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Dynamic Properties of the Monte Carlo Method in Statistical Mechanics

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By means of the Monte Carlo sampling technique the equilibrium thermodynamics of fluids and magnets can be calculated numerically. We show that the questions of convergence and accuracy of this method can be understood in terms of the dynamics of the appropriate stochastic model. Also, we discuss to what extent various choices of transition probabilities lead to different dynamic properties of the system. As examples of applications, we consider Ising and Heisenberg spin systems. The numerical results about the dynamic correlation functions are compared to simple approximations taken from the theory of the kinetic Ising model.

KEY WORDS: Critical slowing down; dynamic susceptibility; Heisenberg model; kinetic equations; master equation; mean field approximation; Monte Carlo; statistical errors; stochastic Ising model; time-dependent correlations; transition probabilities.

1. INTRODUCTION

The task of equilibrium statistical mechanics, to calculate the partition function from a given Hamiltonian, can be solved exactly only in a very few cases (e.g., the one-dimensional[1] and two-dimensional[2] Ising models and the one-dimensional classical Heisenberg model[3]). For three-dimensional magnets and for fluids approximate methods have to be used, and thus numerical techniques such as the Monte Carlo (MC) method[4,5] have a broad range of applications.[2] By this method one calculates thermal averages

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[2] For the large number of calculations on liquids (hard spheres, hard ellipses, Lennard-

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for a finite system using a Markov chain of phase-space points instead of integrating over the whole phase space as is appropriate in statistical mechanics. Specifying the transition probabilities suitably, these MC averages converge to the exact value in the limit of infinite chain length, since the method is ergodic. This has been tested on very small systems where the exact answer is known.[14,27]

However, only heuristic arguments have been given concerning the rate of convergence to this equilibrium state starting from any arbitrary initial configuration of the system. In practice it can be difficult to decide whether one is close to equilibrium or only in a rather long-living metastable state.[8] Since in the numerical computation the chain length is necessarily finite, one always has to deal with a "statistical error." It is not so straightforward to estimate this error very precisely,[3] although the standard procedures of elementary statistics[28] can be applied to this problem.[5,6,27] However, these methods disregard the knowledge that one can draw from the transition probabilities about the well-defined correlations between subsequent configurations.

It is one aim of the present work to show that interpreting the Monte Carlo process in terms of dynamic stochastic models can contribute to elucidating these accuracy problems. In the simplest case of the Ising model one thus can give a rough estimate of the number of MC steps per spin which are necessary to reach a given accuracy.

Furthermore, these dynamic stochastic models are rather interesting from the point of view of nonequilibrium statistical mechanics. For example, the stochastic Ising model has been studied extensively.[29–34] We give some results about time-displaced correlation functions which have been obtained from the MC calculation[4] for three-dimensional systems. These correlation functions have not been evaluated in the few previous applications of the MC method to relaxation phenomena,[12,15,35] while quite recently the power of the MC method has been clearly demonstrated by Stoll *et al.*,[36] who investigated the critical slowing down in the two-dimensional Ising model.

In Section 2 we formulate the dynamic problem in terms of a master equation, restricting the analysis to the case of the Ising and the classical

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Jones fluids, etc.) see the recent review in Ref. 6. For the simulation of liquid droplets in a gas see Refs. 7 and 8; an application to liquid crystals is given in Ref. 9. References 5 and 10–15 contain Ising model calculations, while Heisenberg magnets are treated in Refs. 11 and 16–22. The Blume–Capel model[23,24] has also been investigated.[25] For a generalization to quantum statistics see Ref. 26.

[3] Error estimates of the early work[4,5] seem to be too optimistic in many cases.

[4] A very brief account of these results has been given at the meeting of the Arbeitsgemeinschaft Magnetismus at Freudenstadt, April 1972, Germany; Proceedings in *Int. J. Magn.* 3:113 (1972).

Heisenberg models. In the latter case the relation to the actual dynamics, which is governed by the Hamiltonian of the system via the equations of motion, has to be discussed.

In Section 3 we present some numerical results on time-dependent correlation functions and compare them to simple analytic theories.[31]

In Section 4 the problem of error estimates is treated from the dynamic point of view, and some results on probability distributions are given. The observation of "critical behavior" of the errors near phase transitions leads to the question of the extent to which one can get different dynamic properties by choosing various transition probabilities, and the extent to which one only renormalizes the time scale. This problem is discussed in Section 5, while the main conclusions are given in Section 6.

2. DYNAMIC DESCRIPTION OF THE MONTE CARLO METHOD

Consider a system of N particles where each particle (labeled by index i) is described by a dynamic variable α_i which can be in one of the N_1 states of the set $\{\alpha_i\}$. These particles interact with a given Hamiltonian $\mathscr{H}_N(\{\alpha_i\})$. An example which will be treated explicitly is the Ising $S = 1/2$ model, where α_i is a spin variable σ_i which can take on two ($N_1 = 2$) discrete values $\{\sigma_i\} = \{+1, -1\}$; another example is the $S = \infty$ Heisenberg model, where the angles of spin orientation $\Omega_i = (\vartheta_i, \varphi_i)$ can vary continuously ($N_1 = \infty$), namely $0 \leqslant \vartheta \leqslant \pi$, $0 \leqslant \varphi \leqslant 2\pi$. Assuming only nearest-neighbor interactions, we have the Hamiltonians in zero magnetic field

$$\mathscr{H}_N^{\text{Ising}} = -\tfrac{1}{2}J \sum_{i \neq j(\text{n.n.})} \sigma_i \sigma_j \tag{1a}$$

$$\mathscr{H}_N^{\text{Heisenberg}} = -J \sum_{i \neq j(\text{n.n.})} [(\sin\vartheta_i \sin\vartheta_j)\cos(\varphi_i - \varphi_j) + \cos\vartheta_i \cos\vartheta_j] \tag{1b}$$

Then the expectation value of any variable A which depends on the dynamic variables $\{\alpha_i\}$ of the system is calculated from the canonical ensemble

$$\langle A \rangle = \left[\int d\mathbf{x}\, A(\{\alpha_i\})\, e^{-\beta\mathscr{H}(\{\alpha_i\})}\right] \Big/ \int d\mathbf{x}\, e^{-\beta\mathscr{H}(\{\alpha_i\})}$$

e.g., (2)

$$\langle A \rangle = \left[\sum_{\{\sigma_i = \pm 1\}} A(\{\sigma_i\}) \exp(-\beta\mathscr{H}^{\text{Ising}})\right] \Big/ \sum_{\{\sigma_i = \pm 1\}} \exp(-\beta\mathscr{H}^{\text{Ising}})$$

In approximating an integral $\int f(\mathbf{x})\, d\mathbf{x}$ by a sum with a finite number of terms $\sum_\nu f(\mathbf{x}_\nu)\, \Delta\mathbf{x}_\nu$, it is wellknown[37] that it is advantageous to choose the points $\mathbf{x}_\nu$ at random instead of using a regular set of points if the space of integration is of high dimensionality. The MC method introduced by Metropolis *et al.*[4] is based on the idea of "importance sampling,"[5] that is, one chooses the phase-space points $\mathbf{x}_\nu$ in Eq. (2) not completely at random

but takes them from that region of the phase space where the dominant contributions in Eq. (2) arise. If it is possible to choose a sequence of states $\mathbf{x}_\nu$ with the probability (density)

$$P_\nu^{\mathrm{eq}}\, d\mathbf{x}_\nu = \{\exp[-\beta\mathscr{H}(\mathbf{x}_\nu)]\}\, d\mathbf{x}_\nu \Big/ \int d\mathbf{x}_\nu \exp[-\beta\mathscr{H}(\mathbf{x}_\nu)] \tag{3}$$

the MC estimate $\bar{A}$ for the average $\langle A\rangle$ simply reduces to an arithmetic average

$$\bar{A} = (1/M) \sum_{\nu=1}^{M} A(\mathbf{x}_\nu) \tag{4}$$

where M is the total number of states generated in the MC sequence. In order to construct a sequence of states with the canonical probability distribution of Eq. (3) one introduces transition probabilities $W_{\mu\nu}$ which obey a detailed balance condition with the equilibrium distribution

