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# Monte Carlo renormalization-group studies of critical phenomena

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Monte Carlo renormalization-group (MCRG) methods are described and illustrated for models of current interest. The calculation of critical exponents and the determination of critical temperatures are discussed, as well as the application to multicritical points.

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## INTRODUCTION

The methods of Monte Carlo computer simulation [1, 2] and real-space renormalization-group analysis [3-6] have been used for several years to investigate the properties of thermodynamic systems. Both approaches have great generality and the possibility of calculating non-universal properties (such as the critical temperature) as well as universal properties. Although considerable success has been achieved with these techniques, they each suffer from certain drawbacks, which I shall discuss below. The Monte Carlo renormalization group (MCRG) [6-27] is a combination of the two methods, which has been shown to have important advantages over the individual techniques.

I shall begin with a brief description of the methods on which MCRG is based, and then show a method for combining them. Whenever a new approach to a general class of problems is developed, it is appropriate to test it on special cases for which the answers are known. I shall therefore give examples of applications to the Ising model and the particularly difficult case of the Baxter model to establish the validity of the method.

The determination of critical exponents relies on the ability to locate the critical (or multicritical) point of the system under investigation. Location of the critical point can also be attacked within the framework of the MCRG using techniques developed by Wilson and Swendsen [22]. These methods have been applied by Landau and Swendsen [23] to find tricritical points in the Blume-Capel model and an Ising antiferromagnet in a magnetic field.

The MCRG method is applicable to a very large class of physical models, as are the real-space RG truncation approximations and standard MC simulations. Current requirements are that the operators be classical (although this may not be a limitation in the future [28-35]) and associated with lattice sites. We shall denote the operator on lattice site  $i$  by  $\sigma_i$ . The simplest example is that of Ising spins, for which  $\sigma_i$  takes on only the values  $+1$  and  $-1$ . However, the operators can take on any values, including an arbitrary number of discrete states (as in the  $q$ -state Potts model), a continuum of states, or vectors. The Hamiltonian can be written in the general form

$$H = \sum_{\alpha} K_{\alpha} S_{\alpha}, \quad (1)$$

where the  $S_{\alpha}$ 's are the various possible combinations of the  $\sigma_i$ 's that occur in models of interest or are generated by the renormalization-group transformations. An example is the nearest-neighbor operator

$$S_{nn} = \sum_{\langle ij \rangle} \sigma_i \sigma_j. \quad (2)$$

The equilibrium probability for configuration  $a$  can then be written as

$$P(a) = \exp(H(a)) / Z, \quad (3)$$

where  $Z$  is the partition function. Correlation functions are defined in the usual way by the trace over the equilibrium distribution.

## MONTE CARLO COMPUTER SIMULATIONS

Since good descriptions of standard Monte Carlo simulations exist [1,2], I shall only sketch the method here.

The basic idea is to generate a sequence of configurations with the equilibrium probability distribution (3). This is accomplished by introducing "dynamics" through a Master Equation

$$P(a, t + \Delta t) = P(a, t) + \sum_b [W(b, a) P(b, t) - W(a, b) P(a, t)], \quad (4)$$

where  $a$  and  $b$  are configurations,  $P(a, t)$  is the probability of finding a configuration  $a$  at time  $t$ , and  $W(a, b)$  is the conditional probability of finding  $b$  at time  $t + \Delta t$ , if it were in  $a$  at time  $t$ . The condition of detailed balance

$$W(b, a) P(b) = W(a, b) P(a), \quad (5)$$

and a non-zero probability of reaching any state from any other state then ensure that

$$P(a, t) \Rightarrow P(a) \quad (6)$$

as  $t \rightarrow \infty$ , and we say that the system goes to equilibrium. Equation (6) can be written as

$$\frac{W(b, a)}{W(a, b)} = \exp(H(a) - H(b)) \quad (7)$$

so that the partition function cancels out and allows us to construct an efficient algorithm for the computer if we restrict the allowed transitions to local spin flips.

In the simplest case, as each spin is visited, the probability of changing that spin is compared with the output of a pseudo-random-number generator and, depending on which is larger, the spin is either updated or

left unchanged. This produces a sequence of configurations from which any correlation functions of interest can be calculated. The most serious limitation of standard MC techniques for calculating critical properties is the finite-size effect, which rounds off the critical singularities.

