Digital dynamics and the simulation of magnetic systems

M. Y. Choi
Department of Applied Physics, Stanford University, Stanford, California 94305

B. A. Huberman
Xerox Palo Alto Research Center, Palo Alto, California 94304
(Received 25 April 1983)

This paper investigates the problems associated with simulating many-body systems with finite-state machines such as computers. It is shown that the digital (discrete) character of time brings in features which are not encountered in the usual analytical studies using continuous time. This is illustrated with a thorough study of the dynamics of simple magnetic systems with competing interactions. Whereas continuous dynamics, as derived from the usual master-equation approach, yields asymptotic behavior which is time independent, dynamics in digital time can lead to complex behavior characterized by the existence of multiple basins of attraction, broken symmetries, oscillations, and chaos. These results might provide a dynamical explanation for the breakdown of ergodicity which has been reported in Monte Carlo studies of spin-glasses.

I. INTRODUCTION

The emergence of powerful computing machines has led to the exciting possibility that a number of complex problems, which only a few years ago refused to yield any answers, might be finally understood on a quantitative basis. Large-scale computer simulations are becoming a familiar tool in the study and understanding of the behavior of stressed fluids, chemical reactions, and complex economic organizations, to cite just a few examples. Moreover, Monte Carlo methods have allowed for the study of spin systems of relevance to both condensed-matter physics and elementary-particle theory, and they hold promise of providing realistic insights into kinetic processes such as nucleation and pattern formation.[1]

Besides providing clues to the understanding of complex systems, computer simulations are also assumed to give answers which do not differ in a marked way from the ones one would find by performing experiments on real systems or by solving the differential equation embodying a particular law of nature. Insofar as nature can be thought of as an analog computer integrating a particular equation with given boundary conditions, it would seem that the advantage provided by fast digital machines is one of flexibility (i.e., varying coupling constants or boundary conditions) and ease of observing behavior as parameters are changed.

There are differences, however, between the way a system is simulated by a digital machine and the way it is studied in real experiments or analyzed by solving the differential equations describing its behavior. A very important, if seldom acknowledged, difference is that in a computer, time can only be implemented by discrete processes which correspond to steps of a program. This peculiar digital character of time can in turn have serious consequences in the dynamical behavior of the system simulated and lead to results that might have little resemblance to the real process being studied.

This paper investigates the problems associated with simulating many-body systems with finite-state machines such as computers. It is shown that the digital (discrete) character of time brings in features which are not encountered in the usual analytical studies using continuous time. This is illustrated with a thorough study of the dynamics of simple magnetic systems with competing interactions. Whereas continuous dynamics, as derived from the usual master-equation approach, yields asymptotic behavior which is time independent, dynamics in digital time can lead to complex behavior characterized by the existence of multiple basins of attraction, broken symmetries, oscillations, and chaos. These results might provide a dynamical explanation for the breakdown of ergodicity which has been reported in Monte Carlo studies of spin-glasses.[2-6] A similar picture appears in numerical analysis when algorithms are used for parameter values beyond their range of validity.

This paper consists of five sections and an appendix. Section II deals with the digital dynamics of Ising systems with competing interactions. After obtaining exact results for the time evolution of expectation values, local-field corrections are used to obtain recursion relations for the magnetization and susceptibilities. Section III analyzes the global behavior of the magnetization and susceptibility as a function of coupling constants and shows the existence of broken symmetries and many basins of attraction. Furthermore, it is shown that for systems with competing interactions, the asymptotic behavior of expectation values can have complicated dynamics such as periodic cycles and strange attractors. This in turn implies a breakdown of ergodicity and chaotic behavior, implying that computer simulations of such systems would not converge to meaningful static values of the observables. These results seem to be consistent with reports of lack of convergence in Monte Carlo simulations of spin-glasses. Section IV analyzes the continuum limit in the context of finite-state machines and shows the effective differential form of the master equation that one obtains. Section V summarizes the results obtained and comments on their applicability to Monte Carlo experiments. An appendix provides a derivation of linear-response theory in discrete time, and shows the existence of asymptotic time dependence in the susceptibilities for the case of static external fields.

II. DISCRETE DYNAMICS

A. Exact results

Consider an Ising spin system with both ferromagnetic and antiferromagnetic interactions, and in the presence of an external magnetic field, h_i, acting on each site i. The Hamiltonian of the system is then given by

$$H=-\sum_{i,j} J_{ij}\vec{s}_i\cdot\vec{s}_j-\sum_j h_i s_i \;, \tag{2.1}$$

where the interaction term has the form

$$J_{ij}=\begin{cases} J_1 & \text{for } p \text{ neighbors} \\ -J_2 & \text{for } r \text{ neighbors} \end{cases} \tag{2.2}$$

with both J_1 and J_2 positive, but not necessarily equal, and the summation extends over all $z=p+r$ neighbor spins.

The probability $P(s_1,s_2,\ldots,s_N,t)$ that the system is in a given state, $(s_1,\ldots,s_N)$, at time t evolves in time according to the master equation

$$P(s_1,\ldots,s_N,t+\tau)-P(s_1,\ldots,s_N,t)=-\sum_k [\omega_k(s_k)P(s_1,\ldots,s_N,t)-\omega_k(-s_k)P(s_1,\ldots,s_{k-1},-s_k,s_{k+1},\ldots,s_N,t)] \;, \tag{2.3}$$

where τ is the basic time step, and $\omega_k(s_k)$ the probability that the kth spin flips its configuration in time τ. Following the standard convention we will assume that $\omega_k(s_k)$ is given by

$$\omega_k(s_k)=\tfrac{1}{2}[1-s_k\tanh(\beta E_k)] \;, \tag{2.4}$$

with $\beta\equiv(k_BT)^{-1}$, k_B the Boltzmann constant, and

$$E_k\equiv\sum_l J_{kl}s_l+h_k \;. \tag{2.5}$$

This choice of transition probability not only satisfies the principle of detailed balance, but also produces the correct equilibrium relation for the probabilities determined by Eq. (2.3). Moreover, this transition rate is thought not to differ substantially from that used in Monte Carlo simulations of Ising spin systems.[7]

The quantity of interest is the magnetization of the system at time t, $\langle s_j\rangle_t$, which is given by

$$\langle s_j\rangle\equiv\sum_{\{s\}} s_jP(s_1,\ldots,s_N,t) \tag{2.6}$$

and where the sum extends over all possible spin configurations at time t. With the use of Eq. (2.3), the following equation of motion is obtained:

$$\langle s_j\rangle_{t+\tau}-\langle s_j\rangle_t=-2\langle s_j\omega_j(s_j)\rangle_t \;, \tag{2.7}$$

which, for the particular choice of transition rates given by Eq. (2.4), becomes

$$\langle s_j\rangle_{t+\tau}=\langle\tanh(\beta E_j)\rangle_t \;, \tag{2.8}$$

an exact equation which in equilibrium (i.e., no time dependence[8]) produces the standard known result of statistical mechanics of Ising systems.[9,10]

The approach described above can also be used to evaluate the time evolution of the magnetic susceptibility, a quantity of direct relevance to experiments and Monte Carlo simulations. Assume the existence of a time-independent external field h_i acting on each ith spin: Then the time-dependent susceptibility is defined as

$$\chi_{ij}(t)\equiv\left.\frac{\partial\langle s_j\rangle_t}{\partial h_i}\right|_{h=0} \;, \tag{2.9}$$

which, with the help of Eq. (2.8) becomes

$$\chi_{ij}(t+\tau)=\left.\frac{\partial\langle\tanh\beta E_j\rangle_t}{\partial h_i}\right|_{h=0} \;, \tag{2.10}$$

a result that can also be obtained from linear-response theory. Its digital-time version is developed in the Appendix.

B. Local-field corrections

Equations (2.8) and (2.10) provide an exact description of the discrete dynamics of a general magnetic system with both ferromagnetic and antiferromagnetic interactions. Since the ensemble averages entering their right-hand sides cannot be calculated exactly, an approximate scheme is necessary in order to evaluate them. The simplest such approach is the Weiss molecular-field approximation, in which E_j is replaced by an effective local field h_j^m, such that

$$h_j^m\equiv\langle E_j\rangle=\sum_k J_{jk}m_k+h_j \;,$$

where $m_k\equiv\langle s_k\rangle$. For systems with competing interactions, however, this approximation fails to give behavior consistent with thermodynamics and an improved local-field correction is necessary. In what follows, we will use the scheme proposed by Brout and Thomas,[11] in which E_j is replaced by

$$h_j^{\text{eff}}=\sum_k J_{jk}m_k-\sum_k J_{jk}^2\tilde{\chi}_{kk}m_j+h_j \;, \tag{2.12}$$

where $\tilde{\chi}_{kk}$ represents the response of spin k to the average magnetization at site j ($\neq k$), and it is given by

$$\tilde{\chi}_{kk} = \frac{\partial m_k}{\partial (J_{kj} m_j)} . \tag{2.13}$$

This equation has also been used by Thouless, Anderson, and Palmer[12] in their study of spin-glasses with infinite-range interactions.

With the use of the fact that, to first order,

$$\frac{\partial h_k^{\text{eff}}}{\partial (J_{kj} m_j)} = \frac{\partial}{\partial (J_{kj} m_j)} \left[\sum_l J_{kl} m_l - \sum_l J_{kl}^2 \tilde{\chi}_{ll} m_k + h_k \right] = 1 , \tag{2.14}$$

Eq. (2.13) can be written as

$$\tilde{\chi}_{kk} = \frac{\partial m_k}{\partial h_k^{\text{eff}}} . \tag{2.15}$$

We are now in a position to evaluate the dynamics of both the magnetization and susceptibility. Replacing E_j in Eq. (2.8) by the effective field given by Eq. (2.12), we obtain

$$m_j(t+\tau) = \tanh \left[\beta \left[\sum_k J_{jk} m_k(t) - \sum_k J_{jk}^2 \tilde{\chi}_{kk}(t) m_j(t) + h_j \right] \right] , \tag{2.16}$$

where it has been assumed that the magnetization at site j at time t is determined by the effective field produced a time step earlier [i.e., $h_j^{\text{eff}}(t-\tau)$] and that therefore

$$\tilde{\chi}_{kk}(t) = \frac{\partial m_k(t)}{\partial h_k^{\text{eff}}(t-\tau)} , \tag{2.17}$$

or equivalently, using Eq. (2.12),

$$\tilde{\chi}_{kk} = \beta [1 - m_k^2(t)]_{h=0} , \tag{2.18}$$

which gives the quantity evaluated in several Monte Carlo simulations of magnetic systems with competing interactions.[3,4]

The equation for the time evolution of the susceptibility can also be obtained in a similar fashion. With the use of the same local-field corrections as above, Eq. (2.10) becomes

$$\chi_{ij}(t+\tau) = \left. \frac{\partial m_j(t+\tau)}{\partial h_i} \right|_{h=0} , \tag{2.19}$$

which can be written with the help of Eq. (2.16) as

$$\chi_{ij}(t+\tau) = \beta [1 - m_j^2(t+\tau)] \left. \left[\sum_k J_{jk} \chi_{ik}(t) - \sum_k J_{jk}^2 \tilde{\chi}_{kk}(t) \chi_{ij}(t) + \delta_{ij} \right] \right|_{h=0} . \tag{2.20}$$

The results of this section then show that in the absence of an external field, the magnetization and susceptibilities behave in time according to the equations

$$m_j(t+\tau) = \tanh \left[\beta \left[\sum_k J_{jk} m_k(t) - \beta \sum_k J_{jk}^2 [1 - m_k^2(t)] m_j(t) \right] \right] , \tag{2.21a}$$

$$\begin{aligned} \tilde{\chi}_{jj}(t+\tau) &= \beta [1 - m_j^2(t+\tau)] , \\ \chi_{ij}(t+\tau) &= \tilde{\chi}_{jj}(t+\tau) \left[\sum_k J_{jk} \chi_{ik}(t) - \beta \sum_k J_{jk}^2 [1 - m_k^2(t)] \chi_{ij}(t) + \delta_{ij} \right] . \end{aligned} \tag{2.21b}$$

In what follows, we will study the global behavior of their solutions as a function of both the strength of competing interactions and initial conditions.

III. RESULTS

In the previous section, we derived equations which determine the time evolution of the magnetization and susceptibilities. We will now study the global behavior of their solutions as a function of both the interaction strength and the amount of competition present in the system.

In order to obtain the basic features of the spin dynamics in our system, we will assume that any given spin has the same amount of nearest neighbors and ferromagnetic and antiferromagnetic couplings.[13] This in turn implies that one can write $m_i = m$ and

$$\sum_k J_{kj} = pJ_1 - rJ_2 \equiv J , \tag{3.1}$$

with p the number of ferromagnetic neighbors; J_1 is their strength, and r is the number of antiferromagnetic neighbors with strength J_2. Similarly

$$\sum_k J_{kj}^2 = pJ_1^2 + rJ_2^2 \equiv J'^2 . \tag{3.2}$$

Equations (2.21) then become

$$m_i(t+\tau) = \tanh[(\tilde{J} - \tilde{J}'^2)m_i(t) + \tilde{J}'^2 m_i^3(t)] , \tag{3.3a}$$

$$\tilde{\chi}_{ii}(t+\tau) = 1 - m_i^2(t+\tau) , \tag{3.3b}$$

and

$$\chi_{ii}(t+\tau) = \tilde{\chi}_{ii}(t+\tau)[1 - \tilde{J}'^2\chi_{ii}(t) + \tilde{J}'^2\chi_{ii}(t)m_i^2(t)] , \tag{3.3c}$$

where we have defined

$$\tilde{J} = \beta J, \quad \tilde{J}'^2 = \beta^2 J'^2 , \tag{3.4}$$

and have assumed $J_{ij}\chi_{ii} \ll 1$ in deriving Eq. (3.3c).

Since Eq. (3.3a) is independent of the susceptibility values, we start by analyzing its behavior as a function of the renormalized constants. Consider a system with pure ferromagnetic couplings. In that case, any initial spin configuration relaxes to a simple fixed point which is approximately given by the solution of Eq. (3.3a) with $\tau = 0$, in agreement with earlier studies of Ising systems using continuum dynamics.[14]

As the number of antiferromagnetic bonds is increased even further, new fixed points appear in the dynamics of the system. Starting with a small antiferromagnetic interaction, a new stable fixed point is first encountered. In this case, regardless of the initial spin configuration, the long-time behavior corresponds to a time-independent solution with $m_i = 0$. As the relative strength of the antiferromagnetic interaction is further increased, the solutions of Eq. (3.3a) undergo a bifurcation into asymptotic oscillations such that the average magnetization flips its value from plus to minus periodically at every time step. However, since the values at each instant of time are symmetric about the origin, a time-averaged measurement of the magnetization in this range would produce a zero value.

As the number and strength of both the ferromagnetic and antiferromagnetic couplings is further increased while keeping their difference constant, new fixed points and basins of attraction appear in the dynamics of the system. The existence of different attractors implies that the long-term behavior of magnetic systems with competing interactions, can, when simulated by digital machines, become time dependent and complicated. Furthermore, multiple basins of attraction will make the solutions reach asymptotic values which strongly depend on initial conditions. In what follows, we will describe some of the important dynamical features that are encountered in a magnetic system both as a function of the amount of competition and temperature.

Figure 1 gives a description of the possible asymptotic regimes to be encountered in a magnetic system with $\tilde{J} = 2$ as a function of the total strength $\tilde{J}'^2 = rJ_1^2 + pJ_2^2$, with initial conditions for each value of $\tilde{J}'^2$ set at $m = 0.6$. As $\tilde{J}'^2$ is increased past the point A, a new attractor appears such that the long-time behavior corresponds to a simple fixed point with zero magnetization. A further increase in $\tilde{J}'^2$ produces a bifurcation into a periodic cycle such that the magnetization reverses itself in every cycle, while giving an average value equal to zero.

At $\tilde{J}'^2 = B$, an interesting symmetry-breaking process takes place. Beyond this point, the asymptotic magnetization still reverses itself every time step, but with an asymmetry which produces a nonzero average value. This phenomenon is associated with the appearance of two basins of attraction for the solutions of Eq. (3.3a). Each of these basins traps all solutions started with either a positive or negative magnetization, respectively. (If an initial configuration with negative m were chosen, the broken symmetry state would correspond to a negative average value of m.) For still higher values of $\tilde{J}'^2$, each basin of attraction bifurcates into new periodic states, yielding a finite average magnetization whose actual magnitude depends on the initial value of m. A further increase in $\tilde{J}'^2$ produces new dynamical behavior such that initial configurations can now be trapped into strange attractors.

In this regime, the asymptotic behavior of the magnetization is chaotic, and its average can become either zero or nonzero, depending on initial conditions. Figure 2 shows its time evolution as predicted by Eq. (3.3) for $\tilde{J} = 2$, $\tilde{J}'^2 = 6$. As can be seen, the magnetization wanders in time over a large range of values without any recognizable period. For still higher values of $\tilde{J}'^2$, a variety of basins of attraction, periodic cycles, chaotic, and intermittent behavior is encountered, implying that a discrete simulation of such magnetic systems can lead to nontrivial situa-

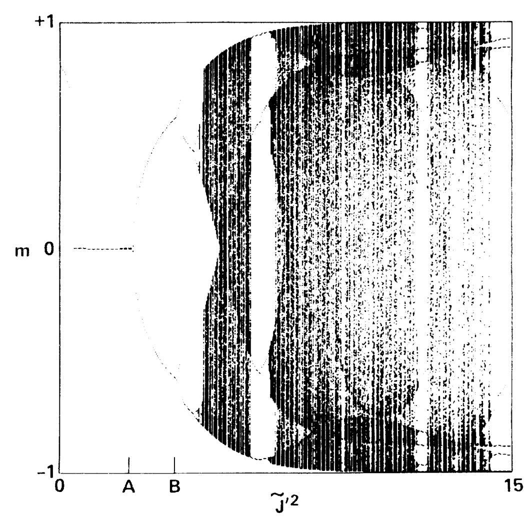

FIG. 1. Asymptotic behavior of the magnetization, as determined by Eq. (3.3a) for $\tilde{J} = 2$ as a function of $\tilde{J}'^2$. The initial configuration for each value of $\tilde{J}'^2$ is $m = 0.6$.

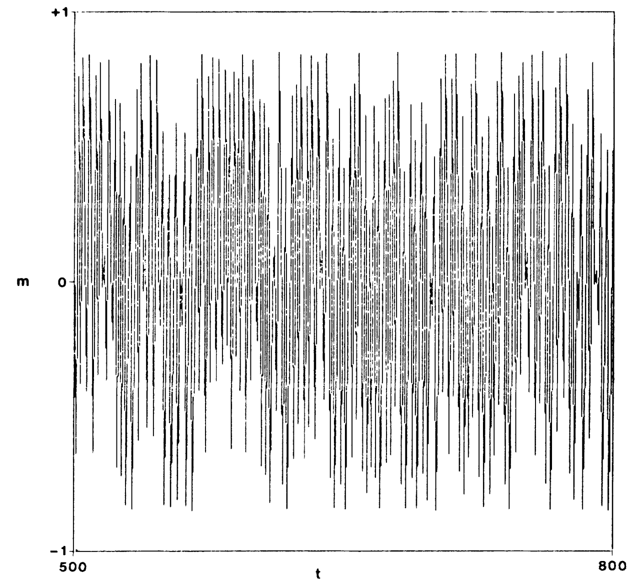

FIG. 2. The solution of Eq. (3.3a) for $\tilde{J}=2$, $\tilde{J}'^2=6$ after an initial transient of 500 steps. Notice the random macroscopic reversals in the magnetization.

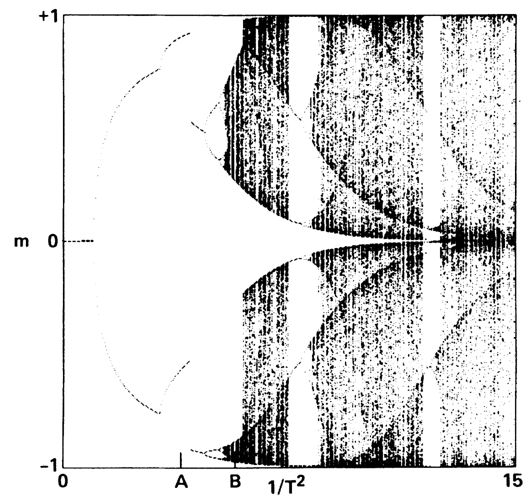

FIG. 3. Asymptotic behavior of the magnetization, for a system with equal amounts of competing interactions, as a function of T^{-2}. The initial value of the magnetization at each point is $m=0.6$.

tions with non-Gibbsian measures.

While it is beyond the scope of this paper to produce a detailed analysis of Eq. (3.3a), it is worth pointing out that in the chaotic regime one observes random switchings of the magnetization with time. Notice that this effect is obtained in the large N limit of our equations and it is therefor *not* a finite-size problem.

Another interesting scenario appears in systems with equal amounts of ferromagnetic and antiferromagnetic couplings. In this fully frustrated limit, $\tilde{J}\equiv 0$ and an increase in the value of $\tilde{J}'^2$ in Eq. (3.3a) can be regarded as a lowering of the temperature. Figure 3 shows the asymptotic behavior of the magnetization as a function of the inverse square temperature, in units of $(rJ_1^2+pJ_2^2)^{-2}$. Some of the features encountered in the previous case are still present, such as solutions with broken symmetries and chaotic behavior. In addition, one encounters a great deal of overall symmetry around the $m=0$ state, although for many values of T (see, for example, A and B) nonzero values of the average magnetization are encountered. Furthermore, the local susceptibility, as given by Eq. (3.3b), also exhibits chaotic behavior, implying lack of convergence into a time-independent fixed point (Fig. 4).

IV. THE CONTINUUM LIMIT AND FINITE-STATE MACHINES

Since the results obtained in the previous sections contain qualitative features which differ considerably from those encountered in studies of spin systems using continuum dynamics,[15–17] we will now discuss the origin of these differences, together with a detailed analysis of how the differential form of the master equation is recovered in a finite-state machine.

Consider time to be given in units of a basic time length, τ, such that $t=n\tau$ and $t+\tau=(n+1)\tau$. The master equation for the time evolution of the probability that a given configuration of the system be $\underline{\alpha}\equiv(s_1,\ldots,s_N)$ is given by

$$P(\underline{\alpha},t+\tau)-P(\underline{\alpha},t) = -\sum[\rho(\underline{\alpha}\rightarrow\underline{\beta})P(\underline{\alpha},t)-\rho(\underline{\beta}\rightarrow\underline{\alpha})P(\underline{\beta},t)] , \tag{4.1}$$

where $\rho(\underline{\alpha}\rightarrow\underline{\beta})$ denotes the probability that the system make a transition from a configuration $\underline{\alpha}$ to another configuration $\underline{\beta}$ in a unit time step τ. As shown in Sec. II, the expectation value of the jth spin at time t, $\langle s_j\rangle_t$, can be simply obtained from Eq. (4.1) yielding

$$\langle s_j\rangle_{t+\tau}-\langle s_j\rangle_t=-2\langle s_j\rho_j(s_j)\rangle_t . \tag{4.2}$$

Since the left-hand side of the equation is a finite difference, it can be written as

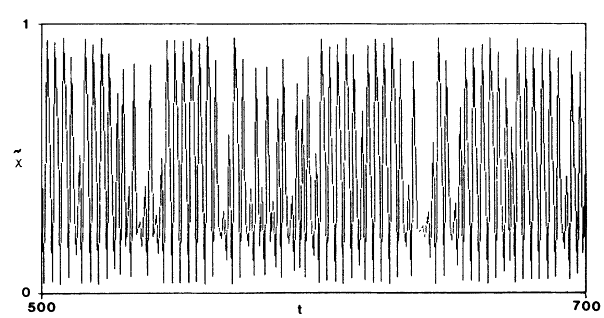

FIG. 4. The time evolution of the local susceptibility for $\tilde{J}=0$, $\tilde{J}'^2=6$ after an initial transient of 500 steps.

$$\langle s \rangle_{t+\tau} - \langle s \rangle_t = \frac{\tau d\langle s \rangle}{dt} + \frac{\tau^2}{2!}\frac{d^2\langle s \rangle}{dt^2} + \frac{\tau^3}{3!}\frac{d^3\langle s \rangle}{dt^3} + \cdots \ . \quad (4.3)$$

Moreover, if the standard assumption is made that the transition probability scales linearly with time (i.e., the golden rule) ρ can be expressed as

$$\rho = \omega\tau \ , \quad (4.4)$$

with ω the transition rate. In the limit $\tau \to 0$, Eqs. (4.2) and (4.3) then give

$$\frac{d\langle s \rangle}{dt} = -2\langle s\omega \rangle \ , \quad (4.5)$$

which is the familiar first-order differential equation that follows from the continuous version of the master equation. For a scalar expectation value, this exact equation can only produce asymptotic behavior consisting of a simple time-independent fixed point. Since, however, Eq. (4.5) obtains because of the assumptions listed above, it is worthwhile to study its validity in the context of studies using finite state machines such as computers.

As is well known, a general computation goes through a series of discrete states which are upgraded by the program at integer multiples of a unit time τ according to a set of given instructions, thus emulating the evolution of the system. It is therefore clear that a finite-state machine violates Eq. (4.4) because in time intervals shorter than τ the probability that the system changes its state is zero, while large changes can occur at the instants when the states are upgraded. Since the golden rule is no longer applicable, an infinite number of derivatives will appear in the resulting differential equation for the expectation values. This enlargement of the dimensionality of the manifold in turn allows for more complex dynamics to take place in the simulation, such as periodic cycles and strange attractors. Thus, in this limit, the results that one obtains agree with those generated by nonlinear recursion relations.

Before concluding, we should mention that, although in real magnetic systems as found in nature there is no evidence of a discrete time, there exist situations where the violation of Eq. (4.4) will lead to results similar to those obtained here. In systems where interactions are mediated via dynamic fields, retardation effects can become important. These delays, which have been shown to be able to affect the critical dynamics of spin systems,[18] will in turn produce evolution equations which are equivalent to recurrence relations with time steps of order of delay times. In such cases, competing interactions of the type discussed in this paper will be expected to produce asymptotic dynamics which can be time dependent, chaotic, and with broken symmetries implying a lack of ergodicity.

V. CONCLUSION

Throughout this paper, it has been shown that discrete time produces a host of new phenomena in the dynamics of spin systems with competing interactions. In particular, asymptotic behavior characterized by complicated time dependence and nonergodicity appears naturally as a result of the existence of multiple basins of attraction and solutions with broken symmetries. Since phenomena of this type have been reported in spin-glasses[19] and the evidence quoted is mainly numerical, it is of interest to ascertain whether our predictions are of relevance to those studies.

In analyzing Monte Carlo simulations, it is important to elucidate the correspondence between Monte Carlo step per spin and the time unit τ that we have used in our theory. Unfortunately, the available data does not provide a conclusive answer. If at each Monte Carlo step a single spin can flip its value, and the new configuration is then used to upgrade the next spin, then it could be argued that in the inifinite limit the simulated dynamics is effectively continuous.[20] On the other hand, spins could be upgraded in such a way that in a given time step the same transition probability is used for all of them, a case that closely resembles our treatment. Which procedure is closer to the true dynamics of a magnetic system is not clear, and it would be of interest to compare each algorithm with available experimental data, if any.

Although Monte Carlo simulations of purely ferromagnetic systems have shown very good agreement with the results of a continuous master equation,[21] we have also shown (Sec. III) that the absence of competing interactions in digital dynamics gives a time-independent fixed point identical to the continuous case. It remains to be seen whether simulations of systems with competing interaction will validate our results.

In spite of these ambiguities, it is suggestive that Monte Carlo simulations of spin-glasses give results which appear to agree qualitatively with the predictions of a digital-time theory. We should point out that in spite of the fact that those results have been obtained in systems with random distributions of coupling constants, we expect them to persist in systems with no explicit randomness.

In closing, we should mention that although the results of our paper are based on a specific problem (i.e., magnetic systems with discrete symmetries), we anticipate them to be of wider applicability. Besides the retardation effects mentioned in the previous section, we have recently noted that networks made up of threshold elements do behave as if time were discrete.[22] In that case their dynamics give rise to complex asymptotic behavior which is similar to that discussed in this paper. At a different level, our results indicate that continuous systems and their corresponding digital simulations do not always display the same behavior.

ACKNOWLEDGMENTS

We have benefited from discussions with J. Helman, T. Hogg, D. d'Humières, and L. P. Kadanoff. Part of this work was supported by the U.S. Office for Naval Research, Contract N00014-82-0699.

APPENDIX: DIGITAL-TIME VERSION OF LINEAR-RESPONSE THEORY

Consider time to be given in integer units of a basic time interval τ, such that $t = n\tau$ and $t+\tau = (n+1)\tau$. The master equation for the time evolution of the probability is then given by

$$P(\underline{\alpha},n+1)-P(\underline{\alpha},n)=LP(\underline{\beta},n)\ , \tag{A1}$$

with $\underline{\alpha}$ denoting a particular configuration of the system, and the right-hand side of the equation given by

$$LP(\underline{\beta},n)\equiv-\sum_{\underline{\beta}}[\omega(\underline{\alpha}\rightarrow\underline{\beta})P(\underline{\alpha},n) -\omega(\underline{\beta}\rightarrow\underline{\alpha})P(\underline{\beta},n)]\ , \tag{A2}$$

with $\omega(\underline{\alpha}\rightarrow\underline{\beta})$ the transition probability in time τ. If by equilibrium it is meant that $P(\underline{\alpha},n+1)=P(\underline{\alpha},n)=P^{(e)}$, Eq. (A1) yields detailed balance in the form

$$LP^{(e)}=0\ , \tag{A3}$$

with $P^{(e)}$ given by

$$P^{(e)}(\alpha)=\frac{e^{-\beta H(\underline{\alpha})}}{\mathrm{Tr}e^{-\beta H}}=\frac{e^{-\beta H(\underline{\alpha})}}{\sum_{\underline{\alpha}}e^{-\beta H(\underline{\alpha})}}\ . \tag{A4}$$

As it is customary,[23] it will be assumed that the Hamiltonian of the system can be written as the sum of two parts, $H=H_0+H_1$, with H_1 a time-dependent Hamiltonian which corresponds to an external perturbation $K(t)$, i.e.,

$$H_1=-AK(t)\ . \tag{A5}$$

This in turn implies that both the probability function P and the operator L can be written as the sum of a time-independent part plus a time-dependent one,

$$P(\underline{\alpha},n)=P_0^{(e)}(\underline{\alpha})+P_1(\underline{\alpha},n)\ , \tag{A6}$$

$$L=L_0+L_1(n)\ . \tag{A7}$$

Substituting these expressions in Eq. (A1) and keeping only linear terms, one obtains

$$P_1(\underline{\alpha},n+1)-P_1(\underline{\alpha},n)=L_0P_1(\underline{\beta},n)+L_1(n)P_0^{(e)}(\underline{\beta})\ . \tag{A8}$$

Furthermore, using Eq. (A4), it is easy to show that in the linear regime

$$P^{(e)}=P_0^{(e)}+P_1^{(e)}\ , \tag{A9}$$

where

$$P_1^{(e)}=-\beta(H_1-\langle H_1\rangle_0)P_0^{(e)}\ , \tag{A10}$$

with

$$\langle H_1\rangle_0\equiv\frac{\mathrm{Tr}(H_1e^{-\beta H_0})}{\mathrm{Tr}e^{-\beta H_0}}\ .$$

With the description given by Eqs. (A6) and (A7), Eq. (A3) also implies that

$$L_1P_0^{(e)}=-L_0P_1^{(e)}=\beta L_0H_1P_0^{(e)} \tag{A11}$$

and therefore the master equation becomes (with $\beta L_0H_1P_0^{(e)}=-\beta K(t)AP_0^{(e)}$)

$$P_1(n+1)=(1+L_0)P_1(n)-\beta K(n)L_0AP_0^{(e)}\ , \tag{A12}$$

an equation which has the solution

$$P_1(n)=-\sum_{k=1}^{n}(1+L_0)^{n-k}\beta K(k-1)L_0AP_0^{(e)}\ , \tag{A13}$$

with the initial condition $P_1(n=0)=0$.

We are interested in ensemble averages of operators such as

$$\langle B(n)\rangle_1\equiv\sum_{\underline{\alpha}}B(\underline{\alpha})P_1(\underline{\alpha},n)\ . \tag{A14}$$

Using Eq. (A13) $\langle B(n)\rangle_1$ can be written as

$$\langle B(n)\rangle_1=-\beta\sum_{k=1}^{n}K(k-1)\Phi_{AB}(n-k)\ , \tag{A15}$$

where $\Phi_{AB}(l)\equiv\langle B(1+L_0)^lL_0A\rangle_0$ is the response function. In the spirit of the standard linear-response theory, let $K(k)$ be written as

$$K(k)=K_0e^{i\omega k\tau} \tag{A16}$$

or

$$K(k-1)=K_0e^{i\omega(k-1)\tau} =K_0e^{i\omega(n-1)\tau}e^{-i\omega(n-k)\tau}\ . \tag{A17}$$

Using the Fourier series representation for $K(k)$, Eq. (A15) becomes

$$\langle B(n)\rangle_1=\chi_{AB}(\omega,n)K_0e^{i\omega(n-1)\tau}\ , \tag{A18}$$

where the susceptibility χ_{AB} is defined as

$$\chi_{AB}\equiv-\beta\sum_{l=1}^{n-1}e^{-i\omega l\tau}\Phi_{AB}(l)\ . \tag{A19}$$

It now remains to compute $\Phi_{AB}(l)$ from its definition above. Writing explicitly the ensemble average as

$$\Phi_{AB}(l)=\sum_{\underline{\alpha},\underline{\beta}}B(\underline{\alpha})(1+L_0)^lL_0A(\underline{\beta})P_0^{(e)}(\underline{\beta})\ , \tag{A20}$$

it can be shown that it is equivalent to

$$\Phi_{AB}(l)=\sum_{\underline{\alpha},\underline{\beta},\underline{\gamma}}B(\underline{\alpha})A(\underline{\gamma})P_0^{(e)}(\underline{\gamma}) \times[(1+L_0)^{l+1}-(1+L_0)^l] \times P_0(\underline{\beta},0\,|\,\underline{\gamma},0)\ , \tag{A21}$$

with $P_0(\underline{\beta},0\,|\,\underline{\gamma},0)$ the conditional probability, or

$$\Phi_{AB}(l)=\langle A(0)B(l+1)\rangle_0-\langle A(0)B(l)\rangle_0\ . \tag{A22}$$

Using this result, the time-dependent susceptibility becomes

$$\chi_{AB}(\omega,n)=\beta\langle A(0)B(0)\rangle_0-\beta e^{-i\omega(n-1)\tau}\langle A(0)B(n)\rangle_0 -\beta(e^{i\omega\tau}-1)\sum_{k=1}^{n-1}e^{-i\omega k\tau}\langle A(0)B(k)\rangle_0\ . \tag{A23}$$

In order to analyze the meaning of this equation and its differences with the continuum theory, it is useful to look at the limit in which the external field becomes time independent. In this "static" limit $\omega=0$ and Eq. (A23) becomes

$$\chi_{AB}(0,n)=\beta\langle A(0)B(0)\rangle_0-\beta\langle A(0)B(n)\rangle_0 , \qquad (A24)$$

which, as can be seen, contains a time-dependent factor in the second term of its right-hand side. If the system is ergodic, one obtains, in the limit of $n\rightarrow\infty$,

$$\chi_{AB}(0,\infty)=\beta[\langle A(0)B(0)\rangle_0-\langle A\rangle_0\langle B\rangle_0] , \qquad (A25)$$

a result which agrees with the standard version of linear-response theory. It should be pointed out, however, that for the spin system treated in this paper, the assumption of ergodicity is by no means obvious, in which case the static-field limit still produces the time-dependent susceptibility given by Eq. (A24).

Another interesting limit is that obtained with a time-dependent field acting on the system. As $n\rightarrow\infty$ Eq. (A23) reduces to

$$\chi_{AB}(\omega,\infty)=\beta\langle A(0)B(0)\rangle_0 -\beta(e^{i\omega\tau}-1)\sum_{k=1}^{\infty}e^{-i\omega\tau k}\langle A(0)B(k)\rangle_0 , \qquad (A26)$$

which for $\tau\rightarrow 0$, becomes the familiar result of linear-response theory, i.e.,

$$\chi_{AB}(\omega)=\beta\langle A(0)B(0)\rangle_0 -i\omega\beta\int_0^{\infty}e^{-i\omega t}\langle A(0)B(t)\rangle_0 dt .$$

[1]See, for example, K. Binder, *Monte Carlo Methods in Statistical Physics* (Springer, New York, 1979).

[2]K. Binder and K. Shröder, Phys. Rev. B 14, 2142 (1976).

[3]A. J. Bray and M. A. Moore, J. Phys. F 7, L333 (1977).

[4]A. J. Bray, M. A. Moore, and P. Reed, J. Phys. C 11, 1187 (1978).

[5]D. Stauffer and K. Binder, Z. Phys. Chem. Abt. B 34, 97 (1979).

[6]K. Binder, in *Fundamental Problems in Statistical Mechanics,* edited by E. G. D. Cohen (North-Holland, Amsterdam, 1980), Vol. V, pp. 21–51.

[7]H. Müller-Krumbbaar and K. Binder, J. Stat. Phys. 8, 1 (1973).

[8]It should be pointed out that the motion of equilibrium as implying no time dependence is somewhat arbitrary, for a higher-order fixed point, i.e., $\langle s\rangle_{t+n\tau}=\langle s\rangle_t$, with n an integer, could also be invoked. It is only in the static case, however, that the well-known continuum limit obtains.

[9]H. B. Callen, Phys. Lett. 4, 161 (1963).

[10]M. Suzuki, Phys. Lett. 19, 267 (1965).

[11]R. Brout and H. Thomas, Physics 3, 317 (1967).

[12]D. J. Thouless, P. W. Anderson, and R. G. Palmer, Philos. Mag. 35, 583 (1977).

[13]This type of problem has been investigated in the static limit by T. Morita, Phys. Lett. 94A, 232 (1983).

[14]R. J. Glauber, J. Math. Phys. 4, 294 (1963); M. Suzuki and R. Kubo, J. Phys. Soc. Jpn. 24, 51 (1968).

[15]W. Kinzel and K. H. Fisher, Solid State Commun. 23, 687 (1977).

[16]S. Kirkpatrick and D. Sherrington, Phys. Rev. B 17, 4384 (1978).

[17]A different approach to continuous dynamics has also been given by H. Sompolinsky and A. Zippelius, Phys. Rev. Lett. 47, 359 (1981). See also J. Hertz, J. Phys. C 16, 1219 (1983); 16, 1233 (1983).

[18]B. A. Huberman and R. M. Martin, Phys. Rev. Lett. 39, 478 (1977); J. B. Boyce and B. A. Huberman, Phys. Repts. 51, 189 (1979).

[19]R. G. Palmer, Adv. Phys. 31, 669 (1982); N. Mackenzie and A. P. Young, Phys. Rev. Lett. 49, 301 (1982).

[20]W. Kinzel, private communication.

[21]E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).

[22]M. