Journal of Statistical Physics, Vol. 16, No. 2, 1977

The Stochastic Models Method Applied to the Critical Behavior of Ising Lattices

Hagai Meirovitch[1] **and Z. Alexandrowicz**[1]

Received November 18, 1975; revised August 31, 1976

The stochastic models (SM) computer simulation method for treating many-body systems in thermodynamic equilibrium is investigated. The SM method, unlike the commonly used Metropolis Monte Carlo method, is not of a relaxation type. Thus an equilibrium configuration is constructed at once by adding particles to an initially *empty* volume with the help of a model stochastic process. The probability of the equilibrium configurations is known and this permits one to estimate the entropy directly. In the present work we greatly improve the accuracy of the SM method for the two- and three-dimensional Ising lattices and extend its scope to calculate fluctuations, and hence specific heat and magnetic susceptibility, in addition to average thermodynamic quantities like energy, entropy, and magnetization. The method is found to be advantageous near the critical temperature. Of special interest are the results at the critical temperature itself, where the Metropolis method seems to be impractical. At this temperature, the average thermodynamic quantities agree well with theoretical values, for both the two- and three-dimensional lattices. For the two-dimensional lattice the specific heat exhibits the expected logarithmic dependence on lattice size; the dependence of the susceptibility on lattice size is also satisfactory, leading to a ratio of critical exponents $\gamma/\nu = 1.85 \pm 0.08$. For the three-dimensional lattice the dependence of the specific heat, long-range order, and susceptibility on lattice size leads to similarly satisfactory exponents: $\alpha = 0.12 \pm 0.03$, $\beta = 0.30 \pm 0.03$, and $\gamma = 1.32 \pm 0.05$ (assuming $\nu = 2/3$).

KEY WORDS: Stochastic models; Monte Carlo; critical behavior; Ising lattice.

1. INTRODUCTION

A computer simulation method for treating many-body systems in thermodynamic equilibrium was suggested some years ago by Alexandrowicz.[1]

[1] Polymer Department, Weizmann Institute of Science, Rehovot, Israel.

© 1977 Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording, or otherwise, without written permission of the publisher.

This method, called the stochastic models (SM) method, was applied preliminarily to the two- and three-dimensional Ising models and to a fluid model consisting of hard cubic molecules with an attractive potential.[2] Most simulation methods (like the Metropolis Monte Carlo[3–6] and molecular dynamics[7,8] methods) are of a relaxation type, i.e., one starts with an arbitrary initial configuration of the system, which relaxes by means of a certain process to the typical equilibrium configurations. In the SM method an equilibrium configuration is obtained in a different way; not as an outcome of a relaxation process, but as an immediate result of a construction procedure based on adding particles gradually to an empty volume. This approach, though approximate in most cases, has several advantages, such as the ability to calculate entropy and the possibility of treating systems close to the critical temperature. In the present work we greatly improve the accuracy of the SM method and extend its scope to calculate specific heat and susceptibility, in addition to energy and entropy, for the two- and three-dimensional Ising models. The efficiency of the method is examined in detail near and at the critical temperature.

2. SAMPLING IN THE CANONICAL ENSEMBLE

Consider a system in equilibrium which can be described by the canonical distribution, e.g., the probability p_i of the ith configuration is given by

$$P_i = Z^{-1} \exp(-E_i/kT) \tag{1}$$

where E_i is its microscopic energy, Z is the partition function, k is the Boltzmann constant, and T is the absolute temperature. With this probability distribution the statistical average $\langle G \rangle$ and the variance $\langle \Delta G^2 \rangle$ of any microscopic quantity G_i are defined by

$$\langle G \rangle = \sum_{\text{all } i} P_i G_i \tag{2}$$

$$\langle \Delta G^2 \rangle = \sum_{\text{all } i} P_i (G_i - \langle G \rangle)^2 \tag{3}$$

To estimate $\langle G \rangle$ one can sample independently n configurations with the probability P_i, calculating the arithmetic average G_n:

$$G_n = n^{-1} \sum_{t=1}^{n} G_{i(t)} \tag{4}$$

where $G_{i(t)}$ corresponds to the configuration i at time t. The mean value of G_n equals $\langle G \rangle$ and its variance $\langle \Delta G_n{}^2 \rangle$ decreases with n as[9]

$$\langle \Delta G_n{}^2 \rangle = \langle \Delta G^2 \rangle / n \tag{5}$$

Therefore, the sample size n required to obtain a good estimation of $\langle G \rangle$ depends on the magnitude of $\langle \Delta G^2 \rangle$. In general, the variance of thermodynamic quantities such as energy per particle decrease as N^{-1}, where N denotes the number of particles. Therefore, n can be relatively small for large enough systems. (Close to the critical temperature the variance decreases much slower with N and one has to increase n.)

In most cases the Boltzmann distribution [Eq. (1)] is unknown and one has to look for approximate probability distributions. In this context, let us consider the free energy functional $F(\mathbf{P}')$:

$$F(\mathbf{P}') = \sum_{\text{all } i} P_i'(E_i + kT \log P_i') \tag{6}$$

where $\mathbf{P}'$ is *any* probability distribution defined on phase space. The minimum free energy principle states that $F(\mathbf{P}')$ is never smaller than the exact free energy

$$F(\mathbf{P}) = \sum_{\text{all } i} P_i(E_i + kT \log P_i) \tag{7}$$

where $\mathbf{P}$ constitutes the Boltzmann distribution [Eq. (1)]. On the basis of this principle, we obtain with the SM method the "best" approximate probability distribution, i.e., one that minimizes the functional $F(\mathbf{P}')$ for given restrictions. Let it be stressed that our minimization is with respect to the sampled values of $F(\mathbf{P}')$. However, this objection is not serious because of the very small fluctuations in $F(\mathbf{P}')$, due to mutual cancellation of the fluctuations in energy and entropy. Indeed, the *exact* free energy $F(\mathbf{P})$ has zero fluctuations.[10,11]