#### REAL-SPACE RENORMALIZATION-GROUP FORMALISM

The renormalization-group approach to problems of the critical behavior of thermodynamic systems attempts to transform the problem in such a way as to focus attention onto the critical properties and thereby simplify calculations [1,2]. RG transformations first integrate out some fraction of the variables associated with short-wavelength fluctuations, producing a new system with fewer degrees of freedom. Usually, a local grouping of the spin variables on neighboring sites into "blocks" is made, and a value assigned to each "block spin" on the basis of the values taken on by the spins in each block. This reduces the linear dimensions of the system by a factor  $b$ . A typical example for the Ising model would be to divide a square lattice into square blocks and assign the block spin,  $\sigma'$ , the value of +1 if the sum of the spins in the block is positive, and -1 if negative. This "majority-rule" transformation will be used below as an example.

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

$$P'(a') = \text{Tr}_a T(a', a) P(a). \quad (8)$$

The new probability distribution can then be interpreted in terms of an effective Hamiltonian  $H'$  for the renormalization block spins

$$P'(a') = \exp(H'(a'))/Z' \quad (9)$$

and this renormalized Hamiltonian can be parameterized in terms of a new set of coupling constants  $\{K'_\alpha\}$ .

Unfortunately, even for very simple models with only nearest-neighbor interactions and simple RG transformations, the renormalized Hamiltonian contains an infinite number of coupling constants. The calculational difficulties this creates are important in all applications of the real-space renormalization group.

To calculate the critical exponents, we follow the usual procedure and linearize the renormalization-group transformation at the fixed point  $\{K_\alpha^*\}$ ,

$$K_\alpha^{(n+1)} - K_\alpha^* = \sum_\beta T_{\alpha\beta} (K_\beta^{(n)} - K_\beta^*), \quad (10)$$

where

$$T_{\alpha\beta} = \partial K_\alpha^{(n+1)} / \partial K_\beta^{(n)}. \quad (11)$$

The critical exponents are then determined from the eigenvalues of  $T_{\alpha\beta}$  [3]. The largest eigenvalue,  $\lambda = b^{y_T}$ , describes how rapidly the renormalized Hamiltonians move away from the fixed point. The eigenvalue exponent  $y_T = 1/\nu$ , for example, gives the divergence of the correlation length as a function of temperature. A deviation from criticality due to a magnetic field would produce a different eigenvalue exponent,  $y_H$ , determining the critical exponents  $\eta$  and  $\delta$ . All other critical exponents can then be found from the scaling equations in the usual way [3].

The usual methods of real-space renormalization-group analysis attack the problem of the infinite number of effective coupling constants by making approximations that eliminate all but a finite number of interactions. This approach has led to the development of successful

approximations for several systems. But there are equally plausible approximations that give very poor results. In principle, the usual real-space renormalization-group approximations can be systematically improved by including more coupling constants in the calculation, but this is generally impractical due to computational difficulties.

Probably the most important advantage of combining Monte Carlo simulations with the renormalization-group analysis is that it allows all approximations to be improved systematically without a major increase in effort.

#### CALCULATION OF CRITICAL EXPONENTS WITH MCRG

MCRG uses an MC simulation to generate a sequence of configurations from which correlation functions can be calculated. Since the explicit configurations are stored in the computer, it is a simple matter to use any reasonable RG transformation to divide the lattice into blocks and apply the exact RG transformation direct to these configurations. This provides a sequence of configurations for the renormalized spins characteristic of the renormalized Hamiltonian. All effective coupling constants that will fit on the lattice are automatically taken into account. The number of such interactions is much larger than in any of the usual truncation approximations and can be easily increased by increasing the size of the lattice. The effective range of the renormalized Hamiltonians must be small with respect to the linear dimensions of the lattice, which can be checked by using different size lattices.

The MC simulation is performed at the critical temperature, and repeated iterations of the RG transformation move the renormalized Hamiltonians towards the fixed point [13]. This produces a sequence of approximations for the critical exponents, converging towards the fixed-point values.

The matrix  $T_{\alpha\beta}$  is found by solving the linear set of chain-rule equations

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \sum_\alpha \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}}. \quad (12)$$

The derivatives in (12) are obtained from MC correlation functions,

$$\frac{\partial \langle S_\alpha^{(m)} \rangle}{\partial K_\beta^{(n)}} = \frac{\langle S_\alpha^{(m)} S_\beta^{(n)} \rangle - \langle S_\alpha^{(m)} \rangle \langle S_\beta^{(n)} \rangle}{\langle S_\alpha^{(m)} \rangle \langle S_\beta^{(n)} \rangle}. \quad (13)$$

The eigenvalues of  $T_{\alpha\beta}$  give estimates of the critical exponents if the effective Hamiltonians are close to the fixed point, as discussed above. Since we can only calculate a small part of the matrix  $T_{\alpha\beta}$ , a second truncation is made at this point. However, more elements of the matrix can be systematically included in the calculation. The analysis is repeated to test the effect of additional matrix elements on the estimates for the critical exponents.

The  $d = 2$  Ising model provides an illustration of how MCRG works in practice. Using a block-spin transformation with scale factor  $b = 2$ , the renormalized block-spin value was determined by majority rule (with ties being decided by a random-number generator). Technical data on the underlying MC simulations is given in [27].

Table I shows the MCRG results for the thermal eigenvalue exponent,  $y_T$ , for various lattice sizes. Since the linear dimensions of a lattice are reduced by the scale factor  $b = 2$  with each RG iteration, the  $64 \times 64$  lattice after  $n$  iterations is reduced to the same size as the  $32 \times 32$  lattice after  $n - 1$  iterations. Consequently, entries along diagonal rows in Table I all refer to the same size renormalized lattices. The numbers in parentheses give the approximate statistical uncertainty in the last digit as estimated from the spread of values obtained from MCRG analyses on groups of data evaluated separately. This procedure is basically the same as the standard error analysis described by Binder [1,2].

In Table I, there is a clear difference between using only a single coupling constant (nearest-neighbor) in the analysis and including second-neighbor interactions. The inclusion of a four-spin coupling and more distant-neighbor interactions does not have a significant effect. Only a few couplings are important for the analysis, although more were used than shown. For the first RG step, the estimate for  $y_T$  is about 3% below the exact value. By the second RG step, the renormalized Hamiltonian has moved close to the fixed point and the

TABLE I. Critical eigenvalue exponent  $y_T$  (exact value is 1.000) for the  $d = 2$  Ising model as a function of the number of RG iterations (Nr), the number of coupling constants in the RG analysis ( $N_c$ ), and the linear dimension of the lattice (L).  $2 \times 2$  RG block transformation.

		Lattice size (L)		
		64	32	16
Nr	$N_c$			
1	1	0.912(2)	0.904(1)	0.897(3)
	2	0.967(3)	0.966(2)	0.964(3)
	3	0.968(3)	0.968(2)	0.966(3)
	4	0.969(4)	0.968(2)	0.966(3)
2	1	0.963(4)	0.953(2)	0.937(3)
	2	0.999(4)	0.998(2)	0.993(3)
	3	1.001(4)	1.000(2)	0.994(3)
	4	1.002(5)	0.998(2)	0.984(4)
3	1	0.957(2)	0.936(3)	
	2	0.998(2)	0.991(3)	
	3	0.999(2)	0.993(3)	
	4	0.999(2)	0.987(4)	
4	1	0.940(7)		
	2	0.993(6)		
	3	0.992(6)		
	4	0.988(5)		

estimates of  $y_T$  have come very close to the exact value. The third iteration comes even closer to the fixed point and no significant change in the estimates for  $y_T$  can be seen, since it is within the statistical errors. Comparison with the data for the  $32 \times 32$  system shows only a very small size effect.

Table II gives similar data for the magnetic eigenvalue exponent,  $y_H$ , for which deviations from the exact value are smaller, as is characteristic of the magnetic eigenvalue.

TABLE II. Critical eigenvalue exponent  $y_H$  (exact value is 1.875) for the  $d = 2$  Ising model under the same conditions as for Table I.

		Lattice size (L)		
		64	32	16
Nr	$N_c$			
1	1	1.8810(1)	1.8807(1)	1.8797(2)
	2	1.8804(1)	1.8803(1)	1.8800(2)
2	1	1.8757(2)	1.8748(2)	1.8719(2)
	2	1.8758(2)	1.8757(2)	1.8747(2)
3	1	1.8731(4)	1.8710(5)	
	2	1.8740(4)	1.8742(5)	
4	1	1.8706(5)		
	2	1.8735(7)		

#### CALCULATION OF RENORMALIZED COUPLING CONSTANTS WITH MCRG

In the calculations of the critical exponents described above, the renormalized Hamiltonians are never explicitly calculated. This is usually an advantage, because many effective couplings can be taken into account implicitly, without introducing the inevitable errors inherent in dealing with them explicitly. On the other hand, to determine the critical temperature with the MCRG method, we must be able to calculate the renormalized Hamiltonians. Recently, techniques have been developed to treat this problem [22,23], based on a method introduced by Wilson for the study of lattice gauge theories [5,6].

Wilson has pointed out the possibility of performing two simulations on lattices of different sizes [6]. If the two systems differ in size by the scale factor  $b$ , one renormalization-group transformation of the larger system will produce a system the same size as the smaller system, making the size effect identical for both. For application to lattice gauge theories, Wilson then suggested adjusting the coupling constants used in the simulation of the smaller system until the correlation functions matched those obtained by renormalizing the larger system.

Unfortunately, we have to be able to deal with many coupling constants, and scanning a many-dimensional space is impractical. However, we can use the differences in the correlation functions to calculate the differences in the coupling constants and to locate the fixed point [22]. Wilson has suggested a particularly simple and efficient procedure, using the derivatives of the renormalized correlation function after  $n$  iterations, with respect to the original coupling constants.

Suppose the Hamiltonian  $H$  is actually the fixed point of the RG transformation, then  $H' = H$  by definition and the correlation functions must be the same on the renormalized large lattice and the small lattice. From non-zero differences in the correlation functions, deviations from the fixed-point Hamiltonian can be calculated.

The changes in the correlation functions are given by

$$\delta \langle S_\alpha^{(n)} \rangle_L = \sum_\beta \frac{\partial \langle S_\alpha^{(n)} \rangle}{\partial K_\beta^{(0)}} \frac{L}{\delta K_\beta^{(0)}} \delta K_\beta^{(0)}, \quad (14)$$

with the derivatives calculated as in Eq. (13). By solving the set of linear equations

$$\langle S_{\alpha}^{(n)} \rangle_L - \langle S_{\alpha}^{(n-1)} \rangle_S = \sum_{\beta} \left[ \frac{\partial \langle S_{\alpha}^{(n)} \rangle_L}{\partial K_{\beta}^{(0)}} - \frac{\partial \langle S_{\alpha}^{(n-1)} \rangle_S}{\partial K_{\beta}^{(0)}} \right] \delta K_{\beta}^{(0)}, \quad (15)$$

we can determine what changes in the coupling constants are necessary to make the correlation functions match and thus calculate an approximate fixed point. As the number of RG iterations increases, the deviations from the fixed point (and from the previous iteration) in the irrelevant directions decrease. The corresponding differences in the correlation functions also decrease and become more difficult to determine accurately.

On the other hand, when the original MC simulation is not exactly at criticality, the deviations in the relevant directions increase upon repetition of the RG transformation, and the corresponding differences in the correlation functions become amplified. The method

TABLE III. Estimates of the deviation of the simulated coupling constant from the true value  $K_c$  (exact value: 0.4406879).  $d = 2$  Ising model.  $2 \times 2$  RG block transformation.

		Lattice sizes being compared		
Nr	Nc	64-32	32-16	16-8
1	1	0.0024(3)	0.0029(1)	0.0037(2)
	2	0.0009(3)	0.0012(1)	0.0017(2)
	3	0.0014(3)	0.0017(1)	0.0023(2)
	4	0.0012(3)	0.0015(1)	0.0022(2)
	5	0.0005(3)	0.0006(2)	0.0012(2)
	6	0.0005(3)	0.0006(2)	0.0012(2)
	7	0.0005(3)	0.0006(2)	0.0012(2)
2	1	0.0002(3)	0.0002(2)	0.0004(2)
	2	0.0000(3)	0.0000(2)	0.0002(3)
	3	0.0001(3)	0.0001(2)	0.0003(3)
	4	0.0000(3)	0.0001(2)	0.0003(3)
	5	-0.0000(3)	0.0001(3)	0.0001(3)
	6	-0.0000(3)	0.0001(3)	0.0001(3)
	7	-0.0000(3)	0.0001(3)	0.0001(3)
3	1	-0.0002(4)	-0.0001(4)	-0.0000(2)
	2	-0.0002(4)	-0.0002(4)	-0.0017(3)
	3	-0.0002(4)	-0.0002(4)	-0.0001(3)
	4	-0.0002(4)	-0.0002(4)	
	5	-0.0002(4)	-0.0002(5)	
	6	-0.0002(4)	-0.0002(5)	
	7	-0.0002(4)	-0.0002(5)	
4	1	-0.0003(4)	-0.0003(6)	
	2	-0.0003(5)	-0.0003(6)	
	3	-0.0003(6)	-0.0003(6)	
	4	-0.0003(6)		
	5	-0.0003(6)		
	6	-0.0003(6)		
	7	-0.0003(6)		

is thus extremely sensitive to the location of the critical temperature. Since we can treat several coupling constants in a single calculation, this method can also be used to find multicritical points [23]. It has proven especially effective to generalize Eq. (15) to perform a least-squares fit of the coupling constants to several correlation-function differences.