$$W_{\mu\nu} P_\mu^{\mathrm{eq}} = W_{\nu\mu} P_\nu^{\mathrm{eq}} \tag{5a}$$

The simplest transitions between subsequent states (configurations) of the whole system are such that the state of only one particle has been changed (Ising model: one spin has been flipped). Then Eq. (5a) reads more precisely

$$W(\alpha_i \to \alpha_i') \cdot P^{\mathrm{eq}}(\alpha_1, \ldots, \alpha_i, \ldots, \alpha_N) = W(\alpha_i' \to \alpha_i) \cdot P^{\mathrm{eq}}(\alpha_1, \ldots, \alpha_i', \ldots, \alpha_N) \tag{5b}$$

or in the continuous case

$$\begin{aligned} &W(\alpha_i \to \alpha_i')\, d\alpha_i' \cdot P^{\mathrm{eq}}(\alpha_1, \ldots, \alpha_i, \ldots, \alpha_N)\, d\alpha_1 \cdots d\alpha_i \cdots d\alpha_N \\ &\quad = W(\alpha_i' \to \alpha_i)\, d\alpha_i \cdot P^{\mathrm{eq}}(\alpha_1, \ldots, \alpha_i', \ldots, \alpha_N) \cdot d\alpha_1 \cdots d\alpha_i' \cdots d\alpha_N \end{aligned} \tag{5c}$$

Starting from some arbitrary initial state, the actual distribution P_ν of the states in the sequence in Eq. (4) will deviate from the equilibrium distribution P_ν^{eq} if M is "small," of course. But from Eq. (5a) it is obvious that $P_\nu \to P_\nu^{\mathrm{eq}}$ if $M \to \infty$; note that the $W_{\mu\nu}$ are chosen to be nonzero for any two states μ, ν; thus the method is ergodic by construction.[38]5,6

[5] The practical realization of this method is as follows: One has to specify the transition probabilities in a simple way, e.g., Eqs. (7a)–(7c), and chooses a starting configuration for the system. Suppose one has random numbers at one's disposal to generate a trial configuration from the previous configuration. The transition probability is then calculated and compared to a random number z_R with $0 < z_R < 1$. If $W_{\mu\nu} < z_R$, the trial configuration is abandoned and the previous configuration is counted once more in the sequence. In the other case the trial configuration is taken to be the new configuration of the system. This step of the procedure is repeated M times.

[6] This property of ergodicity holds for the spin systems considered above. In the general case the phase space can consist of several ergodic classes without transitions between them, e.g., in a system of hard spheres at high density near their hexagonal closest-packing state there may be no transitions to states near the face-centered cubic closest-packing state.[38]

The simple argument[4] we have reproduced here does not say anything about two important problems: 1. How many configurations M_1 must be constructed so that the further states $\nu > M_1$ are close to "equilibrium states" (i.e., have a high probability close to P^{eq})? Clearly the configurations $\nu < M_1$ are influenced by the arbitrary starting configuration and should not be included in the average, Eq. (4). 2. How large must one choose M to have P numerically close to P^{eq} in order to reach some given accuracy $\langle A \rangle - \bar{A}$? In the practical realizations[5,6] one tries to treat these problems using the standard methods of statistical data analysis.[28] Nevertheless these questions have raised some doubt on the usefulness of the method.[39]

Obviously it is natural[5] to associate with the scale ν of subsequent configurations a scale of time t; suppose τ^{-1} single-particle transitions per particle are performed within the unit time (Ising model: $N\tau^{-1}$ trial[7] spin flips). Then the dynamic evolution of the probability $P_\nu = P(t)$ is governed by a master equation:

$$(d/dt)P(\alpha_1,\ldots,\alpha_i,\ldots,\alpha_N,t) = -\sum_{i=1}^{N}\sum_{\alpha_i'\neq\alpha_i} W(\alpha_i \to \alpha_i')P(\alpha_1,\ldots,\alpha_i,\ldots,\alpha_N,t) + \sum_{i=1}^{N}\sum_{\alpha_i'\neq\alpha_i} W(\alpha_i' \to \alpha_i)P(\alpha_1,\ldots,\alpha_i',\ldots,\alpha_N,t) \tag{6a}$$

which we have written down in the discrete case. Note that in the Ising model the sums over the possible one-particle states α_i' can be left out since only one $\alpha_i' \neq \alpha_i$ exists ($N_1 = 2$). Replacing the α_i by their values σ_i for the Ising model, the master equation then is

$$(d/dt)P(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N,t) = -\sum_{i=1}^{N} W(\sigma_i \to -\sigma_i)P(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N,t) + \sum_{i=1}^{N} W(-\sigma_i \to \sigma_i)P(\sigma_1,\ldots,-\sigma_i,\ldots,\sigma_N,t) \tag{6b}$$

and in the case of the classical Heisenberg model, where we have continuous variables,

$$(d/dt)P(\Omega_1,\ldots,\Omega_i,\ldots,\Omega_N,t) = -\sum_{i=1}^{N}\int d\Omega_i'\, W(\Omega_i \to \Omega_i')P(\Omega_1,\ldots,\Omega_i,\ldots,\Omega_N,t) + \sum_{i=1}^{N}\int d\Omega_i'\, W(\Omega_i' \to \Omega_i)P(\Omega_1,\ldots,\Omega_i',\ldots,\Omega_N,t) \tag{6c}$$

[7] See footnote 5.

This master equation given by Eqs. (6a)–(6c) has precisely one stationary (time-independent) solution which is the equilibrium distribution (3) because of the detailed balance conditions (5a)–(5c). Equation (6b) is just the starting equation of the familiar treatments of the kinetic Ising model,[30–34] since in these treatments we measure our times only relative to an arbitrary time scale τ ($\tau = 1$ corresponds to one MC step/spin and unit time). To simulate physical systems as closely as possible, one can consider τ's which depend on parameters like the temperature T in an appropriate way. It is an open question to what extent immediate applications can be made of the stochastic Ising model to physical systems[34]; note that the conditions (5a)–(5c) do not specify $W_{\mu\nu}$ and the dynamics of the system uniquely. We will return below to the question of what actual different cases of dynamic properties are possible.

Note that one does not get any dynamics from the equation of motion $i\hbar\, dA/dt = [A, \mathcal{H}]$ using the Ising Hamiltonian. This situation is different from the case of the Heisenberg model (and also from the case of liquid systems). The dynamic properties of these systems following from the Heisenberg equation of motion are well defined, and it is to be asked how they compare to the dynamics following from the master equation [Eq. (6c)]. From the description of the MC process given above it is immediately clear that in single-particle transition models there exist no conserved quantities, and one cannot define any transport coefficients properly as, e.g., the spin diffusion constant. Although this "stochastic Heisenberg model" which is constituted by the application of the MC method is a nontrivial, well-defined dynamic model, it is somewhat artificial: its dynamics turns out to be much more similar to those of the stochastic Ising model than to the dynamics of the conventional Heisenberg model. However, the static properties of both models are the same; the investigation of the dynamics of the stochastic Heisenberg model is useful for discussing the accuracy of static properties derived by the Monte Carlo method.

