Monte Carlo studies of the kinetic Ising model

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Results are presented for the computer simulation of the time-dependent behavior of the Ising model on a 100×100 lattice. Groups of particles are regarded as samples from an infinite lattice and the interactions between the sample particles and those outside are expressed through new boundary conditions based on extending the concept of mean field in a self-consistent way. These new boundary conditions are explored analytically for a few small samples and a sharp critical point is found in contrast to periodic boundary conditions. The relaxation times for long-range order and nearest-neighbor correlation (energy) for the 100×100 system have been computed and the corresponding critical exponents estimated. The results are $\Delta_{\delta\mu} = 2.30 \pm 0.30$ and $\Delta_{\delta\mathcal{H}} = 0.38 \pm 0.04$; these are compared with other recent results from computer simulations and series calculations.

I. INTRODUCTION

In recent years computer simulation using Monte Carlo techniques has been used to examine various aspects of the behavior of time-dependent statistical-mechanics models for order-disorder phenomena and many useful results have been obtained. Reviews of Monte Carlo investigation in these areas have recently been given by Binder.[1,2] In the present paper we give the results of computer simulation of the time-dependent relaxation towards equilibrium of a two-dimensional Ising system. The primary aim of this work has been to obtain the values of the critical exponents of the relaxation times for the long-range order (magnetization) $\Delta_{\delta\mu}$ and for the nearest-neighbor correlation function (energy) $\Delta_{\delta\mathcal{H}}$. We have found $\Delta_{\delta\mu} = 2.3 \pm 0.30$ in agreement with other authors and $\Delta_{\delta\mathcal{H}} = 0.38 \pm 0.04$ which is a new result.

The simulation process as generally used in statistical mechanics is simulated sampling where "computer observation" of a finite group or sample of particles from an infinite system provides estimates of the parameters describing the behavior of an infinite system. In the simulation of an isolated system, for example, a cluster of particles, the entire system can be "observed" directly and there is usually no need to consider what happens outside the cluster. In the infinite system, however, the sample particles (the inner particles) interact with the particles outside (the outer particles) and some means must be found for simulating this interaction. With Ising systems the particles are usually set at node points of a lattice and the simplest means of allowing for the inner-particle–outer-particle interaction is to consider the sample to be replicated to fill all space. The particles at or near the boundary of the system interact with the particles of the adjacent replicated samples and for the purpose of computing this interaction, these outer particles may be taken as the equivalent inner particles of the actual sample. For computing the interactions in Ising systems this representation of the infinite system is adequate since these interactions involve nearest neighbors and perhaps next nearest neighbors. For other systems, this representation may not be adequate. By imposing this periodic structure on the infinite system we have in fact replaced that part of the infinite system outside the sample by boundary conditions on the surface of the sample. These are referred to as periodic boundary conditions (PBC) and it is hoped that they will satisfactorily mimic the sample-population interaction.

Most of the numerical computations with Ising systems have been made using PBC. However, there is a weakness in these results in that the long-range order does not display a temperature (the critical temperature) at which it falls sharply to zero so that there is no sharp transition and the computed anomalies at the critical temperature are all rounded instead of being singular. This was first noted by Ehrman *et al.*[3] and by Yang.[4] These rounded anomalies in the specific heat of the Ising model have been studied by Ferdinand and Fisher[5] using the Onsager solution and they showed the extent of the rounding region for an

$n \times n$ square lattice to be defined by the temperature-dependent coherence length. This turns out to be $O(n)$ in lattice units and implies the width of the rounding region about the true critical temperature to be $O(1/n)$.

On the other hand, the familiar mean-field approximation (MFA), which is a one-site approximation, gives a sharply defined critical temperature below which the long-range order is nonzero and above which it is identically zero. However, MFA has the disadvantage that it does not give good values for critical exponents, either for equilibrium or time-dependent quantities (Suzuki and Kubo[6]). We are thus led to consider extending the concept of mean field beyond its familiar use for one site to set up boundary conditions which represent the sample-population interaction in a more satisfactory manner. In the present paper we introduce two types of boundary condition based on this extended concept which lead to sharp critical regions. We have explored them analytically for small samples and have used simulation to examine the more important of the two for a sample of 100×100 particles. We call these boundary conditions extended mean-field boundary conditions (EMFBC) and we shall distinguish them later by adding a further Letter. Binder[1,7] has already discussed one of these boundary conditions although only for the case of equilibrium and then for the Heisenberg model.

The structure of the present paper is as follows. In Secs. II and III we briefly discuss the usual interpretation of MFA and show how it can be extended to various samples. Of course the usual way of improving MFA is to use the Bethe-Peierls method and in the present context of time-dependent solutions Huang[8] has given the solution for a Bethe cluster of five spins on the two-dimensional Ising lattice. Our philosophy differs from this because we wish to apply the new boundary conditions to a sufficiently large $n \times n$ sample of the infinite lattice and to perform a computer simulation of the Markov process associated with the master equation. In Sec. IV, we describe the simulation and in Sec. V, we present the results for a 100×100 system.

