformation is known, deviations from the fixed point in the most relevant (least irrelevant) directions could be projected out using eigenvalues and eigenvectors of the matrix T.[7,14,15]

III. MAJORITY-RULE RG TRANSFORMATION WITH $b=2$

The majority-rule RG transformation consists of dividing the system into blocks and assigning a block spin of $+1$ or -1 depending on whether the sum of the spins in the block is positive or negative. I shall consider the most convenient choice of $2\times2\times2$ blocks, with ties being awarded equally.

The calculations presented here are much more detailed than the studies of the two-dimensional model.[2] Instead of seven renormalized coupling constants, I have included 17 in the present analysis, to enable systematic changes to be considered more carefully. Table I contains a list of the interactions used in the analysis of the trajectories.

As in the previous study of the two-dimensional Ising model,[2] preliminary calculations were carried out to check the computer program and the method by calculating coupling constants of the original nearest-neighbor model. After these checks had been completed satisfactorily, calculation of the effective coupling constants for the unrenormalized model was turned off to save computer time

TABLE III. Correlation functions for the original and renormalized lattices from the same MCRG simulations as in Table II.

n	α	First simulation $\langle S_\alpha^{(n)} \rangle$	Second simulation $\langle S_\alpha^{(n)} \rangle$
1	1	0.99(1)	0.996(3)
	2	1.44(2)	1.445(7)
	3	0.80(2)	0.805(5)
	4	0.54(1)	0.545(4)
	5	1.96(5)	1.978(16)
	6	1.82(5)	1.838(17)
	7	0.82(3)	0.828(9)
	8	1.57(5)	1.588(18)
	9	0.48(2)	0.481(6)
	10	0.40(1)	0.400(5)
	11	0.51(1)	0.514(2)
	12	0.81(1)	0.815(4)
	13	1.09(2)	1.091(6)
	14	0.73(1)	0.730(4)
	15	0.21(1)	0.206(2)
	16	0.49(1)	0.493(4)
	17	0.06(1)	0.057(1)
2	1	1.09(2)	1.10(1)
	2	1.17(5)	1.72(2)
	3	0.99(4)	1.00(2)
	4	0.69(3)	0.69(1)
	5	2.58(11)	2.61(4)
	6	2.46(12)	2.50(4)
	7	1.16(6)	1.18(2)
	8	2.26(12)	2.30(5)
	9	0.72(5)	0.73(2)
	10	0.57(3)	0.58(1)
	11	0.60(2)	0.60(1)
	12	0.99(3)	1.00(2)
	13	1.35(5)	1.37(2)
	14	0.89(3)	0.90(2)
	15	0.27(1)	0.27(1)
	16	0.63(3)	0.63(1)
	17	0.08(1)	0.08(1)
3	1	1.34(5)	1.36(2)
	2	2.31(11)	2.35(4)
	3	1.43(8)	1.46(3)
	4	1.09(6)	1.11(2)
	5	4.19(24)	4.27(8)
	6	4.07(25)	4.16(8)
	7	2.02(13)	2.06(4)
	8	3.97(26)	4.05(8)
	9	1.30(9)	1.33(3)
	10		
	11	0.83(4)	0.85(2)
	12	1.47(8)	1.49(3)
	13	2.02(11)	2.06(4)
	14	1.42(9)	1.43(3)
	15		
	16	1.05(7)	1.07(3)
	17	0.13(1)	0.13(1)

TABLE IV. Differences in correlation functions calculated by direct summation (shown in Table III) and using Callen's representation, for the same MCRG simulations as in Tables II and III. The calculations of correlation functions with Callen's representation used the estimates for the renormalized coupling constants given in the first two columns of Table II. Values given below are the deviations from the correlation functions shown in Table III. The differences listed for the first simulation used the "rough estimates" for the coupling constants, and the differences listed for the second simulation used the values for the second approximation in Table II. The errors in the differences for the second approximation were smaller than those for the correlation functions themselves by the ratio given in the last column.