Considerable effort has been spent on the construction of stochastic models with more complicated transition processes, which better simulate the true dynamics (actually not in the classical Heisenberg case, but in the Ising[40] case, e.g., in the lattice gas representation of fluids.[41] Using a two-spin flip process where at one time two spins are simply exchanged, the magnetization is conserved and a spin diffusion constant is well defined.[40] This procedure could be applied to the Heisenberg case in a rather straightforward generalization, but this possibility is less interesting from the computational point of view[8]: One cannot get thermal equilibrium with respect

[8] In special cases of MC calculations such higher spin-flip processes with conserved quantities may be favorable; e.g., in the case of the cluster surface investigation[7] a two-spin-flip process was used keeping the number of reversed spins inside the cluster constant.

to the conserved quantity in the numerical calculation; one would need starting configurations where this quantity has precisely its equilibrium value. Furthermore, one must use non-Hermitian transition matrices $\{W(\alpha_i \to \alpha_i')\}$ in order to get propagating modes[34,41] as sound waves in liquids[41] or spin waves in magnets. The dynamic properties of these systems can be investigated numerically more conveniently using the molecular dynamics method.[42,43][9]

3. TIME-DEPENDENT CORRELATION FUNCTIONS EVALUATED BY THE MC TECHNIQUE

3.1. The Ising Model

Since the condition (5b) together with Eq. (3) does not specify the transition probability $W(\sigma_i \to -\sigma_i)$ in a unique manner, one has the freedom to make a simple choice for W. The two choices we are going to use numerically are

$$W_{\mathrm{MC}}(\sigma_i \to -\sigma_i) = \begin{cases} (\tau')^{-1} \exp(2\sigma_i E_i / k_{\mathrm{B}} T) & \text{if } \sigma_i E_i < 0 \\ (\tau')^{-1} & \text{otherwise} \end{cases} \tag{7a}$$

and

$$\begin{aligned} W_{\mathrm{I}}(\sigma_i \to -\sigma_i) &= (2\tau)^{-1}[1 + \tanh(\sigma_i E_i / k_{\mathrm{B}} T)] \\ &= (2\tau)^{-1}[1 + \sigma_i \tanh(E_i / k_{\mathrm{B}} T)] \end{aligned} \tag{7b}$$

where $\sigma_i E_i$ is the energy of the ith spin in the considered configuration. The factors τ, τ' are still arbitrary and fix only the time scale. While the first choice [Eq. (7a)] is commonly used in the MC work,[4–22,25,36] the second choice [Eq. (7b)] is used in the theory of the kinetic Ising model.[30–34] Both forms are limiting cases of a transition probability with one more parameter ξ (taking $\tau' = 2\tau$)

$$W_\xi(\sigma_i \to -\sigma_i) = W_{\mathrm{I}}(\sigma_i \to -\sigma_i) \left\{ 1 - \sinh^2 \left(\frac{E_i}{k_{\mathrm{B}} T} \right) \left[\frac{\tanh(E_i / \xi k_{\mathrm{B}} T)}{\tanh(E_i / k_{\mathrm{B}} T)} - 1 \right] \right\} \tag{7c}$$

where, putting $\xi \to 0$, we get Eq. (7a), while putting $\xi = 1$, we get Eq. (7b). These various choices for W are also explained in Fig. 1. More general possibilities of choices for $W(\sigma_i \to \sigma_i)$ will be discussed in Section 5.

The expectation value of the magnetization at a lattice site i is defined by

$$\langle \sigma_i(t) \rangle = \sum_{\{\sigma = \pm 1\}} \sigma_i P(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_N, t) \tag{8}$$

[9] An application to the Heisenberg magnet is also contained in Refs. 16 and 17.

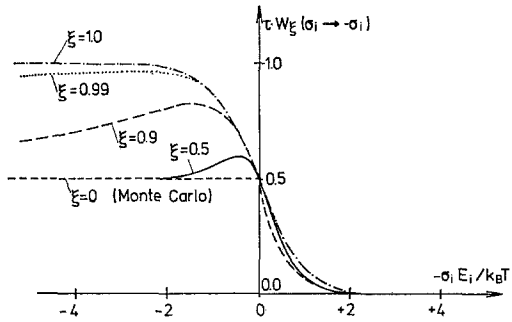

Fig. 1. Transition probabilities $W_\xi(\sigma_i \to -\sigma_i)$ [cf. Eqs. (7a)–(7c)] as a function of $\sigma_i E_i/k_B T$ (the local energy of the spin at lattice site i) plotted for various values of the arbitrary parameter ξ. The limiting cases are a "tanh"-like transition probability (the curve labeled by $\xi = 1.0$—this yields W for the kinetic Ising model), and an "exp"-like transition probability (for $\sigma_i E_i/k_B T < \sigma$; the curve labeled by $\xi = 0$—this yields W for the usual Monte Carlo method).

where the sum is extended over all possible configurations of the system. Using Eq. (7b) and the master equation (6b), it is straightforward to derive[31,34] the kinetic equation for $\langle \sigma_i(t) \rangle$

$$(d/dt)\langle \sigma_i(t) \rangle = -2\langle W_I(\sigma_i \to -\sigma_i)\, \sigma_i \rangle \tag{9a}$$

or more explicitly

$$\tau(d/dt)\langle \sigma_i(t) \rangle = -\{\langle \sigma_i(t) \rangle + \langle \tanh[E_i(t)/k_B T] \rangle\} \tag{9b}$$

Equation (9b) can be solved exactly for one-dimensional systems only.[30] Since we are interested in three-dimensional systems, we have to resort to approximations. We briefly review the mean field approximation[31] since we need these results to give a comparison with the numerical MC results. Treating Eq. (9b) by this approximation,[31] we get

$$\tau(d/dt)\langle \sigma_i(t) \rangle = -[\langle \sigma_i \rangle + \tanh(\langle E_i \rangle/k_B T)] \tag{9c}$$

Since we are interested in the equilibrium dynamic correlations and susceptibilities, we can solve Eq. (9c) by linear response theory introducing an infinitesimal field $\delta H_i(t)$ into the Hamiltonian:

$$E_i = -J \sum_{j(\text{n.n.})} \sigma_j - [H + \delta H_i(t)] \cdot \tfrac{1}{2} g \mu_B \tag{10}$$

Linearizing Eq. (9c) with respect to $\delta H_i(t) = \delta H_i^{\omega} e^{i\omega t}$ and taking Fourier transforms, one gets from Eqs. (9c) and (10)

$$\tau \frac{d}{dt} \langle \delta M_q(t) \rangle = -\langle \delta M_q(t) \rangle + \frac{1}{k_B T} (1 - \langle \sigma \rangle^2) \left[\delta H_q(t) \cdot \left(\frac{g\mu_B}{2} \right)^2 + J(\mathbf{q}) \langle \delta M_q(t) \rangle \right] \quad (11)$$

where the Fourier transform of the exchange $J(\mathbf{q}) = J \sum_{j(\text{n.n.})} \exp(i\mathbf{q}\mathbf{R}_j)$ was introduced, and

$$\langle M_q \rangle = \tfrac{1}{2} g\mu_B \sum_k \langle \sigma_k \rangle \exp(i\mathbf{q}\mathbf{R}_k)$$

Thus one finds for the dynamic susceptibility from $\langle \delta M_q^{\omega} \rangle = \chi(\mathbf{q}, \omega) \cdot \delta H_q^{\omega}$ the result

$$\chi(\mathbf{q}, \omega) = \frac{N(g\mu_B/2)^2}{k_B T} \frac{1 - \langle \sigma \rangle^2}{1 - [J(\mathbf{q})/k_B T](1 - \langle \sigma \rangle^2) + i\omega\tau} \quad (12a)$$

or

$$\chi(\mathbf{q}, \omega) = \frac{N(g\mu_B/2)^2}{k_B T} \frac{\chi_q}{1 + i\omega\tau_q}; \qquad \tau_q = \tau \frac{\chi_q}{1 - \langle \sigma \rangle^2} \quad (12b)$$

where the characteristic relaxation time of the system τ_q exhibits a critical slowing down for $T \to T_c = k_B J(0)$ and $\mathbf{q} \to 0$. Equation (12a) is a simple generalization of the result of Suzuki and Kubo,[31] which is valid also for magnetic fields $H \neq 0$ and for $T \leqslant T_c$ as well as for $T > T_c$. One further derives the time-dependent correlations in ordinary space [$\mathbf{R} = (h, k, l)$, putting the lattice spacing to unity]

$$\langle \sigma_0 \sigma_{\mathbf{R}}(t) \rangle = r_1^{-2} \int_{(2J/k_B T)\, t/\tau}^{\infty} \left[\exp\left(-t' \frac{k_B T}{2J} \right) \right] I_h(t')\, I_k(t')\, I_l(t')\, dt' \quad (13)$$

where the $I_n(x)$ are modified Bessel functions of the first kind. Of course, all these predictions of mean field theory [Eqs. (12) and (13)] are expected to be correct for $T \gg T_c$ and $T \ll T_c$ only; it is well known that this approximation breaks down near the critical point T_c.[44] The simplest idea of improving Eq. (12) is to correct for the true static correlation length κ^{-1} and the susceptibility exponent, replacing the Curie–Weiss prediction of Eq. (12),

$$\chi_0 = (1 - T_c/T)^{-1} \quad (14a)$$

by[44,45]

$$\chi_0 = 1.06(1 - T_c/T)^{-5/4} \quad (14b)$$

and neglecting η, we write for χ_q

$$\chi_q = r_1^{-2}\left[\kappa^2 + z - \sum_{(\text{n.n.})} \exp(i\mathbf{qR})\right]^{-1} \tag{14c}$$

where z is the number of nearest neighbors (over which the sum is extended). A similar change is applied to Eq. (13) so that it fits the approximant Eq. (14c) for $t \to 0$. Of course, this latter approximation is invalid very close to T_c, since it cannot yield the correct critical behavior of the energy if we choose $\mathbf{R}$ a nearest-neighbor vector in Eq. (13).