Table III shows the results of such a calculation of the critical temperature for the simple example of the two-dimensional Ising model. The numbers at the top of each column give the original linear dimensions of the lattices being compared. The second RG iteration is sufficient to reduce the systematic error due to the irrelevant operators below the small statistical uncertainty. Comparison of the  $16 \times 16$  and  $8 \times 8$  lattices shows no systematic deviation from the true critical point at the second RG iteration within the statistical errors.

#### MCRG RESULTS FOR MODEL SYSTEMS

A particularly difficult text is provided by the eight-vertex or Baxter mode [36,37]. This model can be represented by Ising spins on a square lattice with

$$H = K_{\text{nnn}} S_{\text{nnn}} + K_4 S_4, \quad (16)$$

where  $S_{\text{nnn}}$  is the sum over all next-nearest-neighbor products, and  $S_4$  is the sum over all four-spin products around an elementary plaquette. The critical exponents do not take on fixed universal values, but are functions of the coupling constants. This behavior can be represented by a fixed line, instead of a fixed point. The usual truncation approximations have not been able to reproduce the true behavior. Swendsen and Krinsky [14] have shown that the MCRG method does not run into such difficulties and can reproduce the correct function  $v(K_4)$  within 1% for  $v$  ranging from 0.7 to 1.35. Their calculation demonstrated another advantage of this approach in that they were able to calculate several independent critical exponents with a single MC simulation. They correctly obtained the values of  $y_H = 1.875$  (which describes the magnetization) to within 0.3%,  $y_{H_2} = 0.875$  (which corresponds to a three-spin coupling) to within 4%, and  $y_S = 0.75 + 0.25 y_T$  (which corresponds to breaking the symmetry with a nearest-neighbor coupling) to within 0.5%. Similar results have been obtained for the Ashkin-Teller model.

Swendsen and Krinsky [14] also investigated the  $d = 2$  Ising antiferromagnet with nearest- and second-nearest-neighbor interactions. This model had been predicted by van Leeuwen [38] to renormalize onto the Baxter fixed line, and therefore to have critical exponents that depend on the value of the second-neighbor coupling  $K_{\text{nnn}}$  when  $K_{\text{nnn}}$  is large and negative. The convergence of the magnetic eigenvalue was used as a criterion for determining the critical temperatures, and they were able to confirm van Leeuwen's prediction by explicitly calculating the dependence of  $y_T$  on  $K_{\text{nnn}}$ . Later calculations using the two-lattice simulations described above [14,22,23] have given the same critical temperatures as the original work, and the values of  $v$  also agree with the finite-size scaling approach of Nightingale [39].

Extensions of the MCRG method to the Ising model in three and four dimensions have been made by Blöte and Swendsen [16,19] and Sahni and Banavar [26]. The  $q = 3$  Potts model has also been studied by the MCRG method in three and four dimensions, and the phase transition determined to be first order in both cases [15].

Tricritical exponents have been investigated by Landau and Swendsen [23] for the Blume-Capel model and an Ising antiferromagnet in a magnetic field. The major difficulty in the calculation is locating the tricritical point, since two coupling parameters must be specified. This problem was overcome by the methods described above and tricritical exponents were found to be in agreement with existing conjectures [40,44], as shown in Table IV. The efficiency of these methods is expected to be very useful in future investigations of multicritical points.

TABLE IV. Estimates of the tricritical eigenvalue exponents for the  $d = 2$  Blume-Capel model [23]. Data taken from an MC simulation of  $2.24 \times 10^6$  MC-steps/site on a  $32 \times 32$  lattice.

Nr	$\gamma_{T1}$	$\gamma_{T2}$	$\gamma_{H1}$	$\gamma_{H2}$
1	1.785	0.715	1.934	1.12
2	1.799	0.795	1.934	1.14
3	1.805	0.835	1.929	1.14
Conjectured [40-44]:				
	1.8	0.8	1.925	?

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