PHYSICAL REVIEW
LETTERS

VOLUME 37 | 23 AUGUST 1976 | NUMBER 8

Renormalization Group by Monte Carlo Methods

Shang-keng Ma*
Service de Physique Théorique, Centre d'Etudes Nucléaires de Saclay, Gif-sur-Yvette, 91190 France
(Received 18 June 1976; revised manuscript received 29 July 1976)

I discuss the basic ideas in applying the Monte Carlo methods to the renormalization-group study of static and dynamic critical phenomena within the framework of a kinetic Ising model. Simple calculations demonstrating these ideas are presented.

Ever since electronic computers became available, the Monte Carlo method has become a useful tool in studying statistical mechanical problems as well as other problems in science. Basically the method involves generating, with the aid of a random-number generator, a sequence of configurations of the statistical mechanical system of interest in such a way that these configurations follow a canonical distribution.[1-4] Then one can "observe and measure" various physical properties such as the energy and the magnetization. In short, the method is a numerical experiment. The random-number generator simulates the effect of the thermal reservoir with which the system is in contact.

The literature on the application of Monte Carlo methods to the study of critical phenomena is vast (see the review article of Binder[4] and references therein). In spite of the extreme sophistication in programming and the power of the newest computers, there is still difficulty in simulating a system much larger than the correlation length ξ, which becomes infinite at the critical point. The divergence of ξ and other physical quantities is of course that which makes the critical phenomena difficult to study.

The recently advanced renormalization-group (RG) method has been effective in extracting the critical exponents.[5-9] This method does not attempt to calculate the singular quantities directly. It deals with the transformation of the interaction parameters defining the model under a change of length scale. Critical exponents are deduced from the transformation properties. The understanding of this very successful method cannot be regarded as complete, however, because there has been no systematic procedure in carrying out the RG method for three- and two-dimensional systems. Recent numerical works have made many advances.[7-9] They demonstrated not only the power of the method, but also that there is much to be understood.

The idea that a program combining the Monte Carlo and the RG methods should be helpful in the study of critical phenomena and the basic aspects of the RG seems evident. It is the purpose of this note to explain and demonstrate this idea. My preliminary results reported below show an optimistic outlook for developing this program into a powerful tool. The program applies to both static and dynamic RG.

To be specific, I shall carry out the discussion in the framework of a simple kinetic Ising model.[10] Consider Ising spins $\sigma_r = \pm 1$ (r is the coordinate vector), on a two-dimensional square lattice. The dynamics (and hence the statics) is defined by the flip probability

$$w_r(\sigma_r)dt = \Gamma \exp(-\sigma_r B_r)dt \qquad (1)$$

for each spin, which is the probability that the spin at r flips from σ_r to $-\sigma_r$ in the time interval dt. B_r is the magnetic field seen by σ_r, and is

the sum of the applied field $\boldsymbol{h}$ and the field produced by neighbors. Formally, we can write

$$B_r = \partial \mathcal{H}[\sigma]/\partial \sigma_r, \tag{2}$$

where $\mathcal{H}[\sigma]$ is $-$(Hamiltonian)/(temperature) for the spin configuration σ. The quantity Γ is independent of σ_r but may depend on the neighboring spins. Let μ denote the set of parameters specifying the model:

$$\mu = (J, K, L, \Gamma), \tag{3}$$

where J, K, and L refer to, respectively, the nearest-neighbor, the next-nearest-neighbor, and the four-spin interaction parameters. The rate $w_r(\sigma_r)$ given by (1) and the rate $w_r(-\sigma_r)$ for the inverse process satisfy the condition of detailed balance,

$$w_r(-\sigma_r)/w_r(\sigma_r) = \exp(2B_r\sigma_r) = \exp(\mathcal{H}[\sigma] - \mathcal{H}[\sigma'']), \tag{4}$$

where σ'' is the configuration obtained from σ by reversing σ_r. This condition implies that the probability distribution for σ will approach the canonical distribution $\exp(\mathcal{H}[\sigma])$ after a long time.

The basic steps of a Monte Carlo program that carries out the RG transformation $\mu \to \mu'$ are outlined in Fig. 1(a). The first step is to generate a sequence or a "history" of spin configurations according to (1). The second step is to measure the interaction parameters with probes of different scales. This is the step which is very different from the previous Monte Carlo studies. Here we do not measure global quantities like the specific heat, but rather observe how a small number of neighboring spins behave, i.e., we make "local measurements." The "small probe" is a probe measuring interaction parameters among the spins and should give the μ we start with. This serves as a check on the generation procedure and convergence. The large probe is designed to measure the effective interaction parameters $\mu' = (J', K', L', \Gamma')$ among the block spins. The last step is a matter of analyzing the data and extracting exponents. I proceed to explain these steps in more detail.