In making a comparison of these approximations with the MC results, it is useful to assess the accuracy of static properties. Static correlations of the SC lattice are plotted in Fig. 2 as functions of temperature and compared to high-temperature series expansion and extrapolation results.[45] The size of the lattice was $N = 512 = 8^3$ and periodic boundary conditions have been used. Near T_c we see some deviations from the "exact" results:[45] both a rounding of the transition and a shift of the maximum to higher temperatures.[14,20,22,46] Apart from these effects (which have to be expected since the system is very small) the agreement with the "exact" calculation[45] is satisfactory.

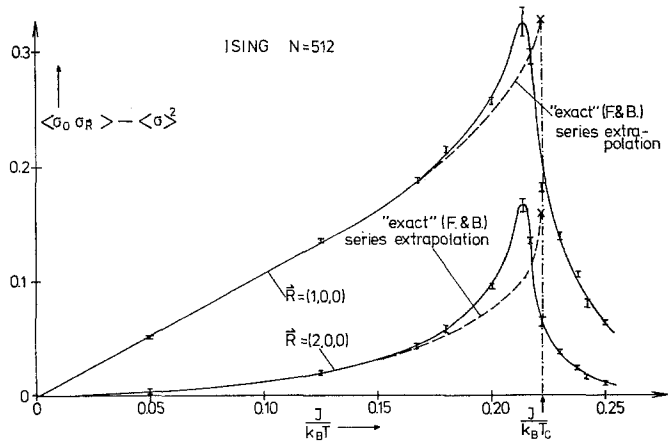

Fig. 2. Static correlations $\langle\sigma_0\sigma_\mathbf{R}\rangle$ of the three-dimensional Ising model plotted versus the reciprocal temperature J/k_BT. The critical point of the infinite systems is also shown ($J/k_BT_c \approx 0.222$[44]). The series expansion of Fisher and Burford[45] is included (dashed curves): for $J/k_BT \leqslant 0.20$ the series have been used as they stand; the critical values are also tabulated[45]; near T_c, a $(1 - T_c/T)\log(|1 - T_c/T|)$ behavior was assumed.

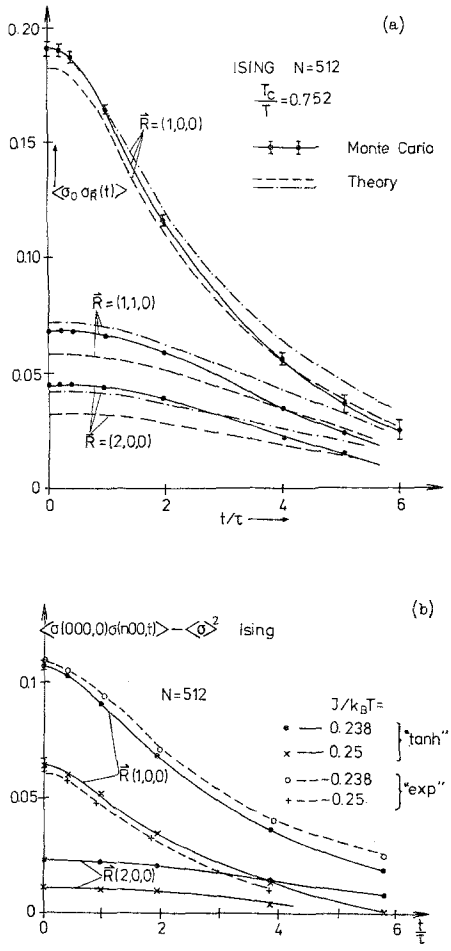

Fig. 3. Dynamic correlations $\langle \sigma_0 \sigma_{\mathbf{R}}(t) \rangle$ of the three-dimensional Ising model plotted versus the time t/τ. Various $\mathbf{R}$ are shown. (a) $J/k_B T = 0.1667$, above T_c. Full curve with error bars: MC result. The dashed curves represent the simple mean field approximation [Eq. (13)], the dashed-dotted curves are given by the same functional form but using the susceptibility (14b) instead of the mean field susceptibility (14a) in the relaxation time; the static MF values have been fitted to the MC results and normalized to $\langle \sigma_0 \sigma_{\mathbf{R}}(0) \rangle$, $\mathbf{R} = (1, 0, 0)$. (b) $J/k_B T_c = 0.238, 0.25$, below T_c. Full curve: MC result with transition probability of the "tanh" form Eq. (7b); broken curve, with transition probability of the exp form Eq. (7a); time scale normalized to the same number of spin flips per unit time as according to Eq. (7b).

In Fig. 3(a) we plot some time-displaced correlation functions at the temperature $J/k_B T = 0.1667$ ($T/T_c = 1.3$). Since this is not very close to T_c, the mean field result [Eq. (13)] for the same value of T/T_c yields rather similar curves. It is not clear if the use of Eq. (12b) together with Eqs. (14b) and (14c) actually leads to an improvement at larger values of t/τ since the accuracy of this MC calculation of time-dependent correlations is rather limited. In Fig. 3(b) similar results for correlations below T_c are shown, and we also include the results of a calculation where the first choice of transition probability (7a) has been used. Since the mean numbers of successful spin flips per Monte Carlo step are different for both choices, we calculated these numbers of spin flips at each temperature for both choices and we normalized the time scale with the ratio of these numbers in Fig. 3; this ratio between Eqs. (7a) and (7b) changes from one-half (at $T \to \infty$) to one (at $T \to 0$). The slight deviations between the correlation functions derived from these two choices can be fully attributed to the statistical error, since the accuracy of this calculation is not very good.

In Fig. 4 we plot the self-correlation function $\langle \sigma_0 \sigma_0(t) \rangle$ for various times as a function of temperature. This function is peaked at a temperature value close to the maximum of the static correlations (Fig. 2) as expected. In Fig. 5(a) we plot the self-correlation function logarithmically versus time; the curvature indicates strong nonexponential behavior. The initial slope of this function is nonzero at T_c. This behavior is different from the correlation function of the magnetization shown in Fig. 5(b). The scatter of the data points demonstrates again that the error of such dynamic calculations is much larger than the error in calculating static properties (cf. Fig. 2) derived

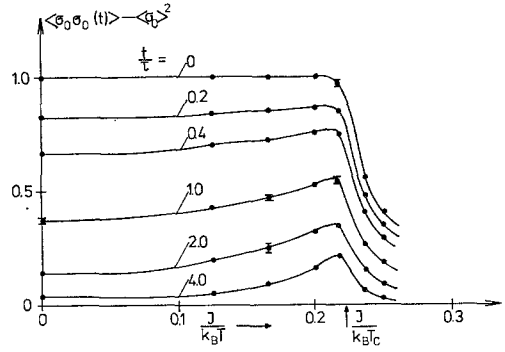

Fig. 4. Self-correlation function of the Ising model plotted versus reciprocal temperature. Parameter of the curves is the time t/τ. For large t/τ the maximum of this function is at the same position as the maximum of the static correlation $\langle \sigma_0 \sigma_{\mathbf{R}} \rangle - \langle \sigma \rangle^2$.