II. MEAN-FIELD APPROXIMATION AND ITS EXTENSION TO EQUILIBRIUM CONFIGURATIONS

In order to present the extensions we shall first define precisely MFA itself. The basic approximation consists essentially in isolating a sample of one particle out of the whole lattice by screening out the rest of the lattice. It is as if we were sampling the entire lattice by looking through a window in an opaque screen. The window is square and is just large enough for us to see one site. We recognize that the particle on this site (the inner particle) interacts with its (outer) neighbors, but we know nothing of this interaction and we must estimate it in some way. We note that the boundary between the inner and the outer spins lies between the sites: Since we are considering only nearest-neighbor interactions we may regard the nearest outer particles as boundary particles in the conventional way; if we were to admit longer-range interactions, we should then have to speak of a boundary region containing more than one line of particles.

The simplest assumption that we can make about the boundary particles is that each particle has an effective spin value of σ, $-1 \leq \sigma \leq 1$, which has to be determined in a self-consistent manner. If the spin variable for the inner particle be $s_1 = \pm 1$, the Hamiltonian for the inner particle is then given by

$$H = -4Js_1\sigma, \tag{2.1}$$

assuming nearest-neighbor interaction only. J is the exchange coupling constant. The partition function is then given by

$$Q = \sum_{s_1=\pm 1} e^{-\beta H}, \tag{2.2}$$

where $\beta = 1/kT$, k being Boltzmann's constant and T the absolute temperature. The ensemble average of s_1 is identified as σ and is given by

$$\sigma = \tanh 4K\sigma, \quad K = \beta J, \tag{2.3}$$

which is the MFA expression and shows a sharp transition at $K_c = \frac{1}{4}$ so that $T_c = 4$ in units of J/k. This is now extended to larger samples by enlarging the sample window. Thus, for the 2×2 sample assuming that the eight boundary spins are given the value of σ, we find that

$$\sigma = \frac{2\sinh 4K\sigma + e^{4K}\sinh 8K\sigma}{2 + 4\cosh 4K\sigma + e^{-4K} + e^{4K}\cosh 8K\sigma}. \tag{2.4}$$

The transition temperature of the 2×2 sample is given by

$$K_c = \tfrac{1}{8} e^{-2K_c}(3 + \cosh 4K_c)/\cosh 2K_c, \tag{2.5}$$

which yields

$$K_c = 0.285\,74, \quad T_c = 3.499\,62$$

in units of J/k. The Onsager solution is $T_c = 2.269\ldots$. The functions on the right-hand side of Eqs. (2.3) and (2.4) can be expanded as power series in $(K - K_c)$ and this yields $\frac{1}{2}$ for the critical exponent for the order, instead of the

correct value $\frac{1}{8}$ which is known to hold for the infinite lattice. We return to this point later. Since we are extending MFA using a self-consistent value for the order, which is the ensemble average of the inner spins, we shall call this boundary condition extended MFA using the average and shall denote it by EMFBCA or EA for short. The nearest-neighbor correlation function ϕ_0 for the 2×2 sample is given by

$$\phi_0 = \frac{e^{4K}\cosh 8K\sigma - e^{-4K}}{2 + 4\cosh 4K\sigma + e^{-4K} + e^{4K}\cosh 8K\sigma}. \quad (2.6)$$

The critical value of ϕ_0 is

$$\phi_0(T_c) = \sinh 4K_c/(3+\cosh 4K_c) = 0.29\ldots. \quad (2.7)$$

The exact value for the infinite lattice is $1/\sqrt{2} = 0.70\ldots$.

The existence of the nonzero value of σ at sufficiently low temperatures is a consequence of the symmetry-breaking term in the Hamiltonian arising from the interactions between the inner and outer particles. Gallavotti[9] discusses the boundary conditions in which the outer spins are, respectively, all up or all down. These also break the symmetry of the Ising Hamiltonian and yield a nonzero value for the long-range order for sufficiently low temperatures. With PBC the symmetry of the Hamiltonian is maintained and accordingly the long-range order is always identically zero.

There is however a much more realistic way of representing these unknown boundary spins. Each of the outer spins, like the inner ones, can have only one of two state values ± 1 and these are the values which must be used in the calculations. We can only make remarks in probability concerning the states of the outer spins and the best we can say about the outer spins considering them one at a time, is that they take the values ± 1 with probabilities such that their average is σ. We thus define the one-particle probability distribution function $p(s_j)$,

$$p(s_j = \pm 1) = \tfrac{1}{2}(1 \pm \sigma), \quad (2.8)$$

where σ must be identified self-consistently as the ensemble average of the long-range order. This is in fact the basis of the simulation process which we describe later. We will call this boundary condition the extended MFA boundary conditions using probability and shall denote it by EMFBCP or EP for short.