n	α	First approximation $\langle \Delta S_\alpha^{(n)} \rangle$	Second approximation $\langle \Delta S_\alpha^{(n)} \rangle$	Error ratio	n	α	First approximation $\langle \Delta S_\alpha^{(n)} \rangle$	Second approximation $\langle \Delta S_\alpha^{(n)} \rangle$	Error ratio
1	1	0.0011(2)	0.0003(1)	0.03		10	−0.0302(5)	0.0007(1)	0.03
	2	−0.0058(5)	−0.0001(3)	0.04		11	−0.0036(5)	0.0006(1)	0.11
	3	−0.0033(3)	0.0000(1)	0.01		12	−0.0097(2)	0.0008(2)	0.07
	4	−0.0026(2)	0.0000(1)	0.03		13	−0.0019(6)	−0.0014(2)	0.03
	5	−0.0082(4)	0.0001(2)	0.01		14	−0.0139(13)	0.0011(2)	0.05
	6	−0.0070(4)	−0.0006(3)	0.02		15	−0.0033(2)	0.0002(1)	0.05
	7	−0.0054(3)	0.0001(2)	0.02		16	−0.0002(7)	0.0004(2)	0.02
	8	−0.0083(5)	−0.0006(2)	0.01		17	0.0006(1)	0.0001(1)	0.11
	9	−0.0026(1)	0.0001(1)	0.01					
	10	−0.0011(3)	−0.0001(1)	0.01	3	1	−0.016(5)	0.001(3)	0.15
	11	0.0013(3)	0.0003(1)	0.03		2	−0.047(6)	0.003(4)	0.10
	12	0.0002(2)	0.0005(2)	0.04		3	−0.036(6)	−0.002(3)	0.09
	13	−0.0021(4)	−0.0001(2)	0.03		4	−0.050(6)	0.001(2)	0.12
	14	0.0018(2)	0.0004(2)	0.05		5	−0.157(14)	−0.005(8)	0.10
	15	−0.0006(1)	−0.0001(1)	0.05		6	−0.144(18)	−0.007(8)	0.10
	16	0.0039(2)	0.0003(2)	0.05		7	−0.076(8)	−0.003(3)	0.08
	17	0.0002(1)	−0.0000(1)	0.06		8	−0.142(16)	−0.004(9)	0.12
						9	−0.008(5)	−0.005(2)	0.06
2	1	−0.0161(7)	0.0015(1)	0.09		10			
	2	−0.0402(8)	0.0004(3)	0.05		11	−0.041(10)	−0.009(4)	0.13
	3	−0.0308(6)	0.0006(1)	0.06		12	−0.000(3)	0.003(2)	0.11
	4	−0.0393(3)	0.0009(1)	0.07		13	−0.003(4)	−0.000(2)	0.07
	5	−0.1334(13)	0.0028(2)	0.05		14	0.007(4)	−0.002(3)	0.06
	6	−0.1228(14)	0.0006(3)	0.03		15			
	7	−0.0592(14)	0.0005(2)	0.03		16	0.007(3)	0.002(2)	0.07
	8	−0.1156(31)	0.0013(2)	0.04		17	0.001(3)	0.001(1)	0.08
	9	−0.0368(3)	0.0004(1)	0.03					

and make the calculation of the RG trajectories more efficient.

In using Eqs. (5) and (6) to calculate the effective renormalized coupling constants, it is necessary to perform at least one or two preliminary iterations of the equations to find values of the parameters close enough to the true values, for a linear approximation to be valid. Particular care was taken to check this sequence of approximations to the true values, to make sure that all assumptions were satisfied.

Table II gives data for three successive approximations to the RG trajectory from the nearest-neighbor critical point towards the fixed point. The "rough estimate" was the result of a very short simulation, starting with the nearest-neighbor parameters. A calculation using these rough estimates in Eq. (6) then produced the values listed as the "first approximation." The statistical errors were determined in the usual manner, by breaking up the MC simulation into a series of separate runs, carrying out the full calculation with data from each of these runs, and calculating the spread in results. As can be seen from Table II, the statistical errors were quite small. To check on possible systematic errors, the entire calculation was then repeated with the new values for the renormalized coupling constants, with the results shown in the last column under "second approximation." Comparison of the first and second approximations show that the nonlinear effects were extremely small, and the differences are generally within the small statistical errors.