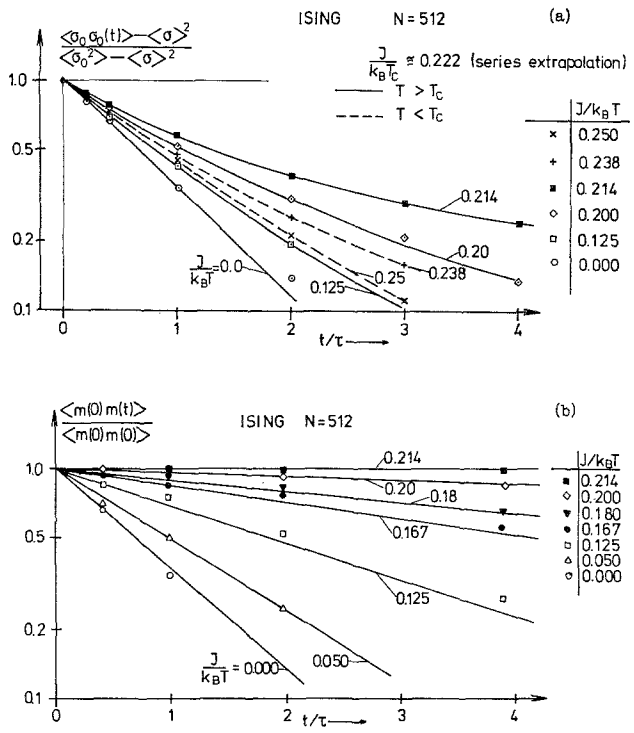

Fig. 5. (a) Self-correlation function $\langle\sigma_0\sigma_0(t)\rangle$ and (b) correlation function of magnetization $\langle m(0)m(t)\rangle$ plotted logarithmically versus time. The statistical error is about as large as the data "points." Paramagnetic temperatures correspond to full curves and ferromagnetic temperatures correspond to broken curves. The straight lines of part (b) are the result of fitting Eq. (15a) to the data; the only adjustable parameter was taken to be T_c (since the finite system has a shifted critical point, which leads to $J/k_B T_c = 0.214$).

from the same total number of configurations. The straight lines in Fig. 5(b) are estimates following from Eqs. (12b) and (14b):

$$\langle m(0)\, m(t)\rangle / \langle m^2\rangle = \exp(-t/\chi_0\tau) = \exp[-(1 - T_c/T)^{5/4} t/1.06\tau] \quad (15a)$$

which should be a reasonable approximation, at least for the small times considered in the diagram.[32,36] The integral of this function,

$$\tau_m \equiv \langle m^2\rangle^{-1} \int_0^\infty \langle m(0)m(t)\rangle\, dt \cong \tau_m{}^0 (1 - T_c/T)^{-\Delta} \quad (15b)$$

characterizes the slowing down of the magnetization, and Δ is the associated critical exponent.[32] At least not too close to T_c, it is legitimate to take $\Delta \approx \gamma = 1.25$.[36] Figure 5 gives indeed some qualitative evidence for the critical slowing down near T_c. We emphasize that the purpose of this investigation is to show (1) that dynamic considerations are valuable for discussing the accuracy of static properties, and (2) that the MC method is, in principle, capable of yielding time-dependent correlation functions even for three-dimensional systems. Since the question of "statistical errors" for dynamic properties is far more subtle[36] than it is for static properties, we make no statements about the critical exponents of the slowing down. This very interesting question is treated in the two-dimensional case only in Ref. 36; in this case a greater accuracy is available.

3.2. The Heisenberg Model

It is important to remember that the dynamics considered here is *not* the dynamics which follows from the Hamiltonian through the equation of motion $i\hbar(d/dt)\,\mathbf{S}_i(t) = [\mathbf{S}_i, \mathscr{H}]$. We consider here the dynamics of a model based upon the master equation (6c) together with appropriate transition probabilities which describe the MC process. This is a well-defined dynamic model, but perhaps somewhat artificial from a physical point of view.

The analog of Eqs. (7a) and (7b) is in this case

$$W_{\mathrm{MC}}(\Omega_i \to \Omega_i') = \begin{cases} (4\pi\tau)^{-1} \exp[(\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_i') \cdot \mathbf{E}_i/k_{\mathrm{B}}T] & \text{if } (\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_i') \cdot \mathbf{E}_i < 0 \\ (4\pi\tau)^{-1} & \text{otherwise} \end{cases} \tag{16a}$$

and

$$W_{\mathrm{H}}(\Omega_i \to \Omega_i') = (4\pi\tau)^{-1}\{1 + \tanh[\tfrac{1}{2}(\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_i')\,\mathbf{E}_i/k_{\mathrm{B}}T]\} \tag{16b}$$

and the analog of Eq. (8) is

$$\langle S_i^z(t)\rangle = (4\pi)^{-N} \int \cdots \int (\cos\vartheta_i) P(\Omega_1, \ldots, \Omega_i, \ldots, \Omega_N, t)\, d\Omega_1 \cdots d\Omega_i \cdots d\Omega_N \tag{17}$$

From Eqs. (6c), (16b), and (17) we again derive a kinetic equation

$$\tau(d/dt)\langle S_i^z(t)\rangle = -\left\{\langle S_i^z\rangle - \tfrac{1}{2}\left\langle K^{-2} \int_{K(S_i^z-1)}^{K(S_i^z+1)} dx\, x \tanh x \right\rangle\right\} \tag{18a}$$

with the abbreviation

$$-K = E_i^z/2k_{\mathrm{B}}T \tag{18b}$$

This reduces in the mean field approximation to

$$\tau(d/dt)\langle S_i^z(t)\rangle = -\{\langle S_i^z(t)\rangle + \mathscr{L}(\langle E_i^z\rangle/k_B T)\} \tag{18c}$$

where we have introduced the Langevin function $\mathscr{L}(x) = \coth(x) - 1/x$. Equation (18c) is completely analogous to Eq. (9c). This already reflects the

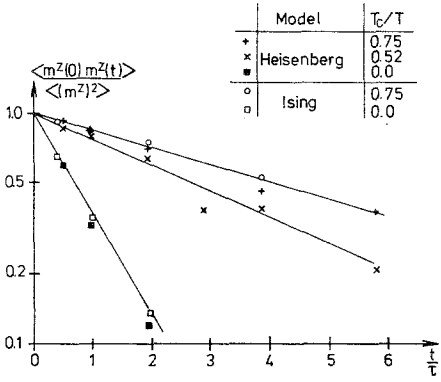

Fig. 6. Correlation function $\langle m_z m_z(t)\rangle$ for the classical Heisenberg model at two temperatures. At $T_c/T = 0.75$ an Ising correlation function is also plotted to show the similarity in the behavior of the stochastic models.

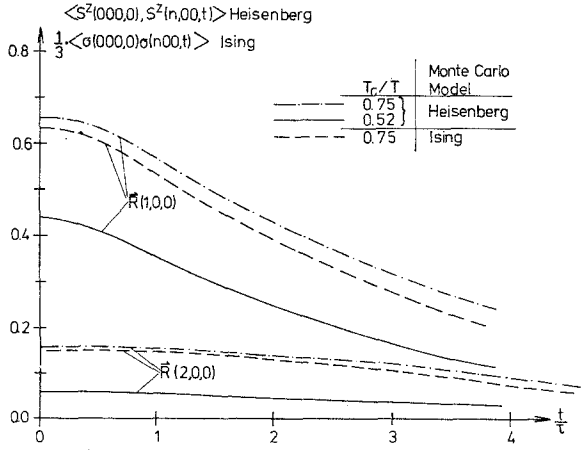

Fig. 7. Dynamic correlation functions $\langle S_0^z S_{\mathbf{R}}^z(t)\rangle$ of the three-dimensional Heisenberg model plotted versus the time t/τ at two (paramagnetic) temperatures. At $T_c/T = 0.75$ a comparison with the Ising correlations is given.

fact that the dynamics of both models are very similar, and this is also exhibited by the numerical calculation. In Fig. 6 we plot $\langle m_z(0)\, m_z(t)\rangle / \langle m_z^2\rangle$ versus t/τ and compare it to results derived for the Ising model. Since the temperatures used are not close to T_c there is only an insignificant difference of the susceptibility in the Heisenberg model[47] $\chi_0 = 0.97(1 - T_c/T)^{-1.37}$ and the Ising susceptibility (14b). Nevertheless, the differences in the time dependence are larger, although the general behavior is similar. In Fig. 7 some correlation functions $\langle S_0^z S_{\mathbf{R}}^z(t)\rangle$ are plotted as functions of the reduced time for the temperatures $T_c/T = 0.75$ and 0.52. The transition probability (16b) was used for this plot and for Fig. 6, but one can argue—as was done in the case of the Ising model—that the dynamics differ only by some less interesting renormalization of the time scale.

