Monte Carlo calculation of renormalized coupling parameters. I. $d=2$ Ising model

Robert H. Swendsen*
IBM Zurich Research Laboratory, International Business Machines Corporation, CH-8803 Rüschlikon, Switzerland
(Received 2 April 1984)

Renormalization-group trajectories produced by various real-space, block-spin transformations of the $d=2$ Ising model are studied, using a recently developed technique for calculating renormalized coupling parameters from a Monte Carlo simulation of a single system.

I. INTRODUCTION

The real-space renormalization-group (RG) approach[1,2] to the study of critical behavior in thermodynamic systems has contributed much to our understanding of such phenomena. However, many assumptions of this approach still need to be justified more fully, and the validity of various approximations must be tested.

The combination of Monte Carlo (MC) computer simulations[3] with the RG formalism has already made progress in this direction by allowing some of the approximations to be investigated systematically.[4,5] For example, the effect of including more renormalized coupling constants in the calculation of critical exponents can be studied with controlled statistical errors.[5–8]

On the other hand, there was no generally applicable, practical way of investigating the renormalization-group trajectories themselves,[9] until the recent development of a method of calculating renormalized coupling constants from a single MC computer simulation.[10] This problem is important for practical computational reasons, since the determination of the RG trajectory, and especially the fixed point, should enable a substantial improvement in the convergence of the calculation of critical exponents. Fewer iterations of the RG transformation would be necessary, meaning that smaller lattices could be used, reducing computational effort, and improving both accuracy and reliability.

Renormalized coupling constants are also important for lattice gauge theories.[11] This would enable RG trajectories to be obtained from a series of MC simulations on small lattices, instead of requiring large linear dimensions for four-dimensional systems.[11,12]

The fundamental difficulty in calculating renormalized coupling constants from an MC simulation arises from the reduction in size of the system used for the MC simulation after the RG transformation. Since correlation functions in the renormalized system are affected by both the change in effective renormalized coupling constants and the change in size, it is necessary to separate the two effects in order to extract RG trajectories from MC simulations.

In principle, a two-lattice comparison of the type introduced by Wilson[13] is capable of calculating renormalized couplings,[14] but the statistical errors involved in finding differences between correlation functions from two independent MC simulations limit its practical application to certain special cases.[7,8,15–20]

The single-lattice approach has smaller statistical errors than any two-lattice comparison (as demonstrated below) and enables practical calculations of renormalized coupling constants to be carried out for any real-space RG transformation of interest.[10]

In this paper I use the two-dimensional Ising model to test this method on a system with well-known properties. To investigate the effect of different RG transformations, I have performed calculations on several different, commonly used RG transformations. The work can be regarded as a continuation of a previous investigation of the calculation of critical exponents for the two-dimensional Ising model using various RG transformations.[6]

After a brief introduction to the real-space RG formalism to establish notation in Sec. II, the single-lattice calculation of renormalized coupling constants is presented in Sec. III. Numerical extrapolation to the fixed point is discussed in Sec. IV. Applications to various RG transformations are discussed in Secs. V–VII, and results are summarized in Sec. VIII.

II. REAL-SPACE RG FORMALISM

Consider a general model in statistical mechanics, for which the Hamiltonian is written in the form

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

where the S_{α}'s are various possible combinations of the "spins" σ_i's that occur in models of interest or are generated by renormalization-group transformations. An important example for the Ising model is the operator describing the nearest-neighbor (NN) coupling

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

where $\sigma_i=+1$ or -1 and 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 $\{K_{\alpha}\}$. Seven operators of this general form were used in the present work, and are listed in Table I.

The equilibrium probability distribution is then

$$P(\sigma)=\exp[H(\sigma)]/Z , \tag{3}$$

where Z is the partition function

TABLE I. Coupling constants used for the MCRG analysis of the $d=2$ Ising model.

α	Even couplings Description
1	Nearest neighbors (10)
2	Next nearest neighbor (11)
3	Third neighbor (20)
4	Fourth neighbor (21)
5	Fifth neighbor (22)
6	Four-spin coupling around a plaquette
7	Four-spin coupling on a sublattice plaquette

$$Z=\operatorname*{Tr}_{\sigma}\exp(H)\ . \tag{4}$$

The renormalization-group formalism integrates out some fraction of the variables associated with short-wavelength fluctuations, transforming the original system into a new one with few degrees of freedom. Transformations are generally characterized by a local grouping of spin variables on neighboring sites into "blocks," and assigning a value to each "block spin" on the basis of the values assumed by the spins in each block.

For example, for the $d=2$ Ising model, a common RG transformation (considered in detail below) is to divide the system up into 2×2 blocks and assign a block spin on the basis of whether the sum of the spins in the block is positive or negative (ties being awarded equally). This replaces four spins in the original system by a single spin in the new, renormalized system. The linear dimensions of the system has been reduced by the scale factor $b=2$.

