JOURNAL OF COMPUTATIONAL PHYSICS 20, 50–63 (1976)

A Comparison of Two Monte Carlo Methods for Computations in Statistical Mechanics

G. W. CUNNINGHAM

Federal Systems Division, IBM, Gaithersburg, Maryland 20760

AND

P. H. E. MEIJER

Catholic University of America, Washington, D.C. 20017
and National Bureau of Standards, Washington, D.C. 20234

Received September 4, 1974; revised June 30, 1975

A comparison of two Monte Carlo methods for computations in statistical mechanics is presented. In the comparison, involving a two-state problem, the transition probabilities introduced by Metropolis *et al.* are compared with the conditional probabilities of the Boltzmann distribution. The analytic relationship between the two is derived. Results of energy computations are given for an Ising spin system on a triangular lattice using first one set of transition probabilities, then the other. Both results are compared with the exact analytic solution. We found greater stability and faster convergence using the conditional Boltzmann probabilities. Also, some results for the Monte Carlo method in general are presented.

1. INTRODUCTION

Since its introduction in 1953 as a method for investigating the behavior of a liquid or a dense gas represented by interacting molecules confined to a box, the Monte Carlo method of Metropolis *et al.* [1] has been used widely and has had extensive description in the literature [2–5]. It has both Markovian and importance-sampling characteristics. It is Markovian in that the sequence of sample points are chained together by having the selection of each successive sample point depend only on the previous sample point. It is importance-sampling in that the criteria for sample selection are based on the known probability distribution of the function that is to be either integrated or summed. (The criteria for sample selection are equivalently referred to as transition probabilities since a system state is associated with each sample point.)

In the comparison presented here, the transition probabilities used by Metropolis *et al.* are compared with the conditional probabilities, suggested by Wood [5] and first used by Flinn and McManus [6], of the known distribution, which in this case [1], is the Boltzmann distribution. The analytic relationship between these two sets of transition probabilities is derived.

As an example of a two-state problem having interest in the literature [7–9], the results for energy computations are given for an Ising spin system [10] on a triangular lattice using first one set of transition probabilities, then the other. Both results are compared with the exact analytic solution [11, 12]. We found greater stability and faster convergence using the conditional Boltzmann probabilities. To gain some measure of the stability of each computation, since it is numerical, we employed techniques for monitoring and evaluating its convergence. Order calculations of general interest to the Monte Carlo method are also given.

2. Framework for Development

To establish a framework in which to develop the revised Monte Carlo method, a description of the specific application used in this study is given. Let us consider a system of magnetic moments on a two-dimensional triangular lattice. The magnetic moments are referred to as spins. Each lattice point is occupied by a spin and is surrounded by six nearest-neighbor sites. Neighbors beyond the nearest are considered to have no interaction with the center spin. Each lattice site, denoted by the subscript i, is assigned a spin variable S_i. This vaiarble can have one of two possible values: $+1$, representing some reference orientation in space, usually taken as up; and -1, representing the opposite, or down orientation. In this, the Ising model, we do not consider the quantum mechanical option of a mixed state which is partially up or partially down. In general, each spin could interact with an external magnetic field. The case studied here is for an isotropic lattice with zero external field. Then, for a given configuration on a lattice of N spins, the total internal energy is defined as

$$E = -\tfrac{1}{2}J \sum_{i=1}^{N} \sum_{j=1}^{6} S_i S_j , \tag{1}$$

where J is the interaction energy between any two spins.

The lattice is called ferromagnetic when $J > 0$, due to a uniform tendency for nearest-neighbor spins to be parallel. When $J < 0$, the lattice is called antiferromagnetic due to a uniform tendency for nearest-neighbor spins to be antiparallel. Both tendencies follow from the physical principal that systems tend towards minimum energy, in conjuction with the definition of energy in (1).