4. DERIVATION OF ERROR ESTIMATES FROM A DYNAMIC THEORY

Suppose one generates M configurations of an Ising lattice with N spins close to thermal equilibrium at some temperature T. The magnetization at one configuration ν of the sequence is given by $m_\nu = (1/N)\sum_{i=1}^{N} \sigma_i^{(\nu)}$ and according to Eq. (4) an estimate for $\langle m\rangle$ is given by $\bar{m} = (1/M)\sum_{\nu=1}^{M} m_\nu$. It is necessary to ask for the accuracy of this estimate. If the m_ν were asymptotically normally distributed and statistically independent of each other, the error estimate would be

$$\Delta \bar{m} \approx \{[\bar{m}^2 - (\bar{m})^2]/M\}^{1/2} \tag{19a}$$

Since subsequent configurations differ only by the value of one spin variable, they are of course not statistically independent and what usually is done is to take an average over subsequent configurations per spin. The total number of configurations per spin is $n = M/N$ and thus $\bar{m} = (1/n)\sum_{\mu=1}^{n} m_\mu$, and M in Eq. (19a) is replaced by n. In most cases subsequent configurations per spin are not yet really statistically independent, however.

Using $n' = \epsilon n$ in the average

$$\bar{m} = (1/n') \sum_{\mu'=1}^{n'} m_{\mu'}$$

one tries several $\epsilon < 1$, applies various tests of elementary statistics[28] to find the largest ϵ (of course one must have $n' \gg 1$) for which subsequent $m_{\mu'}$ are independent, and with this n' one is able to derive a meaningful error estimate

$$\Delta \bar{m} \approx \{[\bar{m}^2 - (\bar{m})^2]/n'\}^{1/2} \tag{19b}$$

If one had chosen M not large enough, however, this whole procedure would

yield ambiguous results. From the considerations of this section one cannot give any *a priori* estimate of the necessary order of magnitude of M.

This difficulty can be overcome using the dynamic interpretation given above. This approach starts by considering the variance of correlated variables[5,28]

$$\langle \delta^2 \rangle = \left\langle \left[\frac{1}{n} \sum_{\mu=1}^{n} (m_\mu - \langle m \rangle) \right]^2 \right\rangle$$

$$= \frac{1}{n^2} \left\langle \sum_{\mu=1}^{n} (m_\mu - \langle m \rangle)^2 \right\rangle + \frac{2}{n^2} \sum_{\mu_1=1}^{n} \sum_{\mu_2=\mu_1+1}^{n} (\langle m_{\mu_1} m_{\mu_2} \rangle - \langle m \rangle^2) \tag{20}$$

which has been split into an uncorrelated and a correlated part. One further gets

$$\langle \delta^2 \rangle \approx \frac{1}{n} (\langle m^2 \rangle - \langle m \rangle^2) + \frac{2}{n} \sum_{\mu=1}^{n} \left(1 - \frac{\mu}{n}\right) (\langle m_0 m_\mu \rangle - \langle m \rangle^2) \tag{21}$$

Associating now with the μth step the time $\tau_\mu = \tau\mu$, one may write for $n \gg 1$

$$\langle \delta^2 \rangle \approx \left(\frac{\tau}{\tau_n}\right) \frac{1}{N} \chi_0 \left[1 + 2 \int_0^{\tau_n} \left(1 - \frac{t}{\tau_n}\right) \frac{\langle m(0) m(t) \rangle - \langle m \rangle^2}{\langle m^2 \rangle - \langle m \rangle^2} \, dt \right] \tag{22}$$

Approximating the integrand in the sense of Eq. (15a) by the exponential $\exp(-t/\tau_0) = \exp(-t/\tau\chi_0)$, one finds ($T > T_c$)

$$\langle \delta^2 \rangle \simeq (1/nN) \chi_0 \{ 1 + 2\chi_0 [1 - (\chi_0/n)(1 - e^{-n/\chi_0})] \} \tag{23}$$

A reasonable estimate for $\langle m \rangle$ and the error $\Delta m = |\langle m \rangle - \bar{m}|$ will be found from the numerical calculation only if

$$\tau_n/\tau_0 \gg 1 \qquad \text{or} \qquad n \gg \chi_0 \tag{24}$$

[note that in this limit $\overline{m(0)\, m(t)}$ can be replaced by $\langle m(0)\, m(t) \rangle$; cf. Eqs. (21) and (22)].

But if Eq. (24) is fulfilled we may also write

$$\langle \delta^2 \rangle \approx (1/nN) \chi_0 (1 + 2\chi_0) \tag{25}$$

i.e., for $\chi_0 \gg 1$ the error $\Delta \bar{m} \approx \langle \delta^2 \rangle^{1/2}$ increases like the susceptibility itself!

Equations (24) and (25) exhibit very clearly the critical behavior of the error for large systems (and are still optimistic, since we have identified τ_m [cf. Eq. (15b)] which follows from Eq. (22) with τ_0, although $\tau_m > \tau_0$ is possible). If the system is very small, the critical anomaly of χ_0 is rounded off[14,20,22,46] and the error behaves in a less critical way. Because of the various approximations, Eq. (25) is a very crude estimate only. Nevertheless, it gives

a feeling for the accuracy which can be obtained and the number of MC steps per spins n which is necessary. If Eq. (24) is not fulfilled, any estimate $\bar{m}$ is certainly highly unreliable; e.g., in a two-dimensional Ising magnet with $N \cong 10^4$, $1 - T_c/T \approx 3 \times 10^2$, we see that $n > 10^4$ is necessary (as also observed "experimentally" in this situation[15] and then the error, according to Eq. (25) is still several per cent, which is consistent with the actual observation.[48] In three-dimensional systems the situation is somewhat more favorable because of the smaller value of the exponent γ and indeed smaller values of n have been sufficient to reach a good accuracy[10,11,14,16] Equation (25) has been used by the authors in a recent investigation of the Heisenberg magnet in an external field H to explain the behavior of the error as function of n, T_c/T, and H/J.[10] A similar treatment as the one sketched in Eqs. (20)–(25) for the magnetization $\langle m \rangle$ applies to other quantities also, e.g., the internal energy $\langle E \rangle$.

It is also necessary to pay some attention to the question of the extent to which the probability distributions $p(m)$, $p(E)$, etc. may be approximated as being Gaussians. This problem can of course be investigated easily by the MC method itself; e.g., in Fig. 8 we plot $p(E_i)$ for the Heisenberg model at various temperatures.[11] In the tails of this distribution there is considerable

[10] Reference 21b, Table II. Although in this case the situation is more complicated due to the boundary conditions used, the agreement between observed and calculated error estimates is satisfactory.

[11] E_i is the local energy at a lattice site [cf. Eq. (16)].

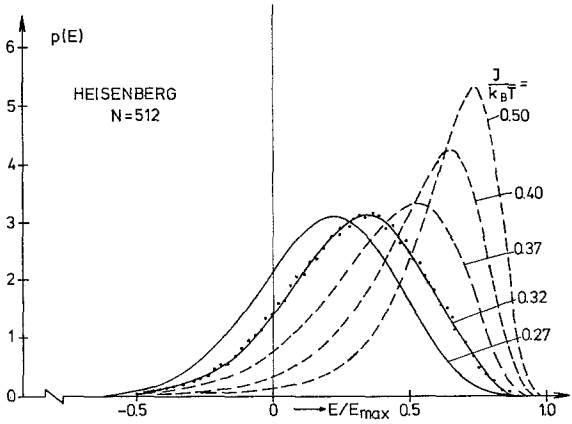

Fig. 8. Probability distribution of the energy $p(E_i)$ versus $E_i/E_{\max}$ for the classical Heisenberg model. Parameter of the curves is the reciprocal temperature J/k_BT. Paramagnetic temperatures correspond to full and ferromagnetic temperatures to broken curves.

asymmetry for $T < T_c$, and this property is even more pronounced for $p(m_i)$ [curves for $p(m_{i_1})$ for $T \ll T_c$ look similar to the curves $p(E_i)$ for E_i, $m > 0$, but are symmetric, $p(m_i) = p(-m_i)$].