Figure 1(b) shows the generation of configurations. Given a configuration σ at time t, one computes the rate $w_r(\sigma_r)$ for each spin. The probability that no spin shall flip during the subsequent period t' is $\exp(-\Omega t')$, where

$$\Omega = \sum_r w_r(\sigma_r) \tag{5}$$

is the probability per second that one of the spins

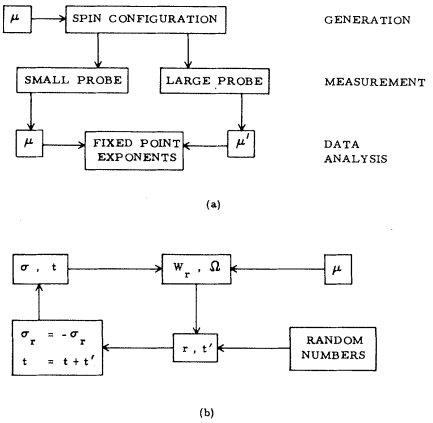

FIG. 1. (a) Outline of the program. (b) Generation of configurations.

flips. Thus the probability that nothing happens for a period t' and then one of the spins flips during the next interval dt' is

$$e^{-\Omega t'}\Omega dt'. \tag{6}$$

The probability that the one which flips is σ_r is

$$w_r(\sigma_r)/\Omega. \tag{7}$$

To choose t' and r, I have the computer generate two uniformly distributed random numbers $0 < x, y < 1$, and set

$$t' = -(\ln x)/\Omega. \tag{8}$$

Then divide the interval (0, 1) into N portions (N being the total number of spins), one for each spin, with lengths given by (7). The spin whose portion contains y gets flipped.[11] The procedure is then repeated.

The interaction parameters are measured by observing how a spin behaves in a given environment. When the range of interaction is no longer than the distance to the next-nearest neighbor, the environment of a spin is defined by the configuration of its eight neighbors (four nearest and four next-nearest). The small probe looks at 3×3 spins and measures τ_+ and τ_-, the lengths of time before flipping that a spin spends in the $+1$ state and that in the -1 state, respectively.[12] The ratio $\tau_+/\tau_- = \exp(2B_r)$ gives an equation for J, K, and L. For example, in the environment where all eight neighbor spins are $+1$, then $B_r = 4(J + K + L)$. By measuring τ_+/τ_- in three or more different environments, one can solve for J, K, and L. The geometrical mean $(\tau_+\tau_-)^{1/2}$ gives Γ. For determining the static parameters J, K, and L, one can simply accumulate the total

times before taking the ratios.

The large probe is the same as the small probe except that it looks at 3×3 *block spins* at a time. Each block spin is a set of 2×2 spins. The value of a block spin is chosen to be $+1$ if the majority of its constituents, excluding one spin arbitrarily to assure a majority, are $+1$, and -1 if the majority are -1. The results of the large-probe measurements give $\mu' = (J', K', L', \Gamma')$, i.e., the interaction parameters at a scale twice as large as that defined by the small probe.

The probes, large and small, can scan through the system to take measurements at different locations. I emphasize that we look at only local properties, i.e., a spin (or a block spin) at a time, and see how it behaves in a given environment, never at any collective property of the system. Thus the size of the lattice for our calculation and the boundary condition do not matter as long as the lattice is larger than the probes and the probes stay away from the boundary. It does not matter if ξ is larger than the lattice.

In principle there should be more parameters in μ and μ' to assure a complete representation of the transformation. A larger probe would be needed. Using only a 3×3 probe and the parameters above is a truncation. The truncation procedure in RG is still not understood. So far our preliminary calculation is not accurate enough to shed light on this problem.

The determination of Γ' is interesting although less well defined. Note that there has been no formulation of the dynamic RG apart from perturbation expansions in very special numbers of dimensions.[13] In the absence of a formalism, we rely heavily on the experimental nature of the Monte Carlo method in defining Γ'. We observe how a block flips in a given block environment and fit the observations with a kinetic Ising model. The block spins actually do not follow a pure exponential law of flipping like the original spins. Qualitatively, there are two time scales. When a block spin flips over, there is an intermediate period during which the block spin fluctuates rapidly. The time scale of this fluctuation is that of the original spin. This is the period when the block spin is determined by a single spin because the other two in the block have opposite signs. The longer time scale is that which describes the collective behavior of a block. We must use Γ' to fit this longer time scale. There are ways to extract the longer times. One can erase any two successive flips of a block spin within a time $t_{\min} \sim$ (original spin-flip time), construct histograms for the distribution of observed times, then plot them on semilog scale and fit straight lines to the longer time tails.