Formally, the RG transformation can be written in terms of the equilibrium probabilities as

$$P'(\sigma')=\operatorname*{Tr}_{\sigma}[T(\sigma',\sigma)P(\sigma)]\ . \tag{5}$$

The new probability distribution can then be interpreted in terms of an effective Hamiltonian for the renormalized block spins

$$P'(\sigma')=\exp[H'(\sigma')]/Z' \tag{6}$$

and this renormalized Hamiltonian can be parametrized in terms of a new set of coupling constants $\{K'_\alpha\}$. It is the calculation of these renormalized coupling constants, $\{K'_\alpha\}$, which is the main subject of this paper.

Even for models with nearest-neighbor interactions and simple RG transformations, the renormalized Hamiltonian requires an infinite number of coupling constants to describe it completely. The effect of the renormalization-group transformation therefore involves a mapping of an infinite-dimensional space of coupling constants onto itself. Fortunately, only a small number of renormalized coupling constants is generally important, and the method discussed below can be used to systematically investigate the effect of additional parameters.

III. CALCULATION OF EFFECTIVE COUPLING CONSTANTS

The difficulty involved in the calculation of effective renormalized coupling constants from configurations of an MC simulation arises primarily from the unknown dependence of all correlation functions on the size of the system. A change in the correlation functions after an RG transformation is due partly to a change in coupling constants and partly to the change in the size of the system upon integrating out some fraction of the degrees of freedom.

The only method previously available for separating these two effects is based on an idea introduced by Wilson.[13] He suggested comparing renormalized correlation functions with those of a second, independent MC simulation on a lattice of the same size as the renormalized system. Even though the finite-size effects might have been large, they would be the same for both MC simulations, so that any differences in the correlation functions had to be attributed to differences in the effective renormalized coupling constants. Methods using matrices of derivatives to systematically investigate the effects of many renormalized coupling constants were than developed and applied to a variety of problems.[7,8,12,15–20]

In principle, the two-lattice comparison solved the problem. In practice, severe numerical difficulties arose, because the statistical errors from two independent MC simulations were too large in comparison with the rather small differences in correlation functions.[7,8]

Although rough approximations to the RG trajectories could be calculated, the information obtained was meager, except for the determination of the location of critical (or multicritical) points. In these cases, the RG transformation amplified small deviations from criticality (relevant directions) and this effect overcame the statistical errors. Two-lattice comparisons have, indeed, become a standard method for highly accurate determinations of critical temperatures from MC simulations.[7,8,12,16,17,19,20]

To overcome the problem of statistical errors encountered in two-lattice comparisons, it was essential to develop a method that only required a single MC simulation. To do that, a second, independent expression for renormalized correlation functions, which depends explicitly on the renormalized coupling constants, is needed.

A representation of the correlation functions satisfying this requirement was suggested in 1963 by Callen[21] and recently applied to lattice gauge theories by Parisi, Petronzio, and Rapuano.[22] This alternative calculation of correlation functions can then be compared with the usual expression, using the same configurations from an MC simulation. Differences in the values of the correlation functions from 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.[12]

To explain the details of this approach, I shall first introduce the usual expressions for the calculation of correlation functions, then alternative expressions, using the same notation. Finally, I shall show how derivative matrices can be constructed to give a sequence of approximations that converges rapidly to the set of values for the renormalized coupling constants.

The standard expression for correlation functions is

$$\langle S_\alpha\rangle=Z^{-1}\operatorname*{Tr}_{\sigma}[S_\alpha\exp(H)]\ . \tag{7}$$

For comparison with Eq. (7), we construct a second expression for the correlation functions, based on an idea due to Callen.[21] The operators $S_{\alpha,l}$ are defined as the sum of all terms in S_α that include σ_l. For example,

$$S_{\mathrm{NN},l}=\sum_{\langle ij\rangle}\sigma_i\sigma_j(\delta_{i,l}+\delta_{j,l})\ . \tag{8}$$

S_α is then given by

$$S_\alpha=m_\alpha^{-1}\sum_l S_{\alpha,l}\ , \tag{9}$$

where m_α is 2 for two-spin operators, 4 for four-spin operators, etc.

Defining

$$H_l=\sum_\alpha K_\alpha S_{\alpha,l}\ , \tag{10}$$

the new correlation functions can be written in Callen's representation as

$$\langle S_{\alpha,l}\rangle=Z^{-1}\operatorname*{Tr}_{\{\sigma_l\ (\neq\sigma_l)\}}[\exp(H-H_l)z_l\langle S_{\alpha,l}\rangle_l]\ , \tag{11}$$

where

$$\langle S_{\alpha,l}\rangle_l=z_l^{-1}\operatorname*{Tr}_{\sigma_l}[S_{\alpha,l}\exp(H_l)] \tag{12}$$

and

$$z_l=\operatorname*{Tr}_{\sigma_l}\exp(H_l) \tag{13}$$

depend on the neighbors of σ_l. Since Eqs. (12) and (13) only involve traces over a single operator, they can be evaluated explicitly from configurations generated by the MC simulation, when the Hamiltonian is known. Depending on the model under consideration, the integration might be done analytically, numerically, or even with MC methods. For the present case of the Ising model, the trace can be carried out analytically. Separating out σ_l, we define

$$\sigma_l\hat{S}_{\alpha,l}=S_{\alpha,l}\ , \tag{14}$$

so that, for example,

$$\hat{S}_{\mathrm{NN},l}=\sum_{\langle i,l\rangle}\sigma_i \tag{15}$$

and

$$H_l=\sigma_l\sum_\alpha K_\alpha\hat{S}_{\alpha,l}\ . \tag{16}$$

Introducing a second set of coupling constants, $\{\tilde{K}_\alpha\}$, for future convenience, we define

$$\langle\tilde{S}_\alpha\rangle=m_\alpha^{-1}\sum_l\left\langle\hat{S}_{\alpha,l}\tanh\left[\sum_\beta\tilde{K}_\beta\hat{S}_{\beta,l}\right]\right\rangle\ , \tag{17}$$

where the large angular brackets still indicate averages with respect to the "true" coupling constants, $\{K_\alpha\}$. The equality $\langle S_\alpha\rangle=\langle\tilde{S}_\alpha\rangle$ is valid *if and only if* $K_\alpha=\tilde{K}_\alpha$ for all α. If the two sets of coupling constants differ, this equality will not hold. To first order, the differences will be given by

$$\langle\tilde{S}_\alpha\rangle-\langle S_\alpha\rangle=\sum_\beta\frac{\partial\langle\tilde{S}_\alpha\rangle}{\partial K_\beta}(\tilde{K}_\beta-K_\beta) \tag{18}$$

with the derivatives

$$\frac{\partial\langle\tilde{S}_\alpha\rangle}{\partial\tilde{K}_\beta}=m_\alpha^{-1}\sum_l\left\langle\hat{S}_{\alpha,l}\hat{S}_{\beta,l}\operatorname{sech}^2\left[\sum_\delta\tilde{K}_\delta S_{\delta,l}\right]\right\rangle\ . \tag{19}$$

By choosing the set $\{\tilde{K}_\alpha\}$ to make $\langle\tilde{S}_\alpha-S_\alpha\rangle=0$, these equations allow the calculation of the effective renormalized coupling constants $\{K_\alpha^{(n)}\}$ after n iterations of the RG transformation. A convenient consistency check is

TABLE II. Correlation functions for the original and renormalized lattices from an MC simulation of a 32×32 lattice with a 2×2 majority-rule RG transformation. The MC simulation ran for 2.5×10^6 MC steps per site (MCS/S), starting from an old, well-equilibrated configuration from a previous simulation. Characteristic relaxation times for the energy of the unrenormalized system were about 100 MCS/S and data were taken every 20 MCS/S. The correlation functions calculated using Callen's representation differed from those shown by the amount in the second to last column, and had very nearly the same accuracy as given below for the correlation functions calculated in the usual manner. The errors in the differences were smaller than those for the correlation functions themselves by the ratio given in the last column.

n	α	$\langle S_\alpha^{(n)}\rangle$	$\langle\Delta S_\alpha^{(n)}\rangle$	Error ratio
0	1	1.4348(8)	0.000 04(4)	0.05
	2	1.3023(11)	−0.000 01(8)	0.07
	3	1.2264(14)	−0.000 02(5)	0.03
	4	2.3749(31)	0.000 03(10)	0.03
	5	1.1300(19)	−0.000 06(9)	0.05
	6	0.6053(5)	0.000 03(3)	0.06
	7	0.4877(7)	−0.000 03(6)	0.08
1	1	1.432(2)	0.000 17(9)	0.06
	2	1.331(2)	0.000 04(22)	0.10
	3	1.247(3)	−0.000 34(20)	0.08
	4	2.440(6)	0.000 35(23)	0.04
	5	1.171(4)	−0.000 22(12)	0.03
	6	0.590(1)	0.000 07(9)	0.10
	7	0.508(1)	−0.000 08(9)	0.08
2	1	1.470(3)	0.000 1(3)	0.10
	2	1.387(4)	0.000 6(3)	0.07
	3	1.319(5)	0.000 8(3)	0.06
	4	2.599(11)	0.001 4(5)	0.04
	5	1.265(7)	0.000 7(3)	0.05
	6	0.610(2)	0.000 1(3)	0.14
	7	0.539(2)	0.000 1(2)	0.08
3	1	1.555(6)	0.000 9(9)	0.15
	2	1.497(8)	0.000 8(10)	0.13
	3	1.477(8)	0.000 9(14)	0.17
	4	2.922(18)	0.002 0(29)	0.16
	5	1.444(10)	−0.000 4(11)	0.12
	6	0.661(4)	0.000 1(5)	0.15
	7	0.610(5)	0.000 3(5)	0.11

the reproduction of the known unrenormalized coupling constants $\{K_\alpha^{(0)}\}$ used in the original MC simulation.

The values of $\{\tilde{K}_\alpha^{(n)}\}$ must be close to $\{K_\alpha^{(n)}\}$ for Eq. (18) to be valid. Starting with $\tilde{K}_\alpha^{(n)}=K_\alpha^{(0)}$, two short preliminary computations were usually sufficient to obtain a good set of values for $\{K_\alpha^{(n)}\}$.

IV. EXTRAPOLATION OF THE RG TRAJECTORIES TO THE FIXED POINT

Estimates for the fixed-point couplings can be made direct from the RG trajectories, using the matrix of derivatives

$$T_{\alpha\beta}=\partial K_\alpha^{(n+1)}/\partial K_\beta^{(n)} \tag{20}$$

which can be calculated by standard Monte Carlo renormalization group (MCRG) methods.[5–8] Going over to an obvious notation, an approximation to the fixed point is given by

$$\underline{K}^*=\underline{K}^{(n)}+(\underline{I}-\underline{T})^{-1}(\underline{K}^{(n+1)}-\underline{K}^{(n)}) \tag{21}$$

and $\underline{I}$ is the identity matrix. This equation can be rewritten to involve only a single matrix inversion and simplify computer programming.

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 full information on the behavior of the RG transformation is available, deviations from the fixed point in the most relevant (least irrelevant) directions could be projected out using eigenvalues and eigenvectors of the matrix $\underline{T}$.

The statistical errors involved in extrapolating to the fixed point are naturally larger than those for the renormalized coupling constants. Explicit examples of such calculations are given below.

V. MAJORITY-RULE TRANSFORMATION WITH SCALE FACTOR $b=2$

The first example of the calculation of renormalized coupling constants for the $d=2$ Ising model will use the 2×2 majority-rule transformation mentioned in the Introduction.

TABLE III. Renormalized coupling constants and extrapolated fixed point for the nearest-neighbor $d=2$ Ising model using a majority-rule transformation with scale factor $b=2$. Same MC simulation as Table II.

n	α	Values in simulation $K_\alpha^{(n)}$	Best estimates for couplings $K_\alpha^{(n)}$	Extrapolated fixed point K_α^*
0	1	0.440 687	0.440 76(24)	
	2	0.0	0.000 04(22)	
	3	0.0	−0.000 15(17)	
	4	0.0	0.000 20(13)	
	5	0.0	−0.000 29(21)	
	6	0.0	0.000 08(18)	
	7	0.0	−0.000 17(16)	
1	1	0.364 212	0.3643(7)	0.3705(17)
	2	0.081 546	0.0814(9)	0.0923(5)
	3	−0.007 484	−0.0068(6)	−0.0178(10)
	4	−0.003 616	−0.0038(3)	−0.0071(2)
	5	−0.002 453	−0.0023(2)	−0.0014(6)
	6	−0.007 572	−0.0075(5)	−0.0113(8)
	7	0.003 029	0.0026(3)	0.0067(5)
2	1	0.354 788	0.3527(7)	0.352(5)
	2	0.093 058	0.0944(10)	0.097(1)
	3	−0.010 410	−0.0094(6)	−0.011(1)
	4	−0.004 736	−0.0046(4)	−0.005(1)
	5	−0.001 800	−0.0019(9)	−0.002(1)
	6	−0.008 112	−0.0075(9)	−0.007(1)
	7	0.005 221	0.0043(5)	0.006(1)
3	1	0.350 144	0.353(3)	0.358(6)
	2	0.095 238	0.095(3)	0.094(3)
	3	−0.012 165	−0.013(2)	−0.014(3)
	4	−0.003 503	−0.002(2)	−0.003(2)
	5	−0.002 313	−0.005(2)	−0.005(2)
	6	−0.002 270	−0.004(3)	−0.002(3)
	7	0.004 343	0.005(2)	0.006(3)

Table II shows the effect of the RG transformation on various correlation functions. The first column gives the number of RG iterations (0 refers to the original MC simulation), and the second column indicates the type of interaction according to Table I. The values of the correlation functions calculated in the usual manner [Eq. (7)] are given in the third column. Even though the simulation was performed at the exact critical temperature of the $d=2$ Ising model and the RG trajectory approaches a fixed point, the correlation functions change significantly under renormalization owing to the size dependence.

Table III shows the calculated values of the original and renormalized coupling constants. The first two columns are the same as in Table II, and the third column gives approximate values of the renormalized coupling constants determined by preliminary calculations using Eq. (18). The differences between the usual correlation functions (third column of Table II) and those calculated with Callen's representation and these parameters are shown in the fourth column of Table II.

The differences in the correlation functions are quite small—well within the statistical errors for the correlation functions themselves (which are the same for both representations of the correlation functions near a critical point). Furthermore, statistical errors for the differences are smaller than for the correlation functions themselves by the factor given in the last column of Table II. The fact that errors in the differences are so much smaller is the reason for the success of this approach. A reduction of statistical error by a factor of 0.1 would have required an increase in computer power by a factor of 100 if a two-lattice comparison had been used. Actually, the gain is substantially more than that, since the single-lattice method does not require the MC simulation of any model more complicated than the original one.

The differences in the correlation functions given in the fourth column of Table II were used to calculate the best estimates for the renormalized couplings found in the fourth column of Table III. The set of values corresponding to $n=0$ represents the consistency check of reproducing the coupling constants used in the original MC simulation. The nearest-neighbor coupling constant agrees with the exact value within a statistical error of about 0.06%, and all other couplings are zero within small statistical errors.

From Table III it can be seen that the critical RG trajectory rapidly approaches a fixed point and that the magnitude of the more distant interactions remains small.

TABLE IV. Renormalization-group trajectories from the nearest-neighbor $d=2$ Ising model using a majority-rule transformation with scale factor $b=2$.

n	$K_{\mathrm{NN}}^{(n)}$	$K_{\mathrm{NNN}}^{(n)}$	$K_{3\mathrm{NN}}^{(n)}$	$K_{4\mathrm{NN}}^{(n)}$	$K_{5\mathrm{NN}}^{(n)}$	$K_{4S(1)}^{(n)}$	$K_{4S(2)}^{(n)}$
0	0.3						
1	0.1838	0.0302	−0.0064	−0.0025	−0.0005	−0.0029	0.0004
2	0.0966	0.0141	−0.0053	−0.0014	−0.0001	−0.0006	−0.0001
0	0.36						
1	0.250	0.051	−0.005	−0.004	−0.002	−0.005	0.001
2	0.173	0.035	−0.009	−0.004	−0.002	−0.003	0.004
0	0.40						
1	0.305	0.067	−0.006	−0.004	−0.002	−0.010	0.001
2	0.248	0.056	−0.010	−0.002	−0.001	−0.005	0.000
0	0.42						
1	0.333	0.072	−0.007	−0.003	−0.001	−0.008	0.002
2	0.298	0.076	−0.012	−0.005	−0.001	0.001	0.001
0	0.46						
1	0.404	0.083	−0.016	−0.002	−0.003	−0.008	0.006
2	0.42	0.10	−0.024	−0.002	−0.001	−0.001	0.008
0	0.48						
1	0.424	0.099	−0.010	−0.006	−0.002	0.004	0.002
2	0.468	0.141	−0.011	−0.013	0.002	0.001	−0.002
0	0.3	0.15					
1	0.420	0.142	−0.009	−0.007	−0.003	−0.009	0.001
2	0.532	0.117	−0.019	0.001	0.028	−0.004	−0.000
0	0.08	0.16					
1	0.1295	0.0501	−0.0033	−0.0018	0.0001	−0.0024	0.0004
2	0.078	0.0145	−0.0037	−0.0001	0.0000	0.0003	0.0005

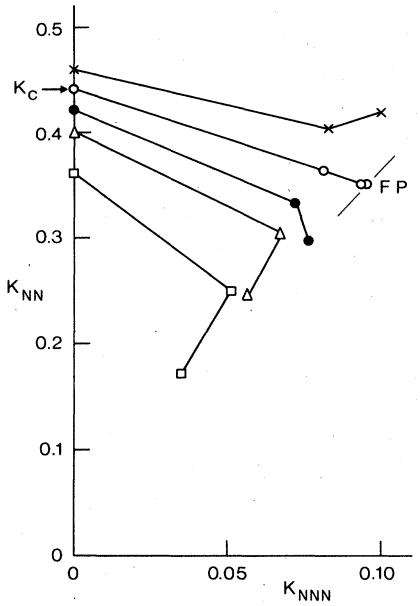

FIG. 1. Renormalization-group trajectories for the 2×2 majority-rule transformation, projected onto the subspace of nearest- and next-nearest-neighbor coupling parameters. Data taken from Table IV.

The interactions between more distant neighbors are negative and are expected to oscillate for still greater distances, as has been seen explicitly in the $d=3$ Ising model.[10]

The last column in Table III shows extrapolated locations of the fixed point using Eq. (21). The first set of values differs slightly from the next two, owing to nonlinear effects arising from the distance of the nearest-neighbor Hamiltonian from the fixed point. The second and third estimates for the fixed point agree with each other and with the third point in the RG trajectory.