Such functions are of interest not only concerning questions of accuracy, but also because $p(m_i)$ is directly accessible to experiment, by analyzing the line shape in ESR and NMR techniques.[49] From Fig. 8 we conclude that the shape of the probability distribution is of minor importance in our case compared to the other approximations necessary to derive Eq. (25). We conclude this section by suggesting that any forthcoming MC work should have selected time correlations and probability distributions as an output, to be sure of a better understanding of all the accuracy problems, thus making it possible to avoid mistakes and counter criticisms such as contained in Refs. 39 and 46.[12]

5. RELATIONS BETWEEN THE TRANSITION PROBABILITIES AND THE DYNAMIC PROPERTIES OF THE MODEL SYSTEM

The critical behavior of the error discussed in the previous section is a serious limitation for numerical applications, of course. It has been suggested[5] that suitable other choices of the transition probability could remove, or at least reduce, this unconvenient behavior. We study this problem now from the dynamic point of view. Generalizing Eq. (7c), we write

$$W(\sigma_i \to -\sigma_i) = W_1(\sigma_i \to -\sigma_i) \cdot g(\{\sigma_j\}) \tag{26}$$

where $g(\{\sigma_j\})$ may depend on any spins except the spin at the lattice site i itself. Then the detailed balance condition (5b) is still fulfilled. If we make the mean field approximation, the master equation reads

$$\tau(d/dt)\langle\sigma_i(t)\rangle = -g(\{\langle\sigma_j\rangle\})[\langle\sigma_i\rangle + \tanh\langle(E_i\rangle/k_B T)] \tag{27}$$

Far from thermal equilibrium the dynamics following from Eq. (27) is completely different from the dynamics contained in Eq. (9c). But if one is only interested in the equilibrium response functions, a treatment similar to Eqs. (10) and (11) leads to a result closely corresponding to Eq. (12b):

$$\chi(\mathbf{q}, \omega) = \frac{N(g\mu_B/2)^2}{k_B T} \frac{\chi_q}{1 + i\omega\tau_q'} \tag{28}$$

with $\tau_q' = \tau_q/g(\langle\sigma\rangle)$, i.e., the only change that has been achieved in the

[12] Reference 46, footnote 20.

dynamic susceptibility is a renormalization of the time scale! It is interesting to investigate to what extent this result holds more generally. We consider a special situation only, where $g(\{\sigma_j\}) = g'(E_i/k_BT)$ is an arbitrary function of the nearest environment of σ_i only,[13] and, more severely, restrict ourselves to the one-dimensional chain. Although the possibility of an exact solution[31] of the general master equation is restricted[34] to the trivial choice $g'(E_i/k_BT) =$ const in Eq. (26), we can still derive a result similar to Eq. (28). We may require that the whole behavior of the system remains unchanged if we change the sign of the magnetic field $\delta H_i(t)$ and those of all spins of the system. Thus we have $g'(E_i/k_BT) = g'(-E_i/k_BT)$.[14] Expanding $g'(E_i/k_BT)$ in powers of E_i and making use of $\sigma_j^2 = 1$ and its consequence

$$(\sigma_{i+1} + \sigma_{i-1})^{2r} = 2^{2r-1}(1 + \sigma_{i-1}\sigma_{i+1}) \tag{29}$$

together with $\delta H_i'(t) = g\mu_B\, \delta H_i(t)/2k_BT$, we obtain the most general form of $g'(E_i/k_BT)$ [Eq. (10) with $H = 0$, and Eq. (29)]:

$$\begin{aligned} g'(E_i/k_BT) = {} & g_0(J/k_BT) + g_1(J/k_BT)\, \delta H_i'(t)(\sigma_{i+1} + \sigma_{i-1}) \\ & + g_2(J/k_BT)(\sigma_{i+1}\sigma_{i-1}) \end{aligned} \tag{30}$$

In the same way one finds for $\tanh(E_i/k_BT)$[30–34]

$$\begin{aligned} \tanh\left(\frac{-E_i}{k_BT}\right) = {} & \frac{1}{2}\left[\tanh\left(\frac{2J}{k_BT}\right)\right](\sigma_{i+1} + \sigma_{i-1}) \\ & + \delta H_i'(t)\left\{1 - \frac{1}{2}\left[\tanh^2\left(\frac{2J}{k_BT}\right)\right](1 + \sigma_{i+1}\sigma_{i-1})\right\} \end{aligned} \tag{31}$$

For a linear response theory it is necessary to keep terms linear in $\delta H_i'(t)$ in Eqs. (30) and (31) only. Introducing the abbreviations

$$\gamma = \tanh(2J/k_BT) \qquad \text{and} \qquad v = \tanh(J/k_BT)$$

and using the property[1,30]

$$\langle \sigma_i \sigma_{i+j} \rangle_{eq} = v^{|j|} \tag{32}$$

the master equation reduces to [$\gamma = 2v/(1 + v^2)$]

$$\begin{aligned} \tau(d/dt)\langle \sigma_i(t) \rangle = {} & -g_0\langle \sigma_i \rangle - g_2\langle \sigma_{i-1}\sigma_i\sigma_{i+1} \rangle + (g_0 + g_2)(\gamma/2)(\langle \sigma_{i+1} \rangle + \langle \sigma_{i-1} \rangle) \\ & + \delta H_i'(t)[\, g_0(1 - \gamma v) + g_2(v^2 - \gamma v)] \end{aligned} \tag{33}$$

[13] This still covers the possibilities (7a)–(7c) and is of practical interest in comparing usual MC work with the kinetic Ising model theories.[30–34]

[14] See footnote 13.

where we were allowed to replace the coefficients of $\delta H_i'(t)$ by their equilibrium values since we are only interested in the *linear* response. To remove the three-spin correlation function from Eq. (33), we make use of the expansions

$$\langle \sigma_{i-1}\sigma_i\sigma_{i+1}\rangle = \sum_{k=-\infty}^{+\infty} \delta H_k'(t)\langle \sigma_k\sigma_{i-1}\sigma_i\sigma_{i+1}\rangle_{\text{eq}} \tag{34a}$$

and

$$\langle \sigma_i\rangle = \sum_{k=-\infty}^{+\infty} \delta H_k'(t)\langle \sigma_k\sigma_i\rangle_{\text{eq}} = \sum_{l=-\infty}^{+\infty} \delta H_{l+i}'(t)\, v^{|l|} \tag{34b}$$

together with the factorization property[50]

$$\langle \sigma_{i1}\sigma_{i2}\sigma_{i3}\sigma_{i4}\rangle = \langle \sigma_{i1}\sigma_{i2}\rangle_{\text{eq}}\langle \sigma_{i3}\sigma_{i4}\rangle_{\text{eq}}\,, \qquad i_1 \leqslant i_2 \leqslant i_3 \leqslant i_4 \tag{35}$$

to derive the formula

$$\langle \sigma_{i-1}\sigma_i\sigma_{i+1}\rangle = \langle \sigma_i\rangle - \delta H_i'(t)(1 - v^2) \tag{36}$$

According to Eqs. (33) and (36), the master equation is simply

$$\tau \frac{d}{dt}\langle \sigma_i(t)\rangle = -\left[g_0\left(\frac{J}{k_{\text{B}}T}\right) + g_2\left(\frac{J}{k_{\text{B}}T}\right)\right] \times \left\{\langle \sigma_i\rangle - \frac{\gamma}{2}\left(\langle \sigma_{i-1}\rangle + \langle \sigma_{i+1}\rangle\right) - \delta H_i'(t)(1 - \gamma v)\right\} \tag{37}$$

Thus also in this case the only change of the dynamics is that the time scale is renormalized by a factor $(g_0 + g_2)^{-1}$ with arbitrary temperature dependence. This fact constitutes an exact proof that the equilibrium response function $\chi(\mathbf{q}, \omega)$ found by Glauber[31] is the same for arbitrary choices of $g'(E_i/k_{\text{B}}T)$ apart from the frequency scale. We have made extensive use of the knowledge one has about the static equilibrium multi-spin-correlations of the Ising chain to derive the main result of this section, Eq. (37). Its extension to higher dimensionality therefore does not seem very straightforward; the numerical results presented in Section 3 and the mean field approximation [Eq. (28)] would be consistent with such an extension. It is to be noted that a renormalization of the time scale in comparison with the scale of Monte Carlo steps per spin could indeed be helpful for the numerical work.