We can now give the analytic solutions for a sample of one spin and for a sample of 2×2 spins. For the one-particle sample, where the four boundary spins are instantaneously s_a, s_b, s_c, and s_d, any term $F(s_1;s_a,s_b,s_c,s_d)$ is replaced by

$$\begin{aligned} &F(s_1;1,1,1,1)p^4(+1) + F(s_1;-1,1,1,1)4p^3(+1)p(-1) \\ &+ F(s_1;-1,-1,1,1)6p^2(+1)p^2(-1) \\ &+ F(s_1;-1,-1,-1,1)4p(+1)p^3(-1) \\ &+ F(s_1;-1,-1,-1,-1)p^4(-1). \end{aligned}$$

It is then straightforward to obtain for the sample of one spin, that

$$\sigma = (X_0^4 - Y_0^4)/(X_0^4 + Y_0^4), \quad (2.9)$$

where

$$X_0 = 1 + \sigma\tanh K$$

and

$$Y_0 = 1 - \sigma\tanh K.$$

This yields the critical temperature at $\tanh K_c = \frac{1}{4}$, so that

$$K_c = 0.25541$$

and

$$T_c = 3.91523,$$

which is a slight improvement on the result using EA.

For the 2×2 sample we have for σ, in EP

$$\sigma = \frac{(X_0^8 - Y_0^8)e^{4K} + 2X_0^2Y_0^2(X_0^4 - Y_0^4)}{(X_0^8 - Y_0^8)e^{4K} + 4X_0^2Y_0^2(X_0^4 + Y_0^4) + 4X_0^4Y_0^4 + 2X_0^4Y_0^4e^{-4K}}. \quad (2.10)$$

The critical temperature is given by $\tanh K_c = F(K_c)$, where $F(K_c)$ is the right-hand side of (2.5). This yields $K_c = 0.29096$, $T_c = 3.4368$. We also get for the nearest-neighbor correlation function

$$\phi_0 = \frac{(X_0^8 + Y_0^8)e^{4K} - 2X_0^4Y_0^4e^{-4K}}{(X_0^8 + Y_0^8)e^{4K} + 4X_0^2Y_0^2(X_0^4 + Y_0^4) + 4X_0^4Y_0^4 + 2X_0^4Y_0^4e^{-4K}}, \quad (2.11)$$

which yields

$$\phi_0(T_c) = \tfrac{1}{8}(1 + e^{-2K_c})^2 = 0.30374.$$

The two examples using our boundary conditions are the first two of a sequence which extends to $n\times n$ samples. The step from 1×1 to 2×2 involving the self-consistency in the order is somewhat arbitrary since all the sites are equivalent: the smallest sample with nonequivalent sites is the 3×3 system. The analysis can be continued to these larger samples, but naturally becomes very involved, and in any case the analysis of the 1×1 and 2×2 samples is sufficient to establish the general pattern of the solutions.

III. NONEQUILIBRIUM BEHAVIOR OF SMALL SAMPLES

We now extend the ideas developed in Sec. II to consider the time-dependent nonequilibrium behav-

ior of small samples. The infinite system of particles is assumed to interact with a heat bath at a given temperature for instance through a spin-phonon interaction which induces transitions in the particle states, no two transitions occurring simultaneously. Assuming a knowledge of the transition probabilities we investigate the behavior of the infinite system by observing a finite sample of neighboring particles.

Consider firstly a sample of one inner particle P. Let the spin variable associated with P be s_1 with values ± 1. The values of the variables for the nearest neighbors of P are unknown and must be estimated from the observed behavior of P. As before, the simplest assumption is to take these spin variables all equal to $s \equiv s(t) = \langle s_1(t) \rangle$, this mean being defined with respect to the probability distribution function for the state of P; this is the boundary condition EA. If $P(s_1;t)$ is the probability that P is in the state s_1 the mean value is defined by

$$s = \sum_{s_1 = \pm 1} s_1 P(s_1;t) = P(+1;t) - P(-1;t), \tag{3.1}$$

and using the normalization $P(+1;t) + P(-1;t) = 1$ we may write generally

$$P(s_1;t) = \tfrac{1}{2}(1 + s_1 s), \quad s_1 = \pm 1, \tag{3.2}$$

which reduces to (2.8) when $s = \sigma$.

That is, the distribution function $P(s_1;t)$ can be represented in linear form in terms of the basis variables $\{1, s_1\}$, the coefficients being functions of the sample variable s which is also to be taken as the mean of the infinite system. We might expect therefore to be able to write the transition probabilities for P in the same form. Thus, if $W(s_1 \to -s_1)$ is the probability per unit time that P being in state s_1 will pass to state $-s_1$, then we should have

$$W(s_1 \to -s_1) = (1/2\alpha) a(s)[1 - s_1 c(s)]. \tag{3.3}$$

The coefficients $a(s)$, $c(s)$ must also depend on the temperature of the heat bath since the transition probabilities derive from the interaction of the heat bath with the Ising system. The parameter α is related to the mean time between transitions. The most important restrictions on $a(s)$ and $c(s)$ come from a consideration of the behavior of P under equilibrium conditions. At equilibrium the condition of detailed balance must hold and we have

$$W(s_1 \to -s_1) P_0(s_1) = W(-s_1 \to s_1) P_0(-s_1), \tag{3.4}$$

where $P_0(s_1) = \frac{1}{2}(1 + s_1 \sigma)$ and σ is the equilibrium value of $\langle s(t) \rangle$.

Using the representation (3.3) in (3.4) and equating coefficients of the variables 1, s_1 we find that $c(\sigma)$ satisfies

$$\sigma = c(\sigma). \tag{3.5}$$

This is an equation for σ which refers to equilibrium and must be identical to (2.3). Thus,

$$c(s) \to \tanh 4K\sigma, \quad \text{as } s \to \sigma. \tag{3.6}$$

Detailed balance does not imply any restriction on $a(s)$. This must come from a consideration of the nature of the coupling between the Ising system and the heat bath.

Using the form (3.3) we may now examine the nonequilibrium behavior of P and hence of the infinite system. The probability function $P(s_1;t)$ satisfies the master equation

$$\frac{dP}{dt}(s_1;t) = -W(s_1 \to -s_1) P(s_1;t) + W(-s_1 \to s_1) P(-s_1;t), \tag{3.7}$$

which on using (3.3) yields

$$\alpha \frac{ds}{dt} = -a(s)[s - c(s)]. \tag{3.8}$$

Equilibrium occurs when $ds/dt = 0$, and this implies

$$s = \sigma, \quad s - c(s) = 0. \tag{3.9}$$

We now examine the solutions to the master equations using EP. To do this we need to express the transition probability in a form similar to (3.3). We begin by fixing the four outer spins s_a, s_b, s_c, s_d and writing

$$W(s_1 \to -s_1) = (1/2\alpha) A(s_a, s_b, s_c, s_d)[1 - s_1 C(s_a, s_b, s_c, s_d)]. \tag{3.10}$$

We now average over each of the outer spins with respect to the one-particle distribution function (3.2) written as

$$P(s_n;t) = \tfrac{1}{2}(1 + s_n s), \quad n = a, b, c, d. \tag{3.11}$$

We can be more explicit about the form of W. In fact, from detailed balance we know that in equilibrium, and in simplest terms,

$$W(s_1 \to -s_1) = (1/2\alpha) \exp(-K s_1 4\sigma), \tag{3.12}$$

and we extend this to nonequilibrium by writing

$$W(s_1 \to -s_1) = (1/2\alpha) \exp[-K s_1 (s_a + s_b + s_c + s_d)]. \tag{3.13}$$

Since s_1 can only take the values ± 1, Eq. (3.12) can be written as the linear form

$$W(s_1 \to -s_1) = (1/2\alpha) \cosh K(s_a + s_b + s_c + s_d) \times [1 - s \tanh K(s_a + s_b + s_c + s_d)]. \tag{3.14}$$

Using (3.14) in the master equation (3.7), averaging over the outer spins first, then averaging over the inner spin s, we readily obtain

$$\frac{ds}{dt} = \frac{4}{\alpha}(X^4 + Y^4)\left(s - \frac{X^4 - Y^4}{X^4 + Y^4}\right), \tag{3.15}$$

where

$$X = 1 + s\tanh K, \quad Y = 1 - s\tanh K.$$

We note that X, Y are the time-dependent values of $X_0 Y_0$ defined in (2.9).

We can now give an analytic expression for the relaxation towards an equilibrium value. We choose an experiment similar to that of Collins and Teh[10] who measured the relaxation of the long-range order in Ni_3Mn by neutron diffraction The temperature was changed discontinuously from $T + \Delta T$ to T. We expand s about the equilibrium order σ writing $s = \sigma + r$.
We find

$$r = r_0 \exp\{-(t/\alpha)[1 - 4K(1 - \sigma^2)]\cosh 4K\sigma\}, \tag{3.16}$$

which shows that the relaxation time is such that its critical exponent is unity. The same result is obtained using EA. This agrees with the result obtained by Collins and Teh experimentally, but there is still doubt about the interpretation of the experiment, which is concerned with a first-order rather than a second-order effect.

We now construct the time-dependent solution to the master equation for two spins. Defining the two-spin correlation function $\phi(t) = \langle s_1 s_2\rangle$ and using $\langle s_1\rangle$ and $\langle s_2\rangle$ we have, in the same way that (3.2) was obtained

$$P(s_1, s_2; t) = (1/2^2)(1 + s_1\langle s_1\rangle + s_2\langle s_2\rangle + s_1 s_2\langle s_1 s_2\rangle). \tag{3.17}$$

Glauber[11] derived (3.2) and (3.17) and similar expressions by a different method using an identity which involved basis functions. Thus, for one particle the basis functions are $\{1, s_1\}$ and for two particles, the basis functions are $\{1, s_1, s_2, s_1 s_2\}$. There is a similar construction for more particles. It is worth noting that these sets of basis functions form groups with respect to multiplication and in particular we recognize the two-particle group as the Klein four group.

We may assume that the transition probabilities W have the convenient form

$$W(s_1 \to -s_1, s_2) = (1/2\alpha)[a(s) - s_1 b(s) + s_2 c(s) - s_1 s_2 d(s)], \tag{3.18}$$

$$W(s_1, s_2 \to -s_2) = (1/2\alpha)[a(s) + s_1 b(s) - s_2 c(s) - s_1 s_2 d(s)], \tag{3.19}$$

where $s = \frac{1}{2}(\langle s_1\rangle + \langle s_2\rangle)$. These two expressions, (3.18) and (3.19) satisfy detailed balance and in equilibrium yield

$$\sigma = [b(\sigma) + c(\sigma)]/2a(\sigma), \tag{3.20}$$

$$\phi_0 = d(\sigma)/a(\sigma). \tag{3.21}$$

It is important to realize that there is an arbitrariness in the forms (3.18) and (3.19) because detailed balance would still be satisfied if an arbitrary factor $h(s)$ appeared on the right-hand sides, similar to (3.3). We have in effect taken $h(s) = 1$ and this sets the time scale. The forms of a, b, c, d can readily be obtained from the partition function using the basis-function expansion. Equations (3.20) and (3.21) reduce to

$$\sigma = \sinh 6K\sigma/(\cosh 6K\sigma + e^{-2K}) \tag{3.22}$$

and

$$\phi_0 = (\cosh 6K\sigma - e^{-2K})/(\cosh 6K\sigma + e^{-2K}). \tag{3.23}$$

On substituting (3.17), (3.18), and (3.19) in the two-spin master equation we obtain three coupled equations for $\langle s_1\rangle$, $\langle s_2\rangle$, and $\langle s_1 s_2\rangle = \phi$. From symmetry $\langle s_1\rangle = \langle s_2\rangle = s$ and so these equations reduce to

$$\frac{ds}{dt} = [-sa(s) + sd(s) + b(s) - b(s)\phi], \tag{3.24}$$

$$\frac{d\phi}{dt} = 2[d(s) - a(s)\phi]. \tag{3.25}$$

We have absorbed α and numerical factors into t.

These equations (3.24) and (3.25) are equivalent to to the equation of motion for any operator $A(s_1 \cdots s_i \cdots s_N)$, namely,

$$\frac{d}{dt}\langle A(s_1 \cdots s_i \cdots s_N; t)\rangle = -\sum_{i=1}^{N}\langle W(s_i \to -s_i)\times[A(s_1 \cdots s_i \cdots s_N; t) - A(s_1 \cdots -s_i \cdots s_N; t)]\rangle$$

given by Binder[1] and Abe.[12]

For two nearest-neighbor spins on a square Ising lattice in EA, we derive from the partition function the following expressions:

$$a(\sigma) = \cosh^2 3K\sigma \cosh K + \sinh^2 3K\sigma \sinh K,$$
$$b(\sigma) = \sinh 3K\sigma \cosh 3K\sigma(\cosh K + \sinh K), \tag{3.26}$$
$$d(\sigma) = \cosh^2 3K\sigma \sinh K + \sinh^2 3K\sigma \cosh K.$$

Because the spin-phonon coupling, which is expressed by the transition probabilities, is the

same in both equilibrium and nonequilibrium we may replace σ by s and use these formulas in the master equation and in particular in (3.24) and (3.25). Expanding the functions to the first order about equilibrium,

$$s(t)=\sigma+x(t),$$
$$\phi(t)=\phi_0+y(t),$$
$$a(s)=a(\sigma)+(s-\sigma)a_1,$$
$$b(s)=b(\sigma)+(s-\sigma)b_1,$$
$$d(s)=d(\sigma)+(s-\sigma)d_1,$$

where $a_1\equiv[da(s)/ds]_{s=\sigma}$, etc., we get

$$\frac{dx}{dt}=a_{11}x+a_{12}y,$$
$$\frac{dy}{dt}=a_{21}x+a_{22}y, \tag{3.27}$$

where

$$a_{11}=-a(\sigma)-a_1\sigma+d(\sigma)+d_1\sigma+b_1-b_1\phi_0,$$
$$a_{12}=-b(\sigma),$$
$$a_{21}=2d_1-2a_1\phi_0, \tag{3.28}$$
$$a_{22}=-2a(\sigma).$$

Writing the time dependence in x and y as $e^{-\lambda t}$, then λ is given by the roots of the determinantal equation

$$\begin{vmatrix} a_{11}+\lambda & a_{12} \\ a_{21} & a_{22}+\lambda \end{vmatrix}=0.$$

The critical properties are given by noting that at T_c, $\sigma=b(\sigma)/a(\sigma)=0$ so that $a_{12}=0$; a_{22} is finite, but

$$a_{11}=-a(0)[1-b_1/a(0)][1-\phi_0(0)]=0,$$

since $a(0)=\cosh K_c$, $b_1=3K_c e^{K_c}$, and because of the equation defining K_c, $a_{11}=0$. This condition expresses the critical slowing down, and both x and y will have the same relaxation time with a critical exponent of unity. This is to be expected for the mean-field condition; for a finite sample of $n\times n$ sites, estimates of the critical properties of the infinite lattice are not given by considerations within $1/n$ of the critical temperature of the sample.

IV. COMPUTER SIMULATION

The essential steps in the computer simulation of the relaxation of the present ferromagnetic Ising system are as follows:

(a) The particles on the 100×100 square array are set in the well-ordered configuration with all spins up, that is, all $s_j=+1$. This is the lowest-energy configuration and is the configuration to be expected at absolute zero.

(b) Using the single-spin-flip strategy the system is allowed to relax to a partially ordered configuration at the nominal high temperature of 10.0. This configuration is not necessarily consistent with equilibrium at temperature 10.0 and is partially disordered to the extent that the number of configurations, counted with multiplicities, which the system is allowed to pass through is $10\,000=100\times100$. Thus, at this high temperature we might expect each particle, on the average, to have suffered at most one spin flip. Since we are proceeding to the critical temperature from above, the configuration resulting from this sequence provides a convenient standard initial state for the relaxation study.

(c) The temperature of the system is then fixed at the relaxation value and the sequence of configurations corresponding to relaxation at this temperature is then generated using the single-spin-flip strategy. The energy (that is, the short-range order) and the long-range order are recorded as the sequence develops. The number of configurations in the sequence is sufficient for the system to reach equilibrium, which is recognized by the fluctuations about zero in the long-range order.

The single-spin-flip strategy for generating the sequence of configurations operates with the following steps.

(1) Using a random-number generator with a uniform distribution select one of the particles of the array. This point will be either an inner point or a boundary point.

(2) Inner point. The four nearest neighbors interacting with the chosen particle all lie within the array and we may simply calculate the energy change due to reversing the spin of this particle.

(3) Boundary point. Here one or two of the neighbors of the chosen particle will lie outside the array (an outer point) and the others will lie within the array. The values for the states of the inner particles are known and we must estimate the value for the outer particles. With periodic boundary conditions each value is that of the corresponding particle on the opposite boundary of the array. With EP the value is chosen according to the one-particle probability mean-field distribution function discussed in Sec. III. In each case we may readily calculate the energy change on reversing the spin of the central particle.

(4) From the single-flip energy change we compute the transition probability. If this transition

probability value is greater than another uniformly distributed random number the configuration resulting from the spin reversal is accepted, otherwise it is rejected.

The random number used in the present simulation was based on a pair of linear congruences with modulus 2^{48} and was especially written in assembly code for the Control Data CYBER 76 computer used for the present computations. One congruence was used to set up a table of integer numbers and the other used to access the table to provide the number to be used, the table entry being replaced from the first congruence. This method gives a very long sequence of uncorrelated uniformly distributed integer numbers whose subsequences appear to have the same properties (Knuth[13]); these integers are packed into a floating-point format in the interval (0, 1) when used in the computations.

V. ANALYSIS OF THE RESULTS OF THE SIMULATION

For the $n\times n$ system, the order $s(t)=\sum_{i=1}^{n^2}s_i/n^2$ and the nearest-neighbor correlation $\phi(t)=\sum_{\langle i,j\rangle}s_i s_j/2n^2$ were computed for a series of temperatures lying between $T=10$ and $T=2.35$. Generating the sequences of configurations through to equilibrium as described in Sec. IV, we estimated the relaxation time on the approach to equilibrium for s and ϕ by fitting a single exponential to the data. The usual method in this field of fitting the exponential $y=y_0e^{-\lambda t}$ to a set of data pairs (t_k,y_k), $k=1$ through N is to integrate over the values of y. We used one of the Prony least-squares methods.[14] Taking $t_k=k\Delta t$

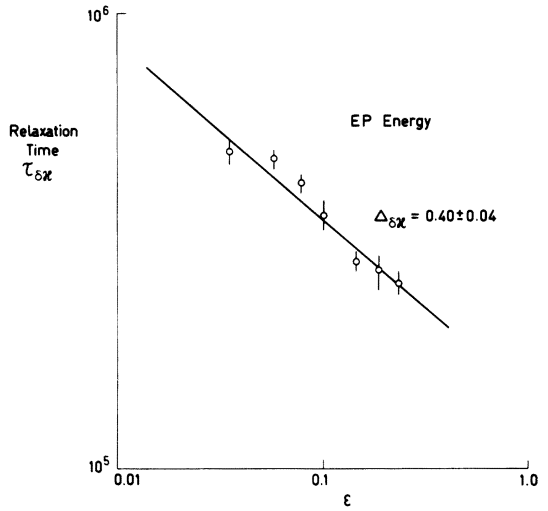

FIG. 1. Calculated temperature dependence of the energy relaxation time $\tau_{\delta\mathcal{H}}$ as a function of $\epsilon=(T-T_c)/T_c$ for the plane square lattice, using extended mean-field boundary conditions using probability.

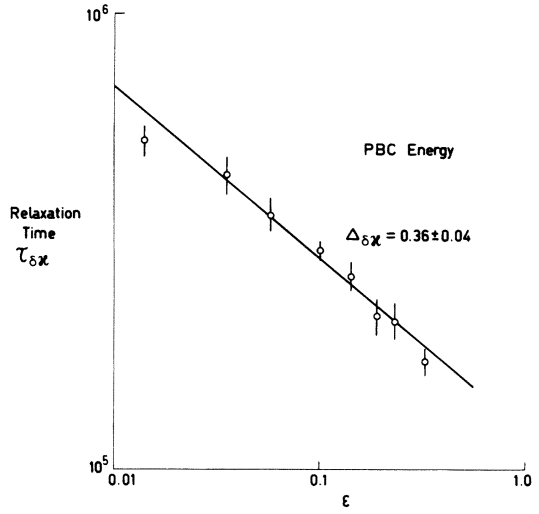

FIG. 2. Calculated temperature dependence of the energy relaxation time $\tau_{\delta\mathcal{H}}$ as a function of $\epsilon=(T_c-T_c)/T_c$ for the plane square lattice, using periodic boundary conditions.

we find

$$e^{-\lambda\Delta t}=\sum_{k=1}^{N-1}y_k y_{k+1}\Big/\sum_{k=1}^{N-1}y_k^2. \tag{5.1}$$

Using EP the equilibrium long-range order is identically zero above the critical temperature and in (5.1) the values of the y_k are taken as the instantaneous values of the order s_k. The equilibrium value ϕ_0 is nonzero and to find the relaxation time for ϕ we take $y_k=\phi_k-\phi_0$. The numerical value of ϕ_0 is obtained by taking the average over several equilibrium sequences.

Using the notation of Binder[1] we call $\tau_{\delta\mu}$ the relaxation time for s and $\tau_{\delta\mathcal{H}}$ that for ϕ. Because of the fluctuations we were unable to get satisfactory estimates of $\tau_{\delta\mu}$; a great deal more computing time would have been needed. The nearest-

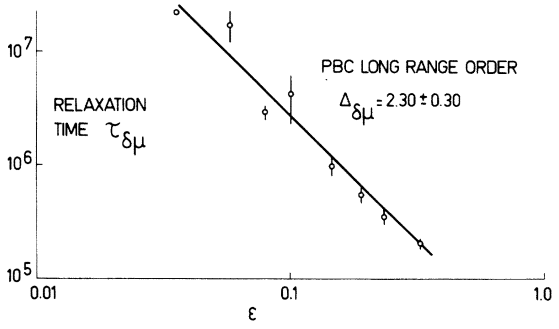

FIG. 3. Calculated temperature dependence of the order-parameter relaxation time $\tau_{\delta\mu}$ as a function of $\epsilon=(T-T_c)/T_c$ for the plane square lattice, using periodic boundary conditions.

TABLE I. Relaxation times and exponents in the kinetic two-dimensional Ising model.

Relaxation time	Exponent	Kawasaki[19]	Yahata[18]	$(4-d)$ expansion[20]	$1/n$ expansion[20]	Suzuki[16,21]	Ogita[15] *et al.*	Stoll[22] *et al.*	Present investigations
$\tau_{\delta\mu\,\delta\mu}$	$\Delta_{\delta\mu\,\delta\mu}$	1.75	~2.0	~2.18	~2.0	2.00 ± 0.05	•••	1.85 ± 0.10	•••
$\tau_{\delta\mu}$	$\Delta_{\delta\mu}$	•••	•••	•••	•••	~2.0	~1.75	1.85 ± 0.10	2.30 ± 0.30
$\tau_{\delta\mathcal{H}\delta\mathcal{H}}$	$\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$	0 (log)	~2.0	•••	•••	0.25 ± 0.05	•••	2.00 ± 0.10	•••
$\tau_{\delta\mathcal{H}}$	$\Delta_{\delta\mathcal{H}}$	•••	•••	•••	•••	•••	~0.3	•••	0.40 ± 0.04 (EP) 0.36 ± 0.04 (PBC)

neighbor correlation function ϕ however exhibited the slowing down more clearly and we were able to measure $\tau_{\delta\mathcal{H}}$ more readily. The plot of $\tau_{\delta\mathcal{H}}$ against $\epsilon = (T - T_c)/T_c$ is given in Fig. 1, and fitting the points in this figure by least squares yielded $\Delta_{\delta\mathcal{H}} = 0.40 \pm 0.04$. It should be emphasized that this is the exponent that characterizes the approach to thermal equilibrium in contradistinction to the critical exponent $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$ characterizing the decay of fluctuations in thermal equilibrium. Some theoretical predictions of these exponents have been given by a number of authors. Thus, from Suzuki[16] we have (i) $\Delta_{\delta\mu\delta\mu} = \Delta_{\delta\mu}$, (ii) $\Delta_{\delta\mathcal{H}\delta\mathcal{H}} = \Delta_{\delta\mathcal{H}}$, and (iii) $\Delta_{\delta\mathcal{H}\delta\mathcal{H}} = \Delta_{\delta\mu\delta\mu} = \gamma + \alpha$, while from Racz[17] $\Delta_{\delta\mu} = \Delta_{\delta\mu\delta\mu} - \beta$. Our value for $\Delta_{\delta\mathcal{H}}$ of 0.40 may be consistent with that of Racz, 0.3. No comparison can be made with the Suzuki estimates since Yahata[18] has shown that Suzuki's analysis for (iii) is incorrect. At present there is no theory which predicts our value of 0.4 for $\Delta_{\delta\mathcal{H}}$. It is worthwhile pointing out that both Suzuki and Racz call the exponent $\Delta_{\delta\mathcal{H}}$ "nonlinear", meaning that the equilibrium is approached from a state with a mean value different from the equilibrium value.

We repeated the calculations using periodic boundary conditions and obtained $\Delta_{\delta\mathcal{H}} = 0.36 \pm 0.04$. The order parameter now yielded $\Delta_{\delta\mu} = 2.30 \pm 0.30$. The results are presented in Figs. 2 and 3. The errors in the exponents were estimated from the goodness of fit of the least-squares line and were found to be consistent with the error observed in computing the ensemble averages for the configuration sequence values at each temperature. We collect the values in Table I, which complements a similar table in Stoll *et al.*[22]

VI. CONCLUSIONS

In introducing the extended mean-field boundary conditions it was hoped that the simulation of Ising systems with these conditions might take into account the physics of the problem more explicitly than would simulation with periodic boundary conditions. However, statistical fluctuations in the simulation and the slow convergence of the order toward its equilibrium value allow us to obtain at best only bounds on the critical exponents. Analytical investigations, such as we have made, of the behavior of small clusters, possibly extending the form of the boundary conditions to include higher-order correlation effects, may provide a means of sharpening these estimates. Also, further computation with larger samples would probably allow the effects of fluctuations to be considerably reduced.

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[1] K. Binder, in *Phase Transitions*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 5, pp. 1–100. See also references to Binder given in this review.
[2] K. Binder, Adv. Phys. 23, 917 (1974).
[3] J. R. Ehrman, L. D. Fosdick, and D. C. Handscomb, J. Math. Phys. 1, 547 (1960).
[4] C-P Yang, Am. Math. Soc. 15, 351 (1963).
[5] A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969).
[6] M. Suzuki and R. Kubo, J. Phys. Soc. Jpn. 24, 51 (1968).
[7] H. Müller-Krumbhaar and K. Binder, Z. Phys. 254, 269 (1972).
[8] H. Huang, Phys. Rev. B 11, 1144 (1975).
[9] G. Gallavotti, Rev. Nuovo Cimento 2, 133 (1972).
[10] M. F. Collins and H. C. Teh, Phys. Rev. Lett. 30, 781 (1973).
[11] R. J. Glauber, J. Math. Phys. 4, 294 (1963).
[12] R. Abe, Prog. Theor. Phys. 39, 947 (1968).
[13] D. E. Knuth, *The Art of Computer Programming. Semi-Numerical Algorithms* (Addison-Wesley, Reading, 1969), Vol. 2.
[14] E. Whittaker and G. Robinson, *The Calculus of Observations* (Blackie, London, 1949).

[15]N. Ogita, A. Ueda, T. Matsubara, H. Matsuda, and F. Yonezawa, J. Phys. Soc. Jpn. 26, 145 (1969).
[16]M. Suzuki, Prog. Theor. Phys. 43, 882 (1970).
[17]Z. Racz (unpublished).
[18]H. Yahata, J. Phys. Soc. Jpn. 30, 657 (1971).
[19]K. Kawasaki, Prog. Theor. Phys. 40, 706 (1968).
[20]B. I. Halperin, P. C. Hohenberg, and S-K Ma, Phys. Rev. Lett. 29, 1548 (1972).
[21]M. Suzuki, Int. J. Magn. 1, 123 (1971).
[22]E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).