For comparison with these results, and RG truncation approximation by Nauenberg and Nienhuis[23] predicted a fixed point for a similar transformation (using a tie-breaker instead of equal probabilities when the sum of spins in a block is zero) at $K_1=0.307$, $K_2=0.084$, and $K_6=-0.004$.

The method for calculating renormalized coupling constants is clearly not limited to the RG trajectory from the critical to the fixed point. The method can be applied to temperatures both above and below the critical value,[24] as shown in Table IV. An interesting feature of this table is that the major effect of the RG transformation is seen in the first two coupling constants, with interactions between more distant neighbors changing less dramatically. This makes it useful to plot these two RG parameters against each other, as shown in Fig. 1. This projection of the RG flow diagram confirms the qualitative picture of the effect of a typical RG transformation, which has formed the basis of all previous work.[1,2]

The RG trajectory from the nearest-neighbor critical point goes rapidly to a fixed point within small statistical errors. For temperatures as little as 4% above or below the critical temperature, the movement away from the fixed point is quite pronounced on the second iteration. The short line through the approximate location of the fixed point in the diagram indicates the projection of the eigenvector of the leading relevant operator onto this two-dimensional subspace, and the deviations of the trajectories are consistent with this direction.

VI. MAJORITY-RULE TRANSFORMATION WITH SCALE FACTOR $b=3$

Since the method of calculating renormalized coupling constants works directly with the renormalized configurations, there is no restriction on the type of transformation that may be analyzed in this manner. Table V shows data for the renormalized correlation functions from an MCRG calculation of a majority-rule RG transformation with scale factor $b=3$. Since there is an odd number of spins in each block for this transformation, no ties ever occur.

It is interesting to note that after two iterations of the $b=3$ RG transformation on a 36×36 lattice, we arrive at the same 4×4 system size as found after three iterations of the $b=2$ transformation of a 32×32 system discussed above. Since the last sets of correlation function in Tables II and V both refer to the same size lattice, differences must reflect different renormalized coupling constants

TABLE V. Renormalized correlation functions for an MC simulation of a 36×36 lattice with a 3×3 majority-rule RG transformation. The format is the same as Table II. The calculation was performed on a 36×36 lattice. The MC simulation ran for 5.76×10^5 MCS/S after discarding 8×10^4 MCS/S, with data taken every 20 MCS/S. Characteristic relaxation times for the energy of the unrenormalized system were about 120 MCS/S.

n	α	$\langle S_\alpha^{(n)}\rangle$	$\langle \Delta S_\alpha^{(n)}\rangle$	Error ratio
0	1	1.431(2)	0.0001(2)	0.10
	2	1.297(3)	0.0002(2)	0.07
	3	1.219(3)	0.0000(2)	0.05
	4	2.358(7)	0.0002(3)	0.05
	5	1.120(4)	0.0001(2)	0.03
	6	0.603(1)	0.0000(1)	0.12
	7	0.485(2)	0.0001(1)	0.08
1	1	1.499(6)	−0.0021(4)	0.07
	2	1.400(8)	−0.0000(4)	0.15
	3	1.315(10)	−0.0002(5)	0.05
	4	2.579(20)	0.0003(6)	0.03
	5	1.242(12)	0.0001(3)	0.02
	6	0.640(4)	−0.0022(3)	0.18
	7	0.558(4)	−0.0002(2)	0.05
2	1	1.61(2)	−0.001(2)	0.14
	2	1.54(2)	0.002(2)	0.11
	3	1.52(2)	−0.000(3)	0.13
	4	3.00(5)	−0.005(5)	0.10
	5	1.48(3)	−0.001(3)	0.12
	6	0.70(1)	−0.000(1)	0.11
	7	0.65(1)	0.000(1)	0.09

TABLE VI. Renormalized coupling constants and extrapolated fixed point for the nearest-neighbor $d=2$ Ising model using a majority-rule transformation with scale factor $b=3$ on a 36×36 lattice. The format is the same as Table III, and the MC simulation is the same as Table V.

n	α	Values in simulation $K_\alpha^{(n)}$	Best estimates for couplings $K_\alpha^{(n)}$	Extrapolated fixed point K_α^*
0	1	0.440 687	0.4409(6)	
	2	0.0	−0.0001(3)	
	3	0.0	−0.0001(4)	
	4	0.0	−0.0005(2)	
	5	0.0	0.0001(3)	
	6	0.0	0.0004(3)	
	7	0.0	0.0000(4)	
1	1	0.407 119	0.408(2)	0.422(6)
	2	0.077 863	0.080(2)	0.081(5)
	3	−0.027 724	−0.027(2)	−0.032(2)
	4	−0.009 074	−0.008(1)	−0.011(2)
	5	−0.001 295	−0.002(1)	0.000(2)
	6	0.005 743	−0.003(2)	−0.008(3)
	7	0.012 115	0.010(1)	−0.014(2)
2	1	0.407 119	0.402(4)	0.439(2)
	2	0.077 863	0.101(5)	0.101(2)
	3	−0.027 724	−0.025(4)	−0.306(2)
	4	−0.009 074	−0.018(3)	−0.018(1)
	5	−0.001 295	−0.001(3)	−0.003(5)
	6	0.005 743	0.006(2)	0.005(1)
	7	0.012 115	0.008(5)	0.009(2)

TABLE VII. Renormalized coupling constants and extrapolated fixed point for the nearest-neighbor $d=2$ Ising model using a majority-rule transformation with scale factor $b=3$. The format, the model, and the RG transformation are the same as Table III, but the MC simulation was performed on a 12×12 lattice. A preliminary MC simulation ran for 2.185×10^6 MCS/S after discarding 11 000 MCS/S, and produced the values shown in the first column. The second column, giving a subsequent refinement, used the values in the first column to extrapolate after one RG transformation. The second MC simulation ran for 2.85×10^6 MCS/S starting with the last configuration of the first simulation. Characteristic relaxation times were about 20 MCS/S.

n	α	Estimates from first extrapolation $K_\alpha^{(n)}$	Best estimates for couplings $K_\alpha^{(n)}$	Extrapolated fixed point K_α^*
0	1	0.4411(5)	0.4411(9)	
	2	−0.0007(7)	−0.0003(8)	
	3	0.0005(8)	−0.0005(8)	
	4	0.0004(3)	−0.0000(5)	
	5	−0.0001(3)	−0.0000(3)	
	6	0.0001(5)	0.0004(6)	
	7	0.0001(7)	0.0000(2)	
1	1	0.400(3)	0.407(3)	0.421(6)
	2	0.082(4)	0.078(3)	0.086(4)
	3	−0.028(2)	−0.028(2)	−0.36(3)
	4	−0.011(2)	−0.009(2)	−0.013(2)
	5	−0.002(2)	−0.001(2)	−0.000(2)
	6	0.007(3)	0.006(3)	0.007(4)
	7	0.016(1)	0.012(1)	0.015(2)

TABLE VIII. Decimation transformation with scale factor $b=2$ for the nearest-neighbor $d=2$ Ising model ($K_c=0.440\,687$). The calculation was performed on a 32×32 lattice, and ran for 2.25×10 MCS/S starting from the last configuration of an old simulation, with data taken every 20 MCS/S. Extrapolations for all levels of renormalization after the original lattice used $K_1=0.2$ and $K_2=0.1$, and all other couplings are equal to zero.

α	$K_\alpha^{(0)}$	$K_\alpha^{(1)}$	$K_\alpha^{(2)}$	$K_\alpha^{(3)}$
1	0.4396(9)	0.254(1)	0.186(2)	0.146(3)
2	−0.0002(7)	0.086(1)	0.089(2)	0.097(5)
3	−0.0004(11)	0.015(1)	0.028(1)	0.033(1)
4	0.0002(5)	0.008(1)	0.016(2)	0.019(2)
5	0.0004(3)	0.004(1)	0.012(3)	0.010(3)
6	0.0011(6)	−0.018(1)	−0.031(1)	−0.043(3)
7	0.0003(6)	−0.009(1)	−0.013(3)	−0.028(4)

and, different fixed points.

That this is indeed the case can be seen in Table VI. The renormalized nearest-neighbor coupling constant is about 0.4 for both iterations, although it was about 0.35 for the $b=2$ transformation. The third-neighbor interaction is negative, but much stronger than for the $b=2$ transformation, balancing the strength of the enhanced nearest-neighbor coupling.

A curious feature is that of the strength of the nearest-neighbor coupling at the extrapolated fixed point is larger than for the first two iterations. Although it is possible that this is indeed the case, it would seem more likely that the effect is due to the use of an insufficient number of coupling constants.

To test the method for finite-size effects, the calculation in Table VI was repeated, using a 12×12 lattice. The renormalized coupling constants calculated with this smaller lattice are shown in Table VII and can be seen to agree very well with data in Table VI.

VII. DECIMATION WITH SCALE FACTOR $b=2$

A decimation transformation is one in which the renormalized spins are simply a subset of the original spins. When the renormalized spin is always given the value of the original spin in the lower left-hand corner of the 2×2 block, we have a decimation transformation with scale factor $b=2$.

The fixed point is known to be a trivial one, in which the range of interaction diverges and magnitudes of the renormalized couplings all vanish. The results are shown in Table VIII. In contrast to previous RG transformations, the renormalized coupling constants do not fall off rapidly with distance. The seven parameters included in the calculation are clearly not enough for a full description of the renormalized system. All pair interactions are positive (ferromagnetic), although other transformations produced a change of sign with distance. Although three iterations are not enough to get a good idea of the asymptotic behavior of the transformation under many iterations, Table VIII appears to be consistent with the expected trivial fixed point.

VIII. SUMMARY AND CONCLUSIONS

The ability to calculate effective renormalized coupling constants for any block-spin RG transformation of interest opens up the systematic investigation of detailed effects of renormalization. This paper has attempted to provide a basis for such investigations, by showing the method in operation using various RG transformations on a simple, well-known model in statistical mechanics.

A later paper will extend these studies to the three-dimensional Ising model,[25] for which there is still no exact solution. This direction is very promising, since current state-of-the-art MCRG calculations already come close to the accuracy of the best competing methods for the calculation of critical exponents.[26]

The three-dimensional model will also be used to investigate the improvement in the convergence of the MCRG calculation of critical exponents by simulating an approximate fixed point, instead of the nearest-neighbor critical point. Such an investigation has not been discussed in this paper, because the first iteration of the $b=2$ RG transformation starting from the nearest-neighbor model is already only 3% away from the exact value, so that a dramatic improvement is not to be expected.[5–8]

I believe that this approach can be useful for studying very general models, including lattice gauge theories, which are important in the theory of elementary particles. The class of RG transformations can also be broadened to include transformations in momentum space.[27] Such future applications appear to be quite feasible on the basis of the present results.

*Present address: Department of Physics, Carnegie-Mellon University, Pittsburgh, PA 15213.

[1]Th. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

[2]K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[3]For a discussion of Monte Carlo methods, see K. Binder, in *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979), Vol. 7, p. 1.

[4]S.-k. Ma, Phys. Rev. Lett. **37**, 461 (1976).

[5]R. H. Swendsen, Phys. Rev. Lett. **42**, 859 (1979).

[6]R. H. Swendsen, Phys. Rev. B **20**, 2080 (1979).

[7]R. H. Swendsen, in *Phase Transitions: Cargese 1980,* edited by M. Levy, J.-C. Le Guillou, and J. Zinn-Justin (Plenum, New York, 1982), p. 395.

[8]R. H. Swendsen, in *Real-Space Renormalization,* Vol. 30 of *Topics in Current Physics,* edited by Th. W. Burkhardt and J. M. J. van Leeuwen, (Springer, Berlin, 1982), p. 57.

[9]In Ref. 2, K. G. Wilson presented a unique calculation of 217 coupling constants for a certain RG transformation of the $d=2$ Ising model. The method is numerical, but is not applicable to Monte Carlo simulations, because it uses negative weighting factors in the RG transformation.

[10]R. H. Swendsen, Phys. Rev. Lett. **52**, 1165 (1984).

[11]M. Creutz, L. Jacobs, and C. Rebbi, Phys. Rep. **95**, 2029 (1983).

[12]R. H. Swendsen, Phys. Rev. Lett. **47**, 1775 (1981).

[13]K. G. Wilson, in *Recent Developments in Gauge Theories,* edited by G. 't Hooft *et al.* (Plenum, New York, 1980).

[14]K. G. Wilson and R. H. Swendsen (unpublished).

[15]S. H. Shenker and J. Tobochnik, Phys. Rev. B **22**, 4462 (1980).

[16]D. P. Landau and R. H. Swendsen, Phys. Rev. Lett. **46**, 1437 (1981).

[17]R. H. Swendsen, D. Andelman, and A. N. Berker, Phys. Rev. B **24**, 6732 (1981).

[18]J. Tobochnik, Phys. Rev. B **26**, 6201 (1982); **27**, 6972(E) (1982).

[19]R. H. Swendsen, Phys. Rev. B **27**, 391 (1983).

[20]R. H. Swendsen and A. N. Berker, Phys. Rev. B **28**, 3987 (1983).

[21]H. B. Callen, Phys. Lett. **4B**, 161 (1963).

[22]G. Parisi, R. Petronzio, and F. Rapuano, Phys. Lett. **128B**, 418 (1983).

[23]M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. **33**, 1598 (1974).

[24]Away from the critical temperature, Callen's representation becomes more efficient in the sense of having smaller statistical errors than the direct summation. However, the differences can still be determined even more accurately.

[25]R. H. Swendsen, Phys. Rev. Lett. **52**, 2321 (1984).

[26]G. S. Pawley, D. J. Wallace, R. H. Swendsen, and K. G. Wilson, Phys. Rev. B **29**, 4030 (1984).

[27]R. H. Swendsen, Phys. Rev. Lett. **47**, 1159 (1981).