3. THE SM METHOD

We shall explain now the SM method as applied to the square Ising model with $N = L \times L$ spins. We denote by σ_k the spin variable at the lattice site k, where σ_k has two possible values: $+1$, -1. The interaction is only between nearest neighbor spins, and it is of a ferromagnetic type (the coupling interaction constant $J > 0$). The microscopic energy E_i and magnetization M_i of a particular configuration are given, respectively, by

$$E_i = -J \sum_{\substack{kl \\ (\text{nn})}} \sigma_k \sigma_l \tag{8}$$

$$M_i = (1/N) \sum_{k=1}^{N} \sigma_k \tag{9}$$

where (nn) denotes nearest neighbors. The construction of the lattice configurations is carried out with a set of transition probabilities $P_{\mathbf{x}}(+|I)$, which depend on a given set of parameters $\mathbf{x}$; the symbol I stands for a *row* configuration of L spins. One begins with an empty lattice and fills the first

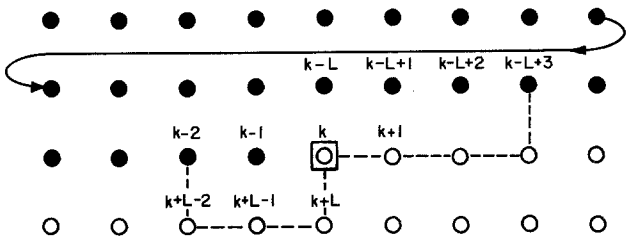

Fig. 1. An illustration of the kth step of the spiral construction of the two-dimensional Ising lattice. Closed circles denote lattice spins already specified in the previous steps of the process, while open circles denote the still empty lattice sites. The dashed lines connecting site k with sites $k - L + 3$ and $k - 2$ represent the paths by which these spins affect the spin that has to be fixed at site k. The solid line indicates the present "spiral" boundary conditions.

row with spins, which are distributed at random. Subsequently, the orientation of the spins on the lattice is fixed step by step by a Monte Carlo lottery according to the $P_{\mathbf{x}}(+|I)$, as explained by the following. Assume that part of the lattice already has been constructed and we want to specify the sign of the spin at site k (Fig. 1). Our computer program checks the signs of the preceding L spins added to the lattice $(\sigma_{k-L} \cdots \sigma_{k-1})$ and determines the transition probability $P_{\mathbf{x}}(+|I_k)$ corresponding to the *row* configuration I_k of these L spins. A random number generator supplies a number between zero and one, which is compared with $P_{\mathbf{x}}(+|I_k)$. The spin at k will be $+1$, with probability $P_{\mathbf{x}}(+|I_k)$, if the random number is smaller than or equal to $P_{\mathbf{x}}(+|I_k)$. If it is larger than $P_{\mathbf{x}}(+|I_k)$, a minus sign is fixed at site k, with the probability $P_{\mathbf{x}}(-|I_k) = 1 - P_{\mathbf{x}}(+|I_k)$. Once the construction of the lattice configuration i has been accomplished, its microscopic energy and the corresponding probability $P_i(\mathbf{x})$ become known. $P_i(\mathbf{x})$ is the product of the N transition probabilities according to which the spins have been chosen:

$$P_i(\mathbf{x}) = \prod_{k=1}^{N} P_{\mathbf{x}}(\sigma_k|I_k) \tag{10}$$

In this way, in principle, each one of the 2^N lattice configurations can be constructed with the corresponding probability $P_i(\mathbf{x})$, which means that a probability distribution $P(\mathbf{x})$ is thus defined on phase space.

The problem is to find the best approximate probability distribution in the sense of Eq. (6). We sample n configurations with $P(\mathbf{x})$, computing the corresponding free energy functional $F(\mathbf{x})$ with the help of the estimator

$$F_n(\mathbf{x}) = n^{-1} \sum_{t=1}^{n} [E_{i(t)} + kT \log P_{i(t)}(\mathbf{x})] \tag{11}$$

where the transition from Eq. (6) to (11) is like that from Eq. (2) to (4). We then seek the optimal set of parameters $\mathbf{x}^*$ giving the minimum value to Eq. (11). For this "best" value one computes the average energy and the

other lattice quantities of interest. Formally, the lattice construction process, using the transition probabilities together with the spiral boundary conditions (Fig. 1), is a Markov chain. The states of the chain are the 2^L row configurations.

The first row of the lattice, which, to recall, is filled with randomly oriented spins, and several following rows, which are significantly dependent on it, are discarded from our calculation of energy, entropy, etc. In practice it is found that the effect of the first row disappears after about ten successive rows.

At this stage, after having described the SM construction procedure and before introducing the transition probabilities in detail, it is worthwhile to comment on several points. Our problem is to determine the probability of fixing $+1$ on site k while only two of its four nearest neighbor spins are known (σ_{k-1}, σ_{k-L}). If the other two neighbors σ_{k+1} and σ_{k+L} were also known, the answer would be simple: The probability for σ_k is proportional to the Boltzmann factor $\exp[\sigma_k(\sigma_{k+1} + \sigma_{k+L} + \sigma_{k-1} + \sigma_{k-L})J/kT]$. But since two spins will be determined only in the future steps, we have to "guess" their signs by taking into account the signs of the last L spins. In order to clarify this last, somewhat vague statement, let us examine, for example, the effect of spin σ_{k-2}. In future the strongest influence of this spin will be on the probability determining the sign of its nearest neighbor, σ_{k+L-2} (Fig. 1). If $\sigma_{k-2} = +1$, this will increase the probability for σ_{k+L-2} to also be $+1$ (ferromagnetic interaction), which will increase in the next step the probability of having $\sigma_{k+L-1} = 1$, and so on. In this way a chain effect favoring $+1$ is established toward the site k via site $k + L$.

We can now summarize the concepts that guide our choice of transition probabilities: (a) Only the last L spins are taken into account explicitly in the transition probabilities (in a ferromagnetic way). (b) The magnitude of the effect of each spin is expressed by a suitable parameter. This effect decreases with increasing distance. We assume that identical parameters correspond to any two spins located at the same distance from site k, except for the spins in the immediate surrounding of site k. Accordingly, the transition probability $P_{\mathbf{x}}(+|I)$ is written as follows:

$$P_{\mathbf{x}}(+|I_k) = (1 + a^{\sigma_{k-1}}b^{\sigma_{k-L}}c^{\sigma_{k-L+1}}d^{\sigma_{k-L+2}}e^{\sigma'}r^{\sigma''}t^{\sigma'''})^{-1} \tag{12}$$

where

$$\sigma' = 2^{-1}(\sigma_{k-L+3} + \sigma_{k-2}) \tag{13}$$

$$\sigma'' = \left[\sum_{m=5}^{l} (\sigma_{k-L+m-1} + \sigma_{k-m+2})m^{-f}\right] \Big/ \sum_{m=5}^{l} 2m^{-f} \tag{14}$$

$$\sigma''' = L^{-1} \sum_{m=k-L}^{k-1} \sigma_m \tag{15}$$

The parameters a, b, c, and d in Eq. (12) express the effect of the four nearest neighbor spins defined by the labels occurring in the exponents. The parameter e is a parameter common to the spins at sites $k-2$ and $k-L+3$, since these two spins are separated from site k by the same number of bonds (broken lines in Fig. 1); σ' [Eq. (13)] is their normalized spin charge. The parameter r belongs to a group of farther placed spins summed by the normalized charge σ'' [Eq. (14)]; in the summation, individual spins are multiplied by a decreasing function m^{-f}, where m is the distance (in lattice steps) from site k, and f is a decay parameter. The number of terms occurring in this summation is defined by another parameter l. The value of σ'' varies in the range $(-1, +1)$, but for practical reasons we have allowed σ'' to take only 20 distinct values. Finally, the "mean field parameter" t belongs to the L spins summed together by the normalized charge σ''' [Eq. (15)]. In this sum, the spins are accorded equal weights. σ''' is allowed to take only two values; if σ''' is greater than zero, it is $+1$ and if σ''' is smaller than zero, it is -1. By the above definition, we obtain a set of approximately 2300 transition probabilities, which means that many row configurations are redundant.

It should be emphasized that although the SM method can be regarded as a type of mean field theory,[12,13] it does not necessarily lead to the mean field critical description. Thus in the present work the effect of *individual* remote spins is expressed with the help of Eq. (14). However, as the correlation length becomes very large close to the critical temperature, three parameters only [r, l, and f in Eqs. (12) and (14)] cannot remain sufficient.

What are the restrictions on the values of the parameters? Clearly, a, b, c, d, e, r, and t vary in the range [0, 1]; a parameter with small values has a higher influence on the probabilities [when all the parameters become 1, the probability in Eq. (12) reduces to the random value of 0.5]. One expects also the relation $a < b < c < d < e^{0.5}$ to be fulfilled because the magnitude of the effect decreases with distance. The spins $k-1$ and $k-L$, in spite of the fact that both are nearest neighbors, should not have the same effect, because spin $k-1$ affects k by an additional path (through $k+L-1$ and $K+L$; see Fig. 1); hence $a < b$.

4. RESULTS AND DISCUSSION

The essential part of the work is the determination of the optimal parameters $\mathbf{x}^*$ giving minimum of the free energy functional $F_n(\mathbf{x})$ averaged over sample n [see Eq. (11)] for each temperature. Using the optimal parameters $\mathbf{x}^*$, the average energy $E_n(\mathbf{x}^*)$, magnetization $M_n(\mathbf{x}^*)$, order parameter

$|M_n(\mathbf{x}^*)|$, and entropy $S_n(\mathbf{x}^*)$ are calculated. The equation for the entropy is

$$S_n(\mathbf{x}^*) = -(k/n) \sum_{t=1}^{n} \log P_{i(t)}(\mathbf{x}^*) \tag{16}$$

and for the order parameter,

$$|M_n(\mathbf{x}^*)| = n^{-1} \sum_{t=1}^{n} |M_{i(t)}| \tag{17}$$

In order to calculate the specific heat C and the isothermal susceptibility per spin χ, the following two relations are used:

$$k^2TC = \langle \Delta E^2 \rangle \tag{18}$$

$$kT\chi = \langle \Delta M^2 \rangle N \tag{19}$$

$\langle \Delta E^2 \rangle$ and $\langle \Delta M^2 \rangle$ are the variances of the energy and the magnetization, respectively. The variance in the energy is estimated by

$$\Delta E^2(\mathbf{x}^*)_n = (1/n) \sum_{t=1}^{n} [E_n(\mathbf{x}^*) - E_{i(t)}]^2 \tag{20}$$

with a similar estimator for the variance in magnetization.

4.1. The Two-Dimensional Lattice

The results are summarized in Table I, together with the corresponding values obtained by the accurate analytical solution and with approximate formulas based on series expansion. For comparison, results we obtained by using the Metropolis method are also given.

It is important to emphasize that caution is needed while comparing results obtained with finite lattices to the thermodynamic limit solutions. The deviations in χ and C are negligible at temperatures where $\xi/L \ll 1$ (ξ is the correlation length[14]), but become dramatically large for $\xi/L \sim 1$. The correlation length corresponding to $K = 0.43$ ($K = J/kT$ is the reciprocal lattice temperature) is $\xi = 23$ lattice sites; hence we have taken a lattice $L = 150$, which was deemed sufficiently large. For the other, noncritical temperatures in Table I, the correlation lengths are smaller than $\xi = 13$; hence we have taken $L = 90$–120.

The SM results for F, S, E, M, $|M|$, and C at both $K < K_c$ and $K > K_c$ and for χ at $K < K_c$ are in good agreement with the corresponding values obtained with the analytical solutions and series expansion approximate formulas. The results for χ in the "cold" region $K > K_c$ are much too low. The present results are incomparably better than the results (for S, E, and

Table I. Results for the Two-Dimensional Ising Lattice[a]

	$-F/NkT$		$-E/NJ$			S/Nk		$\|M\|$			M			C/Nk			χ/N		
K	SM	Theo.	SM	Metr.	Theo.	SM	Theo.	SM	Metr.	Theo.	SM	Metr.	Theo.	SM	Metr.	Theo.	SM	Metr.	Theo.
0.40 $L = 90$	0.87934	0.87936	1.105	1.106	1.106	0.434	0.437	0.065	0.065	n.a.	0.003	0.004	n.a.	0.85	0.82	0.86	60	50	62
0.41 $L = 120$	0.89065	0.89070	1.160	1.163	1.163	0.415	0.414	0.068	0.069	n.a.	0.001	0.01	n.a.	1.00	1.02	1.00	100	100	102
0.42 $L = 120$	0.90256	0.90264	1.224	1.227	1.226	0.389	0.388	0.088	0.097	n.a.	0.0007	0.03	n.a.	1.28	1.17	1.20	180	195	204
0.43 $L = 150$	0.91512	0.91526	1.294	1.302	1.300	0.358	0.356	0.114	0.137	n.a.	0.005	0.11	n.a.	1.65	1.55	1.53	450	350	647
K_c $L = 40$	0.92958	0.93009	1.429	1.441	1.430	0.299	0.300	0.585	0.678	n.a.	0.06	0.677	n.a.	1.98	1.70	1.95	620	24	n.a.
K_c $L = 64$	0.92947	0.92985	1.425	1.419	1.424	0.304	0.302	0.573	0.578	n.a.	0.07	0.540	n.a.	2.34	2.23	2.18	1440	300	n.a.
K_c $L = 90$	0.92944	0.92977	1.419	1.412	1.421	0.304	0.304	0.570	0.678	n.a.	0.07	0.678	n.a.	2.43	2.25	2.35	2700	400	n.a.
K_c $L = 120$	0.92941	0.92974	1.419	1.412	1.419	0.304	0.304	0.567	0.510	n.a.	0.09	0.510	n.a.	2.56	2.50	2.50	4800	350	n.a.
0.455 $L = 90$	0.95092	0.95104	1.551	1.548	1.550	0.245	0.246	0.796	0.787	0.788	0.796	0.787	0.788	1.40	1.45	1.40	5	10	10
0.46 $L = 90$	0.95875	0.95887	1.580	1.583	1.581	0.232	0.232	0.820	0.818	0.815	0.820	0.818	0.815	1.25	1.17	1.25	3.4	4.7	6
0.47 $L = 90$	0.97488	0.97496	1.638	1.636	1.634	0.205	0.207	0.857	0.854	0.852	0.857	0.854	0.852	1.10	1.01	1.05	2.0	2.7	2.8

[a] Free energy F, energy E, entropy S, magnetization M, long-range order $|M|$, specific heat C, and susceptibilty χ, obtained with the SM method, with the asymmetric Metropolis method,[4] and with theoretical methods (analytical or series expansion). K is the reciprocal Ising temperature, $K = J/kT$, and $K_c = 0.44068....$ is its critical value.[28] L is the lattice size. The estimated statistical error of these results is 0.01% for F, 0.08% for E, 0.15% for S, 0.1% for M and $|M|$, and 1–5% for both C and χ. Metropolis' results are for 10,000 lotteries per spin. The exact results for $K \neq K_c$ are calculated using formulas for the infinite lattice.[28] At $K > K_c$ the susceptibility is calculated using a Padé approximant[29] and at $K < K_c$ with the approximate high-temperature expansion formula.[30] At K_c the accurate values of the energy and specific heat are calculated with formulas of Ferdinand and Fisher.[15] Unavailable theoretical values are marked n.a.

M alone) obtained in the original article[1] describing the SM method. That, of course, is due to the present use of much more sophisticated model transition probabilities.

The Monte Carlo results were obtained with the asymmetric Metropolis procedure,[4] using periodic boundary conditions. At each temperature the averages are for 10^4 lotteries per spin. To get rid of the initial relaxation, this averaging was started only after 10^3 lotteries per spin.

Of special interest are the results obtained at the critical reciprocal temperature K_c. We made calculations for four lattices from $L = 40$ to $L = 120$. The values of the free energy, energy, entropy, and specific heat calculated with the Ferdinand and Fisher formulas[15] at K_c are in very good agreement with our results (see Table I). The finite-size behavior of the magnetic properties (χ and $|M|$) is not known analytically; hence we compare our results to Fisher's finite-size scaling theory.[16,17] According to this theory (see also Refs. 18–21) the susceptibility χ of a finite $L \times L$ lattice should increase with L as

$$\chi = BL^{\gamma/\nu} \qquad \text{at } K_c \text{ and for large } L \tag{21}$$

where B is a constant, and γ and ν are the exponents related to the susceptibility and to the correlation length, respectively.[14] A similar relation is expected for $|M|$, the exponent β replacing γ. A plot of $\log \chi$ vs. $\log L$ gave a straight line with slope 1.85 ± 0.08, while the expected theoretical value is 1.75 ($\nu = 1, \gamma = 1.75$), and $B = 0.7 \pm 0.1$ (Landau,[22] using the Metropolis method, obtained $B = 1.00 \pm 0.04$). The absolute magnetization at K_c decreases with increasing L, but the decrease is less than that corresponding to the expected theoretical value $\beta = \frac{1}{8}$. For illustration, pictures of lattices simulated at K_c are also presented in Figs. 2 and 3, showing the ramified structure of the big droplets.

It is of interest to compare the accuracy of the SM and Metropolis methods. With the SM method the configurations are sampled almost independently (except for the last row of one lattice serving as neighbor to the first row of the next lattice). Therefore, a relatively small number of configurations is required to estimate averages. As a matter of fact, the fluctuations also converge quite rapidly. At $K \neq K_c$ we took 1000 configurations. At K_c the sample size has to be increased and we took 3000–4000 configurations. Assuming that the configurations are sampled independently, we can calculate, for instance, the standard deviations $\langle \Delta^2 M_n \rangle^{1/2}$ [see Eqs. (5) and (19)],

$$\langle \Delta^2 M_n \rangle^{1/2} = \chi^{1/2}/n^{1/2}L \tag{22}$$

Taking $n = 1000$ and the χ values from Table I, we obtain for $K = 0.40$, 0.41, 0.42, and 0.43 the corresponding values of the standard deviation

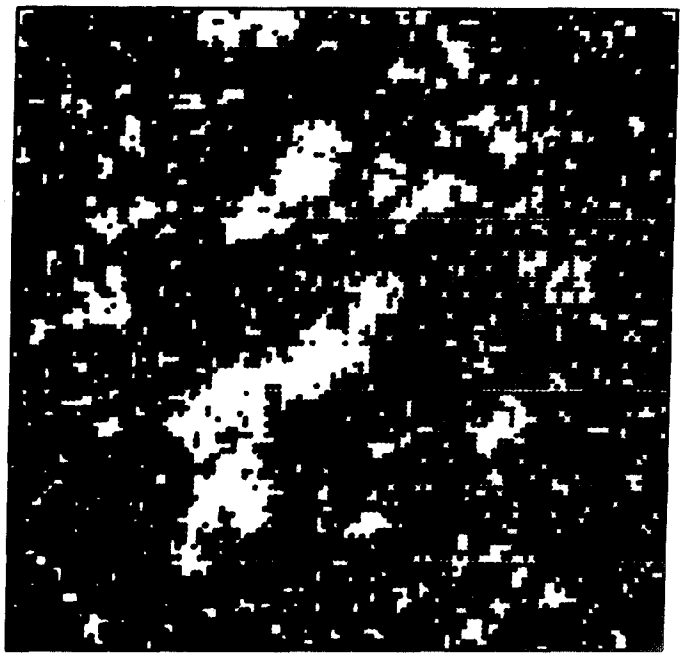

Fig. 2. A typical configuration of a lattice of 120 × 120 spins at K_c. The absolute magnetization $|M| = 0.60$, which is near average.

0.027, 0.0026, 0.0035, and 0.0041, which are all larger than the values of M in Table I. This seems to justify the use of Eq. (22) for statistical error estimation of the SM results at $K < K_c$. However, at K_c itself the standard deviation calculated by Eq. (22) is ~ 0.01 for all the lattices, which is several times smaller than the observed values of magnetization. This might be because lattice configurations sampled at K_c are not entirely uncorrelated.

It is incorrect to use Eq. (22) for the Metropolis method, due to the strong correlations between successive configurations in the sample. In order to check the rate of convergence of the Metropolis relaxation, we shall use an approximated formula derived by Müller-Krumbhaar and Binder.[23] The formula for the standard deviation of the average magnetization for n correlated lotteries per spin $\langle \Delta^2 M_n \rangle^{*1/2}$ is

$$\langle \Delta^2 M_n \rangle^{*1/2} = A\chi / n^{1/2} L \tag{23}$$

where A is a constant. The $\langle \Delta^2 M_n \rangle^{*1/2}$ values for $K = 0.40$, 0.41, 0.42, and 0.43 are, respectively, 0.00066, 0.0083, 0.017, and 0.043 if we take $A = 1$ in Eq. (23). Comparison to the corresponding M values in Table I shows that actual A values are about 2–6 times larger than that.

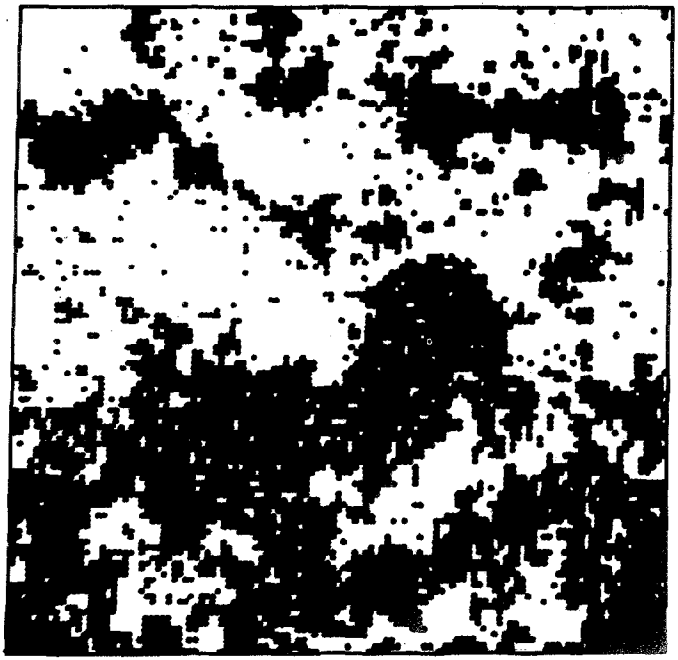

Fig. 3. A typical configuration of a lattice of 120 × 120 spins at K_c. The absolute magnetization $|M| = 0.06$, representing the nonmagnetized configurations of the ensemble.

At K_c itself Eq. (23) is not valid and the convergence of the Metropolis method becomes exceedingly poor due to the very strong correlation between the sampled lattice configurations. This can be seen from the results for M and $|M|$ in Table I. For $L = 40$ and 64 we found $M \sim |M|$, even though during the process the lattice reversed its magnetization twice. For $L = 90$ and 120, the magnetization was not reversed at all and the corresponding values of χ are, of course, meaningless. These difficulties can be removed to some extent by calculating averages over several runs, each starting from a different initial configuration.[22]

The conclusion from the foregoing discussion is that for a comparable accuracy the Metropolis method requires a sample size which is larger by $\chi^{1/2}$ than that of the SM method [or even larger than that in view of $A \simeq 2$–6 in Eq. (23)]. The difference becomes important as χ increases sharply near K_c. Indeed, the difficulty of obtaining statistically adequate samples with the Metropolis method gives rise to a great uncertainty as to whether a process has been run long enough to yield reliable equilibrium values of M, χ, C, etc. In practice one tends to discontinue the process when averages of these quantities become approximately equal to values known from other

sources. How misleading such judgments can be is illustrated by the following typical examples: At $K = 0.43$ and $L = 150$, we carried out 12,000 lotteries per spin (lps) with the Metropolis method. The average χ values between 7000 and 10,000 seemed to reach stability around $\chi = 350$, but after 11,000 lps χ "jumped" suddenly to the (correct) value of 650. The opposite occurred at $K = 0.45$ and $L = 64$; we obtained between 8000 and 12,000 apparently steady values $\chi = 15$, which is near the correct value. However, after 13,000 lps, χ jumped to 80, since for some time the lattice magnetization fell to almost zero. The SM method, which requires a much smaller sample size, avoids such a difficulty, but has a price to pay. First, more parameters are needed to define an adequate set of transition probabilities, and second, longer computer time is required for the calculation of a particular transition probability as more and more spins need to be taken into account in Eqs. (14) and (15), due to increasing correlation length.

Turning to K_c itself, the SM method enabled us to estimate reasonably well the critical exponents directly from experimental data and for quite large lattices. This feat we could not achieve with the help of the Metropolis method. True critical behavior has been studied with the help of Metropolis measurements of relatively small lattices not at, but near, K_c. Such a study has been carried out recently by Landau,[22] relying on Fisher's finite-size scaling theory.[16,17] However, (1) the critical exponents are not calculated directly from raw experimental data, which makes their accuracy difficult to judge, and (2) the most important data are those near K_c and it is not quite certain whether the lattices are large enough to obey the asymptotic behavior. (This doubt we raise in view of measurements we have carried out with comparable lattices; similar doubts have been discussed by Binder[24,25] and Landau.[26]) We now give an example of the times required by each of the two methods (on an IBM 370/165 computer) at $K = 0.42$ and $L = 120$, at which their accuracy is about the same. The SM method required 0.8 sec for constructing one lattice configuration [using $l = 16$ in Eq. (14)]; the sample size for the initial optimization was ~ 100, and about 50 points (distinct sets of parameter values) are tested. About the same computing time was required for a second improved optimization which used a larger sample size and fewer points. Thus the total time amounted to about 3 h. With the Metropolis method, one lattice cycle required 0.2 sec; hence a run of 12,000 lps amounted to about $\frac{3}{4}$ h. At K_c ($L = 120$) the SM method required about four times larger sample size, hence four times larger operation. The time of the Metropolis method remains, of course, the same, but the results, for χ especially, are very far from any sort of convergence.

Finally, we comment on the behavior of our parameters. Typical values are presented in Table II. The prediction from the previous section, namely that $a < b < c < d < e^{0.5}$, is borne out. We verified also our conjecture

Table II. Optimal Parameters for the Two-Dimensional Ising Lattice for Three Temperatures[a]

K	a	b	c	d	e	r	t	f	l
0.46	0.357	0.402	0.704	0.856	0.872	0.856	0.590	3.0	9
K_c	0.354	0.407	0.700	0.833	0.852	0.714	0.853	2.4	14
0.41	0.381	0.441	0.719	0.852	0.852	0.784	0.994	2.4	11

[a] K is the reciprocal Ising temperature. The parameters are defined in Eqs. (12)–(14).

that two spins with the same distance from site k have the same influence. This was done at $K = 0.40$, where ξ is small, by constructing a model of transition probabilities which accords a separate parameter to each of the eight nearest spins to site k. After optimization, equal values of parameters were obtained for any pair of equidistant spins. As for the decay parameter f, which determines the decay of correlations with distance, it was found to be greater for $K > K_c$ than for $K < K_c$. This agrees with the asymptotic form for the spin–spin correlation function (near K_c for large separation distance r)[14]

$$\exp(-\xi^{-1}r)/r^2 \quad \text{for } K > K_c \qquad \text{and} \qquad \exp(-\xi^{-1}r)/r^{1/2} \quad \text{for } K < K_c \tag{24}$$

The mean field parameter also behaves as expected: It is small [hence important in Eq. (12)] for $K > K_c$ and becomes ~ 1 for $K < K_c$. We also checked the assumption (a) from the previous section that only the effect of the last L spins has to be taken explicitly into account in the transition probabilities. This verification was carried out by including explicitly in the transition probabilities the influence of the "covered" spins (i.e., those with site indices smaller than $k - L$). These models of transition probabilities gave much larger free energy, which justifies our assumption of considering the last "uncovered" spins only.

All these properties greatly facilitate the minimization procedure and enable one to consider a relatively large number of parameters. The search for optimal parameter values is also facilitated by, first, their smooth variation from one temperature to another, and second, the fact that the optimal value of one parameter does not depend very much on the trial values accorded to the other parameters.

4.2. The Three-Dimensional Lattice

The simulation of the three-dimensional Ising model constitutes a straightforward generalization of the procedure used for the two-dimensional

case. One starts with an empty simple cubic lattice ($L \times L \times L$) and fills the first layer with spins at random. The spins in the rest of the lattice are determined layer after layer, while in each layer the process is carried out row after row. The allotments are accomplished according to a set of parametrized transition probabilities. In the three-dimensional case they depend at each step of the construction on the L^2 "uncovered" spins that have been already determined. Spiral boundary conditions between any two successive layers and between two successive rows in each layer are imposed.

We shall describe now the transition probabilities in some detail. Assume that $n-1$ layers of the lattice are already filled with spins and the spin at site k belonging to a certain row of the nth layer is to be determined. The probability $P(+|I_k)$ to assign $+1$ at the site, where the configuration of the last L^2 spins is I_k, is written

$$P(+|I_k) = 1\Big/\left(1 + \prod_{i=1}^{6} a_i^{\sigma_i} r^{\sigma'} t^{\sigma''}\right) \tag{25}$$

The parameters a_1, a_2, and a_3 belong to the three nearest neighbor spins at sites $k-1$, $k-L$, and $k-L^2$, respectively (σ_1, σ_2, and σ_3 are their signs). The parameters a_4, a_5, and a_6 belong to the three next nearest neighbor spins at sites $k-L+1$, $k-L^2+L$, and $k-L^2+1$, respectively. The effect of the farther placed spins is expressed, in an approximate way, by the parameter r and the normalized charge σ':

$$\sigma' = \sum_{m=3}^{l} \sum_{i=1}^{j_m} \sigma_i m^{-f} \Big/ \sum_{m=3}^{l} \sum_{i=1}^{j_m} m^{-f} \tag{26}$$

This expression is analogous to σ'' defined in Eq. (14) for the square lattice. The contribution of each spin in the summation above is proportional to the factor m^{-f}, where m is the shortest distance from site k measured on empty lattice sites. Here j_m is the number of spins located at distance m from site k. The parameter f is a decay parameter. As in the two-dimensional model, only 20 distinct values between -1 and 1 were allowed. The parameter l is the range parameter for this summation. Finally, in Eq. (25) t is the mean field parameter; the corresponding charge σ'' takes the value $+1$ or -1 according to whether the magnetization of the layer configuration I_k is respectively greater or smaller than zero.

The data are summarized in Table III and compared with results obtained by approximate series expansion formulas. At $K \neq K_c$ we have measured cubes of $L = 30$. The results for F, E, S, $|M|$, and C are in good agreement with the series expansion results; this also holds for χ at temperatures not too close to K_c. Calculations were made also at the accepted critical temperature $K_c = 0.22169$[27] for $L = 10$, 16, 20, and 30. Results

Table III. Results for the Three-Dimensional Ising Lattice[a]

	$-F/NkT$		$-E/NJ$		S/Nk		$\lvert M\rvert$		M	C/Nk		χ/N	
K	SM	Series	SM	Series	SM	Series	SM	Series	SM	SM	Series	SM	Series
0.210	0.76728	0.76738	0.836	0.846	0.592	0.590	0.030	n.a.	0.0002	0.42	0.40	38	42
0.213	0.76982	0.76993	0.863	0.875	0.586	0.583	0.036	n.a.	0.0003	0.47	0.46	55	60
0.217	0.77334	0.77348	0.897	0.922	0.579	0.573	0.048	n.a.	0.001	0.56	0.59	96	130
0.22169	0.77809	n.a.	1.033	n.a.	0.549	n.a.	0.273	n.a.	0.011	1.10	n.a.	98	n.a.
$L = 10$													
0.22169	0.77782	n.a.	1.006	n.a.	0.554	n.a.	0.222	n.a.	0.017	1.45	n.a.	250	n.a.
$L = 16$													
0.22169	0.77777	n.a.	0.997	n.a.	0.557	n.a.	0.200	n.a.	0.002	1.50	n.a.	400	n.a.
$L = 20$													
0.22169	0.77774	0.77782*	0.996	0.992*	0.557	0.558*	0.185	n.a.	0.006	1.65	n.a.	1050	n.a.
$L = 30$													
0.226	0.78261	0.78248	1.226	1.262	0.506	0.497	0.450	0.451	0.450	2.05	1.92	20	37
0.230	0.78788	0.78782	1.393	1.403	0.467	0.465	0.550	0.546	0.550	1.85	1.75	9.5	13
0.235	0.79522	0.79520	1.550	1.559	0.431	0.429	0.623	0.622	0.623	1.70	1.57	6.0	6.4

[a] Free energy F, energy E, entropy S, magnetization M, long-range order $|M|$, specific heat C, and susceptibility χ, as obtained with the SM method and with approximate series expansion formulas. $K = J/kT$ is the reciprocal Ising temperature and $K_c = 0.22169$ is the best estimate for the critical temperature by series expansion.[27] The SM results for $K \neq K_c$ were obtained with $L = 30$. The estimated statistical errors are comparable to those in Table I. The series expansion results for χ and C at $K < K_c$ were calculated with formulas taken from Refs. 27 and 31. At $K > K_c$, χ and $|M|$ were obtained by Padé approximants.[29] C was calculated by us with a [10, 10] Padé approximant. E, S, and F were obtained by numerical integrations of the specific heat with respect to temperature. The values marked with an asterisk are the best high-temperature series expansion estimates for the respective quantities at K_c for the infinite lattice.[27] Values not available are marked by n.a.

Table IV. Optimal Parameters for the Three-Dimensional Lattice for Three Temperatures[a]

K	a_1	a_2	a_3	a_4	a_5	a_6	r	f	l	t
0.230	0.602	0.617	0.631	0.897	0.900	0.900	0.714	3.7	7	0.777
0.22169	0.608	0.625	0.646	0.893	0.907	0.907	0.583	3.6	10	0.961
0.210	0.624	0.640	0.654	0.901	0.910	0.910	0.618	3.5	10	1

[a] K is the reciprocal Ising temperature. The parameters are defined in Eqs. (25) and (26).

for E, S, and F obtained at K_c by series expansion for the infinite lattice[27] are in good agreement with the SM results for $L = 30$. The dependence of C, χ, and $|M|$ on L at K_c was interpreted with the help of the following relationships [see Eq. (21)]:

$$|M| = B_1 L^{-\beta/\nu}, \qquad \chi = B_2 L^{\gamma/\nu}, \qquad C = B_3 L^{\alpha/\nu} \qquad \text{for large } L \quad (27)$$

The log-log plots of our data, assuming $\nu = \frac{2}{3}$, give as follows: $\beta = 0.30 \pm 0.03$, $\gamma = 1.32 \pm 0.05$, and $\alpha = 0.12 \pm 0.03$. These results agree quite well with the accepted theoretical values[14] $\beta = 0.312$, $\gamma = 1.25$, and $\alpha = 0.125$. [In the case of $|M|$ and χ the result for $L = 30$ deviates somewhat from the line; in the case of C the result for $L = 10$ deviates completely from the line but such a lattice size seems to be too small to fit the asymptotic equation (27); see Ref. 26.]

For the sake of concreteness, the optimal parameters for three temperatures are presented in Table IV. Their behavior is similar to that obtained for the two-dimensional lattice, i.e., the effect of the spins decreases with distance. Among "equidistant" spins the strongest influence is caused by the spin with greatest number of pathways to site k ($a_1 < a_2 < a_3$). In the three-dimensional case our treatment is much more time-consuming. Here one considers in each step the effect of 200 spins (through $\sigma_1\sigma_2 \cdots \sigma_6$ and σ'). For example, the construction of one configuration of $L = 30$ (and $l = 10$) required 8 sec.

4.3. Conclusions

The present work greatly improves the accuracy of the SM method as compared to its original description.[1] The improvement is achieved through the use of more sophisticated model transition probabilities, which carefully distinguish among near neighbor spins and represent the individual effect of remote spins with the help of Eq. (14).

The relative merit of the SM and of the conventional Monte Carlo (Metropolis) method with respect to the critical behavior of Ising lattices is

not easy to judge unequivocally. A conventional Monte Carlo simulation of the Ising lattice, like that of any other system at equilibrium, constitutes a trivial extension of the basic concept of computer simulation proposed by Metropolis *et al.*[3] In contrast, the SM method is certainly much more complicated to use, first, because it calls for an ingenious choice of the set of transition probabilities, and second, because of the need to perform a parameter optimization of these probabilities. The finding of the transition probability at each step is also relatively time-consuming, because of the dependence on a large number of nonneighbor spins. Yet, with the help of the SM method we have been able to describe reasonably well the behavior of quite large lattices at K_c, and such measurements seem to be impractical with the conventional Monte Carlo method. The infinite lattice behavior near K_c is also quite well described by the SM method, with the exception of the rather poor results for χ in the cold region. We did not study the finite-size behavior near K_c (a study comparable in scope to that of Ref. 22 would require a great deal of parameter optimizations), but in principle the SM method is expected to perform in that respect as well as at K_c itself. Furthermore, the SM method calculates the entropy, hence the free energy, in addition to the other thermodynamic quantities. Finally, we dare say that it certainly seems desirable to have a reasonably accurate simulation technique, which is independent and different in its scope from the conventional method.

ACKNOWLEDGMENTS

We are very much indebted to Dr. D. C. Rapaport, for helpful discussions and for kindly providing us with the program for calculating the Padé approximants, and to Dr. D. P. Landau for providing us with preprints of Refs. 22 and 26.

REFERENCES

1. Z. Alexandrowicz, *J. Chem. Phys.* **55**:2765 (1971); see also Z. Alexandrowicz, *J. Stat. Phys.* **5**:19 (1972).
2. Z. Alexandrowicz and M. Mostow, *J. Chem. Phys.* **56**:1274 (1972).
3. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**:1087 (1953).
4. L. D. Fosdick, in *Methods of Computational Physics*, Academic Press, New York (1963), Vol. 1, p. 245.
5. D. P. Landau, *AIP Conf. Proc.* **18**:819 (1974).
6. K. Binder, *Adv. Phys.* **23**:917 (1974).
7. B. J. Alder and T. E. Wainwright, *J. Chem. Phys.* **31**:459 (1959).
8. I. R. McDonald and K. Singer, *Quart. Rev.* **24**:238 (1970).

9. W. Feller, *An Introduction to Probability Theory and its Applications*, Wiley, New York (1968), Chapter IX.
10. W. Gibbs, *Elementary Principles in Statistical Mechanics*, Yale University Press (1902), Chapter XI.
11. H. Meirovitch and Z. Alexandrowicz, *J. Stat. Phys.* **15**:123 (1976).
12. H. Bethe, *Proc. Roy. Soc. (Lond.) A* **150**:552 (1935).
13. R. Kikuchi, *Phys. Rev.* **81**:988 (1951).
14. M. E. Fisher, *Rep. Prog. Phys.* **30**:615 (1967).
15. A. E. Ferdinand and M. E. Fisher, *Phys. Rev.* **185**:832 (1969).
16. M. E. Fisher, in *Proc. Int. Summer School Enrico Fermi, 1970*, Course 51 (Varrena, Italy), Academic Press, New York (1971).
17. M. E. Fisher and M. N. Barber, *Phys. Rev. Lett.* **28**:1516 (1972).
18. C. Domb, *Proc. Phys. Soc.* **86**:933 (1965); C. Domb, *J. Phys. C* **3**:256 (1970).
19. J. D. Gunton, *Phys. Lett.* **26**:406 (1968).
20. P. G. Watson, in *Phase Transition and Critical Phenomena*, Academic Press, London (1972), Vol. 2, pp. 150–159.
21. H. Müller-Krumbhaar and K. Binder, *Z. Physik* **254**:269 (1972).
22. D. P. Landau, *Phys. Rev. B* **13**:2997 (1976).
23. H. Müller-Krumbhaar and K. Binder, *J. Stat. Phys.* **8**:1 (1973).
24. K. Binder, *Physica* **62**:508 (1972).
25. K. Binder and P. C. Hohenberg, *Phys. Rev. B* **9**:2194 (1974).
26. D. P. Landau, *Phys. Rev. B*, in press.
27. M. F. Sykes *et al.*, *J. Phys. A: Gen. Phys.* **5**:667 (1972).
28. G. F. Newell and E. W. Montroll, *Rev. Mod. Phys.* **25**:352 (1953).
29. J. W. Essam and M. E. Fisher, *J. Chem. Phys.* **38**:802 (1962).
30. M. F. Sykes *et al.*, *J. Phys. A: Gen. Phys.* **5**:624 (1972).
31. M. F. Sykes *et al.*, *J. Phys. A: Gen. Phys.* **5**:640 (1972).