It is helpful in understanding the process (and the difficulties encountered by any method using a comparison of two separate MC simulations to calculate effective coupling constants[9–11,16] to consider the renormalized correlation functions. These are shown in Table III for both simulations used in Table II. As can be seen, the values for the coupling constants change substantially under renormalization, primarily due to the change in size of the lattice (the linear dimensions of the renormalized system are reduced by the factor $b=2$).

Table IV contains the differences between the values shown in the previous table and the correlation functions calculated from Callen's representation, using the parameters in Table II. For both simulations, the statistical errors in calculating the differences are substantially smaller

TABLE V. Estimates for the fixed point for the $b=2$ majority-rule RG transformation in the *nearest-neighbor* $d=3$ Ising model from the simulations used in Tables II–IV.

	RG iterations	
	1 to 2	2 to 3
α	K_α^*	K_α^*
1	0.1666(15)	0.1659(41)
2	0.0311(3)	0.0322(4)
3	0.0075(4)	0.0081(1)
4	−0.0099(3)	−0.0105(4)
5	−0.0036(3)	−0.0043(5)
6	−0.0018(3)	−0.0018(1)
7	−0.0001(1)	−0.0007(2)
8	0.0000(2)	0.0000(2)
9	−0.0001(2)	−0.0001(3)
10	0.0011(2)	
11	−0.0021(4)	0.0001(5)
12	0.0005(2)	0.0020(6)
13	0.0032(2)	0.0038(3)
14	0.0005(3)	0.0004(1)
15	0.0012(2)	
16	0.0015(1)	0.0019(1)
17	0.0006(4)	0.0000(6)

than the error in calculating the correlation functions themselves. The last column in Table IV gives the ratio of the errors in the differences to that in the correlation functions themselves. The fact that the statistical error is generally reduced by a factor of 10 or better is the primary advantage of this method of calculating the effective renormalized coupling parameters. A corresponding accuracy could be achieved by a two-lattice simulation only with the use of at least 2 orders of magnitude more computer time.

Table IV also demonstrates the dramatic improvement in agreement of the two methods of computing correlation functions from an improved set of coupling constants. Returning to the last column of Table II, which gives the best estimates for the renormalization-group trajectory, it can be seen that the renormalized coupling constants confirm a number of the assumptions of the real-space renormalization-group formalism. The first ten values demonstrate the rapid decay of coupling strength with distance. A comparison of the (100) with the (200) interaction shows a reduction in magnitude by a factor of 20. Comparing the (110) with the (220) interaction gives a change by a factor of 100.

An oscillation of the sign of the interaction as a function of distance is also apparent. After three positive (ferromagnetic) interactions, the fourth- through eighth-nearest-neighbor interaction parameters are negative (antiferromagnetic). The ninth interaction (222) is zero within statistical error, and the tenth neighbor returns to positive values.

Differences in the significance of various multispin operators are visible, enabling improved choices of parameters for future work. Some four-spin operators are clearly more important than others. The eight-spin operator is completely unimportant.

Looking at successive iterations of the RG transformation, the changes are consistent with the approach to a fixed point, but differences still exist between the effective

TABLE VI. Confirmation of approximation to the fixed point. Estimates of effective renormalized coupling constants from an MC simulation of a 17-parameter model on a $16\times16\times16$ lattice using a $2\times2\times2$ majority-rule RG transformation. The MC simulation used 1.32×10^5 MC steps per site (MCS/S), after discarding 1.8×10^4 MCS/S to equilibriate from the last configuration of an old nearest-neighbor model simulation, with data taken every 10 MCS/S. Relaxation times for the energy on the unrenormalized lattice were typically 25 MC steps per site.