6. CONCLUSIONS

In this paper we have described the Monte Carlo process for computing averages for Ising and classical Heisenberg systems in terms of the appropriate

master equations, and the appropriate dynamic correlations and susceptibilities. An extension of this description [Eq. (6a)] to other model systems is straightforward. The MC calculation readily yields information about the dynamic properties of the system. A comparison of the dynamic correlations with mean field predictions showed that this approximation seems to yield rather reasonable results, contrary to the situation in usual "nonstochastic" Heisenberg magnets. We stress the fact that the dynamics of these stochastic models are not characteristic of the Hamiltonian governing the equilibrium properties, but are mainly determined by the properties of the simple stochastic process producing new configurations: A single spin-change stochastic Heisenberg model has no quantities conserved and its dynamic properties are very similar to the single spin-flip Ising model, while a higher spin-flip Ising model with energy and magnetization conservation can have dynamic properties more similar to the usual Heisenberg magnet.

We further have given a dynamic interpretation of the "statistical errors" in the MC method, and have related them to a simple model of critical relaxation. We have shown how one can estimate in this case the number of configurations necessary to reach a given accuracy. The influence of the various kinds of transition probabilities on the dynamic behavior have also been discussed. While these probabilities lead to entirely different dynamic properties far from the thermal equilibrium, they lead only to a renormalization of the time (or frequency) scale near the thermal equilibrium—at least if one is not too close to a critical point of the system. For a fairly general class of transition probabilities it is proven that this scaling property holds exactly for the one-dimensional kinetic Ising model.

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REFERENCES

1. E. Ising, *Z. Physik* **31**:253 (1925).
2. L. Onsager, *Phys. Rev.* **65**:117 (1944); C. N. Yang, *Phys. Rev.* **85**:809 (1952).
3. M. E. Fisher, *Am. J. Phys.* **32**:343 (1964).
4. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**:1087 (1953).
5. L. D. Fosdick, in *Methods of Computational Physics*, Vol. 1, Academic, New York (1963), p. 245; and references contained therein.

6. W. W. Wood, in *Physics of Simple Liquids*, H. N. V. Temperley, J. S. Rowlinson, and G. S. Rushbrooke, eds., North-Holland Publ. Co., Amsterdam (1968), Chapter 5.
7. K. Binder and D. Stauffer, *J. Stat. Phys.* **6**:49 (1972).
8. E. Stoll, K. Binder, and T. Schneider, *Phys. Rev.* **B6**:2777 (1972).
9. P. A. Lebwohl and G. Lasher, *Phys. Rev.* **A6**:426 (1972).
10. E. A. Harris, *Phys. Rev. Lett.* **13**:158 (1964).
11. K. Binder and H. Rauch, *Phys. Lett.* **27A**:247 (1968); K. Binder and H. Rauch, *Z. Physik* **219**:201 (1969).
12. N. Ogita, A. Ueda, T. Matsubara, H. Matsuda, and F. Yonezawa, *J. Phys. Soc. (Japan)* **26**:Suppl. 146 (1969).
13. D. P. Landau, *Phys. Rev. Lett.* **28**:449 (1972); *J. Appl. Phys.* **42**:1284 (1971).
14. K. Binder, *Ber. Bunsenges. Physikal. Chem.* **76**:201 (1972); *Physica* **62**:508 (1972).
15. E. Stoll and T. Schneider, *Phys. Rev.* **A6**:429 (1972).
16. R. E. Watson, M. Blume, and G. H. Vineyard, *Phys. Rev.* **181**:811 (1969).
17. R. E. Watson, M. Blume, and G. H. Vineyard, *Phys. Rev. B***2**:684 (1970).
18. K. Binder, *Phys. Lett.* **30A**:273 (1969); *Z. Angew. Phys.* **30**:51 (1970).
19. K. Binder, H. Rauch, and V. Wildpaner, *J. Phys. Chem. Solids* **31**:391 (1970).
20. K. Binder, *Phys. Stat. Sol.* **46**(b):567 (1971).
21a. H. Müller-Krumbhaar and K. Binder, *Z. Phys.* **254**:269 (1972).
21b. K. Binder and H. Müller-Krumbhaar, *Phys. Rev.* **B7**:3297 (1973).
22. V. Wildpaner, K. Binder, and H. Rauch, *J. Phys. Chem. Solids*, to be published.
23. M. Blume, *Phys. Rev.* **141**:517 (1966).
24. H. W. Capel, *Physica* **32**:966 (1966).
25. D. P. Landau, preprint.
26. D. C. Handscomb, *Proc. Cambr. Phil. Soc.* **58**:594 (1962); **60**:115 (1964).
27. R. Friedberg and J. E. Cameron, *J. Chem. Phys.* **52**:6049 (1970).
28. W. Feller, *Introduction to Probability Theory and its Application*, New York (1966).
29. Yu. Ya. Gotlib, *Soviet Phys.—Solid State* **3**:1574 (1962).
30. R. J. Glauber, *J. Math. Phys.* **4**:294 (1963).
31. M. Suzuki and R. Kubo, *J. Phys. Soc. (Japan)* **24**:51 (1968).
32. M. Suzuki, H. Ikari, and R. Kubo, *J. Phys. Soc (Japan)* **26**: Suppl. 153 (1969); H. Yahata and M. Suzuki, *J. Phys. Soc. (Japan)* **27**:1421 (1969); H. Yahata, *J. Phys. Soc. (Japan)* **30**:657 (1971).
33. B. U. Felderhof, *Rep. Math. Phys.* **1**:215 (1971); **2**:151 (1971); B. U. Felderhof and M. Suzuki, *Physica* **56**:43 (1971); B. V. Felderhof, *J. Stat. Phys.* **6**:21 (1972).
34. K. Kawasaki, in *Phase Transitions and Critical Phenomena*, Vol. 2, Academic, London and New York (1972), p. 443; and references contained therein.
35. W. Matthes, *J. Comp. Phys.* **6**:157 (1970).
36. E. Stoll, K. Binder, and T. Schneider, *Phys. Rev.* **B**, to be published.
37. J. M. Hammersley and D. C. Handscomb, *Monte Carlo Methods*, Methuen, London (1964).
38. I. Z. Fisher, *Soviet Phys.—Uspekhi* **2**:783 (1960).
39. Z. Alexandrowicz, *J. Stat. Phys.* **5**:19 (1972); *J. Chem. Phys.* **55**:2765 (1971); **55**:2780 (1971).
40. K. Kawasaki, *Phys. Rev.* **145**:224 (1966); **148**:375 (1966); **150**:285 (1966).
41. L. P. Kadanoff and J. Swift, *Phys. Rev.* **165**:310 (1968).
42. B. Alder and T. Wainwright, *J. Chem. Phys.* **27**:1208 (1957).
43. B. Alder, in *Physics of Simple Liquids*, H. N. V. Temperley, J. S. Rowlinson, and G. S. Rushbrooke, eds., North-Holland, Amsterdam, (1968); L. Verlet, *Phys. Rev.* **159**:98 (1967).

44. M. E. Fisher, *Rept. Progr. Phys.* **30**:615 (1967); L. P. Kadanoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. V. Palciauskas, M. Rayl, J. Swift, D. Aspnes, and J. Kane, *Rev. Mod. Phys.* **39**:385 (1967); H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena*, Oxford Univ. Press (1971).
45. M. E. Fisher and R. J. Burford, *Phys. Rev.* **156**:583 (1967).
46. M. E. Fisher and A. E. Ferdinand, *Phys. Rev. Letters* **19**:169 (1967); A. E. Ferdinand and M. E. Fisher, *Phys. Rev.* **185**:832 (1969).
47. D. S. Ritchie and M. E. Fisher, *Phys. Rev.* **B5**:2668 (1972).
48. E. Stoll, private communication.
49. K. A. Müller and W. Berlinger, *Phys. Rev. Letters* **29**:539 (1972).
50. D. Bedeaux, K. E. Shuler, and I. Oppenheim, *J. Stat. Phys.* **2**:1 (1970).