The static exponent ν is related to the largest eigenvalue $\lambda_T = 2^{1/\nu}$ of the matrix $\partial J_i'/\partial J_j$ ($J_1 = J$, $J_2 = K$, and $J_3 = L$). The exponent η is related to the largest eigenvalue $\lambda_H = 2^{2-\eta/2}$ of $\partial h_i'/\partial h_j$ ($h_1 = h$ is the applied field and h_2 is the three-spin interaction). These matrices can be calculated directly through averages at given block configurations when the large probe scans through the system.[14] For example

$$\frac{\partial}{\partial J}(J'+K'+L') = \frac{\partial}{\partial J}\frac{1}{8}\ln(\tau_+'/\tau_-') = \langle \partial\mathcal{H}/\partial J\rangle_+ - \langle \partial\mathcal{H}/\partial J\rangle_-, \quad (9)$$

where $\tau_\pm$ is the time that a block spin spends in ±1 states given all eight neighboring blocks in $+1$ state, and

$$\langle A\rangle_\pm \equiv \textstyle\sum_\sigma^\pm e^{\mathcal{H}} A / \sum_\sigma^\pm e^{\mathcal{H}}, \quad (10)$$

which means averaging over the original spins at the fixed block configuration with the center one at ±1 and the eight neighbors at $+1$. Equation (9) follows from the fact that

$$\tau_\pm \propto \textstyle\sum_\sigma^\pm e^{\mathcal{H}}. \quad (11)$$

The dynamic exponent z is obtained through $\Gamma/\Gamma' = 2^z$.

There are alternatives and variations to the program described above. One which I tried is to impose an additional field $\tilde{B}_r[\sigma']$ defined by a given block-spin configuration σ'. It is so strong that only those spin configurations which are consistent with σ' can occur. Explicitly for the block containing σ_1, σ_2, σ_3, and σ_4, we have $\sigma_r \tilde{B}_r[\sigma'] = a(\sigma_1+\sigma_2+\sigma_3-\sigma_1\sigma_2\sigma_3)\sigma'$, for $r = 1,2,3$ and $\tilde{B}_4 = 0$. The constant a is fairly large, ~ 10. One can also leave some blocks unimposed.

Flexibility is a great virtue of the Monte Carlo method. Generalizations to three-dimensional models and other definitions of RG seem to be straightforward. The major disadvantage seems to be the imprecision. An increase of precision by 10 means roughly 100 times longer computing for the same program.

Table I shows the results of the four trial programs. The errors indicated are in a large part due to the uncertainty in the fixed point. The probes could determine only J (5%) and K (20%), but not L. The static fixed point of Ref. 8 was used in these programs. The dynamic part of the fixed point is less well known. The one-param-

TABLE I. Preliminary results.

Block	Lattice	Time[a]	$1/\nu$	$(d+2-\eta)/2$	z
2×2	15×15	2.5	0.96 ± 0.04	1.87 ± 0.08	1.4 ± 0.4
3×3	15×15	1.5	1.02 ± 0.10	1.96 ± 0.10	...
2×2[b]	12×12	0.7	0.93 ± 0.10	1.85 ± 0.10	...
2×2[b]	12×12	2.5	...	...	1.4 ± 0.4
			1[c]	1.875[c]	~2 (Ref. 15)

[a] Minutes on a Saclay CDC 7600 computer.
[b] $\tilde{B}$ imposed.
[c] Onsager value.

eter fit here is too crude. A better approximation to the dynamic fixed point would need to include some memory and perhaps additional modes such as energy fluctuations. In view of the inefficiency of these trial programs and the relatively trivial amount of time and effort spent, I find these results very encouraging.

I thank Professor J. M. J. Van Leeuwen, Professor E. Brézin, Professor M. T. Beal-Monod, Professor D. Levêsque, Dr. L. Senbetu, and Mr. M. Kolb for helpful conversations and comments. The hospitality of Professor C. De Dominicis and members of the Theoretical Physics Division at Saclay is gratefully acknowledged.

*On leave of absence from University of California, San Diego, La Jolla, Calif. 92093.

[1]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).

[2]J. M. Hammersley and D. C. Handscomb, *Monte Carlo Methods* (Methuen, London, 1964).

[3]E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 6, 2777 (1972).

[4]K. Binder, in "Phase Transitions and Critical Phenomena," edited by C. Domb and M. S. Green (Academic, to be published), Vol. 5.

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

[6]S. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, Mass., 1976).

[7]Th. Niemeijer and J. M. J. Van Leeuwen, Physica (Utrecht) 71, 17 (1974), and review article in "Phase Transitions and Critical Phenomena," edited by C. Domb and M. S. Green (Academic, to be published), Vol. 6.

[8]M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. 33, 344 (1974), and Phys. Rev. B 11, 4152 (1975).

[9]L. P. Kadanoff and A. Houghton, Phys. Rev. B 11, 377 (1975).

[10]See Refs. 3 and 4, and R. Glauber, J. Math. Phys. (N.Y.) 4, 234 (1963).

[11]Note that this is not the procedure commonly used (the "Metropolis method," which is meant for statics only).

[12]In practice, the whole history of the 3×3 spins is recorded and the durations of the configurations which occurred are sampled.

[13]See Ma, Ref. 6, Chaps. XI–XIV.

[14]These matrices converge much faster than μ' itself in our calculations and allow the calculation of static exponents without accurate information of μ^*.

[15]H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. 27, 1421 (1969), and Ref. 3. The results are quite crude. K. Kawasaki [Phys. Rev. 148, 375 (1966)] showed that $z\geq2-\eta$ $(=1.75)$.