α	$K_\alpha^{(0)}$ MC values	$K_\alpha^{(0)}$	$K_\alpha^{(1)}$	$K_\alpha^{(2)}$
1	0.161 737	0.161 63(14)	0.1688(1)	0.1706(19)
2	0.030 586	0.030 72(2)	0.0317(3)	0.0323(3)
3	0.007 500	0.00753(10)	0.0088(2)	0.0096(3)
4	−0.008 166	−0.008 23(2)	−0.0096(7)	−0.0100(3)
5	−0.003 125	−0.003 22(2)	−0.0040(3)	−0.0039(5)
6	−0.001 087	−0.001 06(6)	−0.0013(3)	−0.0016(6)
7	−0.000 279	−0.000 16(13)	−0.0004(1)	−0.0004(5)
8	−0.000 238	−0.000 29(7)	−0.0003(1)	−0.0004(2)
9	0.000 342	0.000 33(18)	0.0003(3)	0.0005(6)
10	0.000 703	0.000 78(15)	0.0011(2)	
11	−0.001 951	−0.001 87(13)	−0.0026(2)	−0.0043(4)
12	0.000 495	0.000 47(5)	0.0004(2)	0.0005(8)
13	0.002 920	0.002 97(8)	0.0029(1)	0.0037(2)
14	0.000 330	0.000 26(7)	0.0005(1)	0.0002(1)
15	0.000 430	0.000 38(5)	−0.0002(3)	
16	0.001 216	0.001 29(7)	0.0012(2)	0.0028(4)
17	0.000 297	0.000 09(11)	0.0000(1)	0.0004(13)

TABLE VII. Estimates for the fixed point for the $b=2$ majority-rule RG transformation in a $d=3$ Ising model *with 17 coupling constants* from the simulations used in Table VI. The first column used the true values used in performing the MC simulation for the extrapolation to the fixed point. The results should be compared with those of Table V.

	RG iterations	
	0 to 1	1 to 2
α	K_α^*	K_α^*
1	0.1792(12)	0.171(25)
2	0.0320(15)	0.030(4)
3	0.0094(2)	0.006(1)
4	−0.0129(19)	−0.008(7)
5	−0.0058(2)	−0.004(3)
6	−0.0017(2)	0.001(1)
7	−0.0008(6)	0.001(1)
8	0.0002(5)	−0.000(1)
9	0.0009(8)	0.000(1)
10	0.0018(6)	
11	−0.0041(11)	−0.004(2)
12	−0.0000(3)	−0.001(2)
13	0.0031(5)	−0.003(1)
14	0.0003(2)	0.000(1)
15	−0.0011(8)	
16	0.0017(3)	0.002(1)
17	0.0008(2)	0.002(1)

renormalized coupling constants at the second and third iterations. The slow approach to the fixed point (in comparison with two-dimensional trajectories[2]) is consistent with the results of extensive MCRG calculations of the critical exponents using this transformation. Even after three iterations, the estimates for the critical exponents had not converged to their final values and the results had to be extrapolated to the fixed point.[21]

One of the reasons for undertaking the current study was to try to avoid this problem by simulating an approximation to the fixed point instead of simply using the nearest-neighbor model. An attempt to calculate the location of the fixed point direct from the data in Table II and Eqs. (7) and (8) is shown in Table V. Aside from the fact that the statistical errors are larger for the extrapolated fixed-point values, there appears to be a discrepancy in the results that might point to a systematic error due to the finite number of coupling constants used in the analysis. Although the nearest-neighbor coupling went steadily down under renormalization (see Table II), the extrapolated fixed-point value is higher than for either the second or third RG iterations. Such behavior is, of course, possible, but seems unlikely.

Since the values on the second RG iteration are rather accurately calculated, I used them in a new MC simulation to improve the convergence to the fixed point. The results are shown in Table VI. (The actual values used differed slightly from those shown in Table II because this simulation was begun before the simulations reported in Table II had been completed.)

The first column in Table VI gives the number of coupling constants used in the MC simulation, and the second column gives the actual values. The third column gives the estimates for these values using Eqs. (5) and (6), which acts as a check on the method for a rather complicated Hamiltonian.

If the MC simulation had reproduced the effective Hamiltonian perfectly after two RG iterations from the nearest-neighbor critical point, the values in Table VI listed under $K_\alpha^{(1)}$ should have agreed with the third RG iteration in Table II. Differences are due to the truncation of the renormalized Hamiltonian and statistical errors. However, the shift in coupling constants is not very large, certainly not in comparison with the initial change from the nearest-neighbor model after one RG transformation. In addition, perhaps accidently, they also tend towards the fixed-point estimates in Table V.

Under the assumption that the Hamiltonians in Table VI are reasonably close to the fixed point, I have used them for extrapolations, with the results shown in Table VII. Again, the nearest-neighbor coupling appears to be too strong, but a rough agreement with Table V is found.

Although there are still considerable uncertainties involved, the best estimate for the fixed point is probably given by the first column in Table V. Performing an MC simulation of this model on a relatively small ($16\times16\times16$) lattice led to the MCRG estimates for the critical exponents shown in Table VIII. The first iteration is somewhat disappointing, since it shows that the model is still "far" from the fixed point, in the sense that the eigenvalues of the derivative matrix do not give the correct critical exponents. However, they are considerably better than the values of $Y_T=1.43$ and $Y_H=2.46$ given by the nearest-neighbor model.[19,21] The second iteration is far better; the thermal eigenvalue is in agreement with

TABLE VIII. Leading thermal and magnetic critical exponent estimates for a 17-parameter $d=3$ Ising model from a simulation on a $16\times16\times16$ lattice. The MC simulation used the first estimates in Table V for the coupling constants at the fixed point. The simulation used 1.8×10^5 MCS/S, after discarding 1.1×10^4 MCS/S, with data recorded every MCS/S. n is the number of RG steps and α the number of couplings included in the analysis.

n	α	y_T	y_H
1	1	1.483(2)	2.4853(4)
	2	1.518(2)	2.4814(3)
	3	1.516(2)	2.4807(3)
	4	1.507(2)	2.4804(3)
	5	1.506(2)	
	6	1.505(2)	
	7	1.491(3)	
2	1	1.56(1)	2.507(3)
	2	1.61(1)	2.496(3)
	3	1.61(1)	2.494(3)
	4	1.60(1)	2.493(3)
	5	1.59(1)	
	6	1.58(1)	
	7	1.58(1)	

TABLE IX. Estimates for the fixed point of the $d=3$ Ising model for the $b=2$ majority-rule RG transformation from a two-lattice comparison on $6\times6\times6$ and $12\times12\times12$ lattices, using a six-parameter MC simulation. The small lattice averaged over 1.1×10^6 MCS/S and the larger lattice over 2.2×10^5 MCS/S. The statistical errors were in the third digit, but were not determined accurately, since the systematic errors, owing to the small number of couplings, clearly dominated.

α	K_α^*
1	0.1965
2	0.0374
3	0.0069
4	−0.0194
5	Not included
6	0.0088
7	0.0002
8	0.0001
9	Not included
10	Not included
11	0.0049

the best estimates (within fairly large statistical errors) and the magnetic eigenvalue is only about 0.3% too high, probably because of a small error in the simulated coupling constants, corresponding to being slightly off the critical hypersurface.[14,15]

IV. SUMMARY AND CONCLUSIONS

The advantages of the new method for calculating renormalized coupling constants can be seen even more clearly by comparison with the results from a two-lattice comparison given in Table IX. The older method shows large systematic errors owing to the small number of coupling constants that could be conveniently handled, as well as the intrinsically larger statistical errors, as discussed above.

In this paper, a new method of calculated renormalized coupling parameters was applied to the three-dimensional Ising model.[1] A partially successful attempt was made to improve the convergence of the MCRG calculation of critical exponents by simulating an approximate fixed point. The basic validity of the approach was confirmed, but a fully satisfactory determination of the fixed point was not achieved, probably owing to the finite number of coupling constants, as well as statistical errors. Both of these difficulties can be reduced in future work through the improved availability of high-speed computers and the inclusion of more parameters in the analysis, based on the present study.

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