Since a physical measurement involves macroscopic quantities, and the internal energy in (1) is, by definition, microscopic, an average of (1) is required. The one used in this study is based on the canonical ensemble [9]. According to the formalism of statistical mechanics, the expectation value of any function F of the ensemble parameters is given for the canonical ensemble by

$$\langle F \rangle = \sum_{\mu=1}^{2^N} F_\mu e^{-E_\mu/kT} \Big/ \sum_{\nu=1}^{2^N} e^{-E_\nu/kT} \tag{2}$$

where k is Boltzmann's constant and T is the absolute temperature. The subscript μ denotes a specific member of the ensemble, and E_μ and F_μ are the energy and the value of F for that member. A member of the ensemble corresponds to a configuration or state of the system.

Since the Monte Carlo method is numerical, we are restricted to a finite value of N. Thus, the lattice has boundaries. The quantities to be computed are intensive (i.e., we will actually compute the energy and the order per spin). Thus, they are not supposed to be influenced by boundary effects. Thereore, we impose periodic boundary conditions on the lattice to minimize these effects.

We will now describe the Monte Carlo method used by Metropolis *et al.* for the evaluation of (2).

3. The Monte Carlo Method

Because of the astronomical value of the upper limit of the summation in (1) for a lattice of any significant size, the direct computation of (2) is impractical even on the fastest computers. In a simple Monte Carlo approach, we would attempt to approximate (2) by selecting at random a sample of the 2^N possible configurations of the lattice, computing F_μ for each configuration and weighting it with $e^{-E_\mu/kT}$ in forming the numerator. The denominator would be formed in the same process with unity replacing F_μ. The chances of attaining a representative sample of the ensemble in this manner are very small due to the large size of the ensemble. A technique that can form a relatively small but representative sample of the ensemble is needed.

From the form of (2), it can be seen that each point is weighted by the normalized Boltzmann probability density distribution:

$$P_\mu = e^{-E_\mu/kT} \Big/ \sum_{\nu=1}^{2^N} e^{-E_\nu/kT} \tag{3}$$

As can be seen, the ensemble is strongly weighted in the direction of the ground state where P_μ is a maximum (since $E_\mu < 0$). If we could somehow steer our Monte

Carlo sampling process in the direction of these more important points, we would attain a better estimate of $\langle F \rangle$. This is called in statistics the method of "importance sampling."

The Monte Carlo method for attaining an estimate of $\langle F \rangle$ based on the foregoing considerations will now be given. It was introduced by Metropolis *et al.* [1] to make equation of state calculations on substances with models similar to that used here for the triangular magnetic lattice. This method has been described extensively in the literature [2–5]. We will simply give the probabilities used by Metropolis *et al.* [1] for transition from any point μ in the ensemble to any point ϵ, and then describe their application in the Monte Carlo method.

The probabilities are:

$$\begin{aligned} P_{\mu\epsilon} &= 0 && \text{for } \epsilon \text{ not one spin reversal removed from } \mu. \\ &= 1 && \text{for } \Delta E \leqslant 0 \\ &= e^{-\Delta E/kT} && \text{for } \Delta E > 0 \end{aligned} \tag{4}$$

where $\Delta E = (E_\epsilon - E_\mu)$.

The application of (4) is as follows. We pass through the lattice reversing spins. At each step we compute ΔE and generate a random number n between 0 and 1. Then, if $n \leqslant p_{\mu\epsilon}$, we make the transition from configuration μ to configuration ϵ (i.e., leave the spin reversed), and compute F_ϵ and add it to a running sum of F. If $n > p_{\mu\epsilon}$, we stay in configuration μ (i.e., put the spin back the way it was), and compute F_μ and add it to the running sum of F. (Actually, F_μ was already computed from the previous step.) We continue making passes through the lattice until, say, R points have been sampled. Then our estimate of (2) is

$$\langle F \rangle \cong \frac{1}{R} \sum_{\epsilon=1}^{R} F_\epsilon \tag{5}$$

It has been shown (e.g., [16]) that (5) is exact in the limit as $R \to \infty$ for transition probabilities (4). Convergence considerations will be made in a later section.

In the next section we describe a method that is different from the above only in the transition probabilities, $P_{\mu\epsilon}$, which have been shown (e.g., [3]) to be not unique.

4. The Revised Monte Carlo Method

We argue that, as before, what we need as we go from one point in the ensemble to the next (by reversing spins) is a transition probability at each point that is derived from the Boltzmann distribution, i.e., we want to make transitions from one point in the ensemble to another according to the Boltzmann distribution. For

the desired transition probabilities we now take the two-point conditional probabilities [14] (suggested by Wood [5] and first used by Flinn and McManus [6]) given by

$$P_{\mu\epsilon} = P_\epsilon/(P_\mu + P_\epsilon) \tag{6}$$

where, as in (4), $P_{\mu\epsilon}$ is the probability of a transition from point μ in the ensemble to point ϵ, and where P_μ and P_ϵ are the unconditional normalized Boltzmann probabilities at points μ and ϵ given by (3). Combining (6) with (3) and adding the condition for reversing one spin only, we get

$$\begin{aligned} P_{\mu\epsilon} &= 0 \text{ for } \epsilon \text{ not one spin reversal removed from } \mu. \\ &= 1/(1 + e^{\Delta E/kT}) \end{aligned} \tag{7}$$

where $\Delta E = (E_\epsilon - E_\mu)$.

The proof that the transition probabilities given by (7) result in expression (5), including its exact form in the limit of large N, follows that of Ref. [16], which considers the transition probabilities of Metropolis *et al.* given by (4). To avoid a lengthy repetition, here we will give only those parts of the proof that are different due to the differences between (4) and (7). A familairity with the material of Ref. [16] is assumed.

The transition matrix, P (for one pass through the lattice), with $2^N \times 2^N$ elements, $p_{\mu\epsilon}$, must be stochastic. That is, $p_{\mu\epsilon} \geqslant 0$ and $\sum_\epsilon p_{\mu\epsilon} = 1$ must hold. This is clearly the case for (7), the first condition being satisfied by inspection, and the second by the fact that the application of (7) is the same as for (4). That is, $p_{\mu\mu} = 1 - p_{\mu\epsilon}$, and these are the only nonzero elements in row μ of P.

The transition matrix P must result in a homogeneous Markov chain. That is, $p_{\mu\epsilon}$ must be independent of the sequence of steps in the Markov chain. Again this is the case for (7) since, as with (4), only the energy difference between two successive states is involved.

Proof that the Markov chain resulting from (7) is irreducible (all states are of the same ergodic class) is the same as in Ref. [16] for (4) except that it is not possible when using (7) for $p_{\mu\mu} = 0$, as it is when using (4).

Proof of the aperiodicity of the Markov chain resulting from (7) is also the same as that given in [16] for (4), except that at least one diagonal element of P is seen to be nonzero without recourse to the configuration of minimum energy.

Finally, we must show that for P defined by (7), the probability distribution on step $n + 1$ of the Markov chain, given by

$$\psi_{n+1} = \psi_n P, \tag{8}$$

approaches the Boltzmann distribution (3) as n becomes infinitely large; that is

$$\lim_{n\to\infty} \psi_n = \psi$$

where ψ is given by (3). Because of the uniqueness of this limit [16], it suffices to show that a vector with components given by (3) is an eigenvector of P with eigenvalue unity. This can be done by demonstrating that ψ is an eigenvector with eigenvalue unity of $P(k)$ for all k, where $P(k)$ is the 2^N dimensional square stochastic matrix of transition probabilities corresponding to the reversal of the spin on site k. That is, we need only show that

$$\psi P(k) = \psi \tag{9}$$

where ψ is the Boltzman distribution. It follows that this will hold for the product

$$\psi \prod_{k=1}^{N} P(K) = \psi. \tag{10}$$

As previously defined, $P = \prod_{k=1}^{N} P(k)$ is the transition matrix for one pass through a lattice of N sites. Rewriting (9) in element form,

$$\sum_j \psi_j p_{j\epsilon} = \psi_\epsilon \,. \tag{11}$$

We must show that for $p_{\mu\epsilon}(k)$ given by (7) and ψ_μ given by the Boltzmann distribution (3), ψ_ϵ is also equal to (3). On any spin reversal, at most two states are involved, say μ and ϵ, with the following four possible transitions:

$$\mu \to \epsilon, \qquad \mu \to \mu, \qquad \epsilon \to \mu, \qquad \epsilon \to \epsilon. \tag{12}$$

Thus, $P(k)$ has only four nonzero elements. We have

$$p_{\mu\epsilon} = 1/(1 + e^{(E_\epsilon - E_\mu)/kT}), \qquad p_{\mu\mu} = 1 - p_{\mu\epsilon} \tag{13}$$

and

$$p_{\epsilon\mu} = 1/(1 + e^{(E_\mu - E_\epsilon)/kT}), \qquad p_{\epsilon\epsilon} = 1 - p_{\epsilon\mu} \,. \tag{14}$$

Computing ψ_ϵ, letting $D^{-1} = \sum_{i=1}^{2^N} e^{-E_i/kT}$, we have

$$\psi_\epsilon = De^{-E_\mu/kT}[1/(1 + e^{(E_\epsilon - E_\mu)/kT})] + De^{-E_\epsilon/kT}[1 - 1/(1 + e^{(E_\mu - E_\epsilon)/kT})].$$

Reducing the expression, we get

$$\psi_\epsilon = De^{-E_\epsilon/kT} \tag{15}$$

and we have the Boltzmann distribution. The procedure is similar for the other component of ψ.

In conjunction with Ref. [16], this completes the proof of the validity of (5), including its exact form, for the transition probabilities (7).

The transition probabilities derived here (7) can be related to those used by Metropolis *et al.* [1] by expanding (7) in a power series: For $\Delta E < 0$

$$p_{\mu\epsilon} = 1 - e^{-|\Delta E|/kT} + e^{-2|\Delta E|/kT} - + \cdots. \tag{16}$$

For $\Delta E > 0$

$$p_{\mu\epsilon} = e^{-\Delta E/kT} - e^{-2\Delta E/kT} + - \cdots. \tag{17}$$

Dropping all terms but the first in each series, we have (4).

At first sight, (4) might seem to be a poor approximation to (7). However, the most important characteristic of any satisfactory approximation to (7) is that it has the same relative strength of transition about $\Delta E = 0$. This is the case, as is found by taking the ratio of (16) to (17) and comparing it to the ratio of (7) for $\Delta E < 0$, to (7) for $\Delta E > 0$. These ratios are both equal to $e^{\Delta E/kT}$.

A plot of both sets of probabilities is shown in Fig. 1. Note that for $\Delta E = 0$ (i.e., three surrounding spins up and three down), we keep changing the lattice with a 50% chance using the conditional probabilities (7), rather than always accepting the modification, as would result from using the conventional method (4). This is consistent with the use of transition probabilities in relation to the Boltzmann distribution because two states of equal energy have equal probability of occurrence.

The preceding is a special case of the general statement that the conventional method has a greater strength of transition, i.e.,

$$\int p_{(4)}\, d(\Delta E) > \int p_{(7)}\, d(\Delta E). \tag{18}$$

This results in more movement of the lattice through phase space. If the initial configuration of the lattice is far removed from the mean configuration, this could tend to improve results. Unfortunately, for the cases of greater interest (no analytic exact solution), we usually do not know the relationship between the initial and the mean configurations.

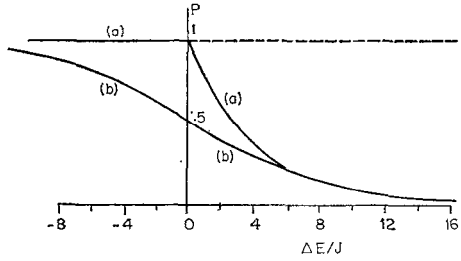

FIG. 1. Plots of conventional transition probabilities (a) and Boltzmann conditional propabilities (b) for $kT/J = 4°K$. P is the probability that a given change is accepted.

5. Calculations

In the calculations, the selection of each subsequent spin for reversal and the definition of an iteration were both based on the method of Ehrman *et al.* [3, 15]. Starting at spin (1, 1), each spin in the first row was selected in turn, then each spin in the second row, and so on until each spin in the entire lattice had been considered. This defined one iteration. Then, spin (1, 1) was selected again, starting the second iteration, and so on. The expectation value per spin of the energy, of the long-range order, and of the short-range order, were computed in the manner indicated by (5). For a lattice of N spins, γ nearest-neighbors, and with M iterations, the equations used in the calculations of energy and long-range order are given below.

Energy:

$$\frac{\langle E\rangle}{JN} = \frac{1}{NR}\sum_{\mu=1}^{R}\frac{E_\mu}{J} \tag{19}$$

where $R = NM$, the number of samples taken from the ensemble.

Long-range order per spin:

$$\langle L\rangle = \frac{1}{NR}\sum_{\mu=1}^{R} L_\mu\,, \tag{20}$$

where L_μ is the long-range order of the system in the μth state. The short-range order per spin calculated [3] is the fraction of nearest-neighbor sites that are occupied by an antiparallel pair of spins.

$$\langle f\rangle = \frac{1}{NR}\sum_{\mu=1}^{R} f_\mu \tag{21}$$

where

$$f_\mu = \frac{1}{2\gamma N}\sum_{i=1}^{N}\sum_{j=1}^{\gamma}(1 - S_iS_j). \tag{22}$$

In terms of $\langle E\rangle$,

$$\langle f\rangle = \frac{1}{\gamma}\left(\frac{\langle E\rangle}{JN}\right) + \frac{1}{2}\,. \tag{23}$$

Once expression (19) was computed, $\langle f\rangle$ was evaluated from Eq. (23).

To verify these Monte Carlo calculations, the energy results were compared with the exact Onsager solution [17] as performed by Wannier [11] and Houtappel [12]. (Initial comparison with [12] showed discrepancies. After two typographical errors were found in the formulation and confirmed by Houtappel in private communication, the comparison became very good [18].) The percentage deviations of

the Monte Carlo results from the exact values are tabulated in Table I. The signs of the deviations were found to be random.

TABLE I

Comparison of Monte Carlo Energy Calculations with Exact Values for the Two-Dimensional Triangular Isotropic Lattice

	Exact	Percentage deviation from exact				
	Lattice size	20 × 20	10 × 10	20 × 20	20 × 20	30 × 30
	Number of iterations	500	8,000	2,000	8,000	8,000
$kT/\|J\|$	Total number of spin flips	200,000	800,000	800,000	3,200,000	7,200,000
	Ferromagnetic using transition probabilities (7)					
1	−2.99992	0.40	0.02	0.10	0.003	0.052
2	−2.96748	0.65	0.03	0.15	0.05	0.059
3	−2.68033	1.11	0.07	0.26	0.04	0.174
4	−1.51468	1.92	2.12	0.36	1.17	0.344
5	−0.98955	0.05	0.35	0.20	0.45	0.015
6	−0.74284	1.00	0.13	0.64	0.001	0.027
7	−0.59548	0.21	0.32	0.82	0.47	0.107
8	−0.49705	0.82	0.37	0.79	0.25	0.044
9	−0.42656	1.25	0.01	0.20	0.37	0.128
10	−0.37359	1.25	1.27	0.49	0.30	0.019
Average percentage deviation		0.87	0.47	0.41	0.31	0.096
	Antiferromagnetic using transition probabilities (4)					
1	−0.931143	0.29	0.39	0.04	0.05	0.087
2	−0.730472	0.28	0.22	0.10	0.01	0.009
3	−0.590302	0.64	0.01	0.51	0.05	0.014
4	−0.494415	0.01	0.19	0.60	0.34	0.077
5	−0.425084	0.21	1.50	0.41	0.25	0.136
6	−0.372688	0.15	0.32	0.74	0.33	0.142
7	−0.331731	0.45	0.23	0.63	0.17	0.116
8	−0.298843	0.28	0.09	1.51	0.19	0.177
9	−0.271873	4.30	1.44	1.80	1.43	0.375
10	−0.249349	3.60	0.70	2.53	0.80	0.452
Average percentage deviation		1.00	0.51	0.90	0.37	0.158

Comparison between analytic results and Monte Carlo calculations of the short-range order is implicit in the comparison of the energy values, as is evident from (23). An exact solution for the long-range order has not yet heen obtained,

since the energy as a function of the field strength is not known. However, its general behavior is indicated by the presence (ferromagnetic lattice) or absence (antiferromagnetic lattice) of a phase transition, for zero field strength. Fig. 2 is

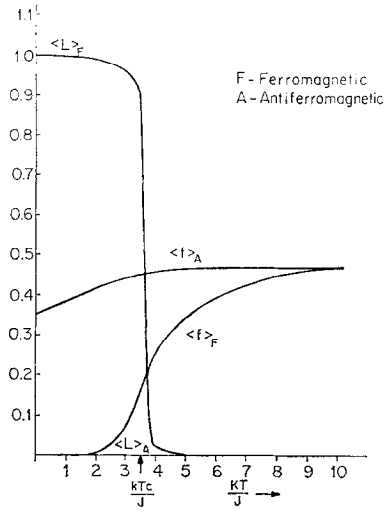

FIG. 2. Long- and short-range order for the ferromagnetic and antiferromagnetic lattices; Done with 30 × 30 lattice and 8000 iterations, and using Boltzmann conditional probabilities.

a graph of long- and short-range order versus kT/J, displaying both the ferromagnetic and antiferromagnetic lattices. These calculations were made using only the Boltzmann conditional probabilities (7) and are of general interest to the Monte Carlo method rather than for comparison of (7) with (4).

6. Discussion of Results

A. *Comparison of Transition Probabilities*

As indicated in Table I, the ferromagnetic calculations were made using the transition probabilities given by (7), and the antiferromagnetic calculations were made using the transition probabilities of Metropolis *et al.* [1] given by (4). A direct comparison of the two sets of transition probabilities for this two-state problem is given in Table II. It can be seen from Table I that the conditional Boltzmann probabilities produce more consistent results, particularly when it is noticed that the ferromagnetic lattice has a critical point at $kT/J = 3.641$, in the neighborhood of which the energy undergoes large fluctuations. As can be seen

TABLE II

Direct Comparison of Transition Probabilities (in Terms of the Percentage Deviation from the Exact; in Same General Format as Table I)

	Ferromagnetic					
	20 × 20 500 200,000		10 × 10 8,000 800,000		20 × 20 2,000 800,000	
$kT/\|J\|$	(4)	(7)	(4)	(7)	(4)	(7)
1	0.36	0.40	0.07	0.02	0.09	0.10
2	0.55	0.65	0.01	0.03	0.76	0.15
3	1.12	1.11	0.23	0.07	0.33	0.26
4	2.24	1.92	7.23	2.12	1.60	0.36
5	0.17	0.05	0.77	0.35	0.62	0.20
6	1.30	1.00	0.60	0.13	0.24	0.64
7	0.56	0.21	0.74	0.32	0.91	0.82
8	0.78	0.82	0.30	0.37	0.88	0.79
9	0.32	1.25	0.60	0.01	0.51	0.20
10	1.27	1.25	0.22	1.27	0.02	0.49
Average	0.90	0.87	1.07	0.47	0.60	0.41

	Antiferromagnetic					
	20 × 20 2,000 800,000		20 × 20 8,000 3,200,000		30 × 30 8,000 7,200,000	
	(4)	(7)	(4)	(7)	(4)	(7)
1	0.04	0.01	0.05	0.04	0.016	0.052
2	0.10	0.05	0.10	0.03	0.046	0.059
3	0.51	0.18	0.05	0.08	0.135	0.174
4	0.60	0.31	0.34	0.02	0.313	0.344
5	0.41	0.01	0.25	0.20	0.220	0.015
6	0.74	0.23	0.33	0.01	0.190	0.027
7	0.63	0.45	0.17	0.41	0.208	0.107
8	1.58	0.21	0.19	0.36	0.095	0.044
9	1.80	0.31	1.43	0.11	0.145	0.128
10	2.53	0.23	0.80	0.39	0.193	0.019
Average	0.90	0.20	0.37	0.16	0.156	0.097

in Table II, the conditional Boltzmann probabilities yield noticeably better results, including the important characteristic of greater regularity in response to changes in process parameters, such as lattice size and the total number of spin reversals. As mentioned, this characteristic is also evident in Table I. The greater strength of transition, inherent in (4) as pointed out earlier, was experienced in the comparison. Typically, (4) resulted in the acceptance of 20 to 40 % more spin reversals than did (7).

B. *General Monte Carlo Considerations*

General estimates of the influence of lattice size, the number of iterations, and the total number of spin reversals on the accuracy can be inferred from Table I. For example, for the ferromagnetic case, increasing the number of iterations significantly (by a factor of 4) for a 20×20 lattice, does not appreciably increase the accuracy. Increasing the lattice size to 30×30 and holding the number of iterations constant (which results in an increase of the total number of spin reversals by a factor of 9/4), produces a significant increase in accuracy (by a factor greater than 3). The maximum percentage deviation also must be considered in any such estimates. In this example, it was significantly reduced (from greater than 1 % to less than 0.4 %).

No attempt was made to assign an absolute uncertainty to the results of the calculations because no such measure of accuracy can be given for any finite Monte Carlo process when applied to an unknown distribution, as is the case here. In a manner similar in principle to that used by Salsburg *et al.* [7], we compute the standard deviations of the running averages of the energy over successively longer portions of the Markov chain. For W estimates of $\langle E\rangle$, we computed

$$\sigma_W = \left[\frac{1}{W}\sum_{j=1}^{W}(\langle E\rangle_{R_j} - \langle \bar{E}\rangle_W)^2\right]^{1/2}, \tag{24}$$

where

$$\langle \bar{E}\rangle = \frac{1}{W}\sum \langle E\rangle_j . \tag{25}$$

In the energy calculations, the average of the expectation values and the corresponding standard deviations were computed from Eqs. (25) and (24) over the entire sample, over the last 90 % of the sample, over the last 80 %, 70 %, etc., to over the last 10 % of the sample. Also, the value of $\langle E\rangle_{R_j}$ was printed out for

$$R_j = jR/100 \qquad j = 1, 2, \ldots, 100, \tag{26}$$

where R is the total number of steps in the Markov chain.

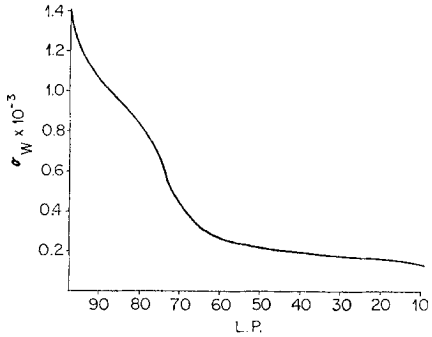

FIG. 3. Fluctuations in $\langle E \rangle$ for a ferromagnetic 30×30 ($kT/J = 8$; 8000 iterations). L. P. is the last percentage of the sample over which σ_W was computed.

The σ_W values were helpful in establishing a convergent pattern, as shown in Fig. 3, which gives a typical set of σ_W values. In the ferromagnetic case near the critical point, the σ_W values are larger by an order of magnitude, but still reflect the same convergent pattern.

The effect of the initial configuration of the lattice was also investigated in terms of random versus ordered. It was found that a configuration that had an energy closer to the exact value of $\langle E \rangle$ produced better results. For example, an ordered initial configuration gave better results by factors of from 1.5 to 4 for the ferromagnetic lattice, and worse by the same factors for the antiferromagnetic lattice. For a random initial configuration, the previous results weer reversed with respect to ferromagnetic and antiferromagnetic systems.

Finally, the results of the order calculations presented in Fig. 2 show the expected [11, 12] transition from the disordered to the ordered state for the ferromagnetic lattice as the temperature decreases through the critical value. An inflection in the short-range order is clearly distinguishable at the critical point. One can expect this from the fact that $\langle E \rangle$ has such an inflection (using Eq. (23)). Also, the slope of $\langle f \rangle$ shows the $1/\gamma$ factor of Eq. (23) with $\gamma = 6$, i.e., $d\langle f \rangle/dT = (1/\gamma)\, d(\langle E \rangle/JN)/dT$. This flattening effect of the $1/\gamma$ factor tends to make the infinite slope at the critical point less obvious. The results for the antiferromagnetic lattice are also as expected [11, 12]. They do not show a critical point, as is evident from the fact that the long-range order is near zero everywhere, and that the short-range order does not have an infinite slope. The magnitude of $\langle L \rangle$ is of the order of 10^{-5}, which is remarkably good for this type of numerical calculation, since a 30×30 lattice in the μth configuration and only one spin reversal removed from zero microscopic long-range order yields $L_\mu \simeq 10^{-3}$.

REFERENCES

1. N. METROPOLIS, A. W. ROSEBLUTH, N. N. ROSENBLUTH, A. H. TELLER, AND E. J. TELLER, *J. Chem. Phys.* **21** (1953), 1087.
2. L. D. FOSDICK, *Phys. Rev.* **116** (1959), 3.
3. J. R. EHRMAN, L. D. FOSDICK, AND D. C. HANDSCOMB, *J. Math. Phys.* **1** (1960), 6.
4. J. M. HAMMERSLEY AND D. C. HANDSCOMB, "Monte Carlo Methods," Chap. 9, Wiley, New York, 1964.
5. W. W. WOOD, "Physics of Simple Liquids," (H. N. V. Temperley, Ed.), Chap. 5, North-Holland, Amsterdam, 1968.
6. P. A. FLINN AND G. M. MCMANUS, *Phys. Rev.* **124** (1961), 54.
7. Z. W. SALSBURG, J. D. JACOBSON, W. FICKETT AND W. W. WOOD, *J. Chem. Phys.* **30** (1959), 65.
8. D. A. CHESNUT AND Z. W. SALSBURG, *J. Chem. Phys.* **38** (1963), 2861.
9. D. A. CHESNUT, *J. Chem. Phys.* **39** (1963), 2081.
10. E. Z. ISING, *Physica* **31** (1925), 253.
11. G. H. WANNIER, *Phys. Rev.* **79** (1950), 357.
12. R. M. F. HOUTAPPEL, *Physica* **16** (1950), 425.
13. K. HUANG, "Statistical Mechanics," 156–162, 189–197, 329–373, Wiley, New York, 1967.
14. W. FELLER, "An Introduction to Probability Theory and Its Applications," Vol. 1, Chap. 5, Wiley, New York, 1957.
15. The method of Ehrman, *et al.* [3] is to make systematic passes through the lattice. We tried both the systematic selection and the random selection of each subsequent spin and found essentially no difference in the results. We chose the systematic selection because it executes more efficiently on the computer.
16. L. D. FOSDICK, *Math. Comp. Phys.* **1** (1953), 255.
17. B. KAUFMAN AND L. ONSAGER, *Phys. Rev.* **76** (1949), 1244.
18. The errors (mentioned but not identified by C. Domb, *Advan. Phys.* **9** (1960), 213, footnote p. 241) are both on p. 452 of [12]. The first is the upper limit of integration for the complete elliptical integrals of the first and second kinds. It should be $\pi/2$ for both, instead of 2π. The second is in the definition of α for the antiferromagnetic case. Part of the denominator, $(1 - x)^2$ should be $(1 - x^2)$.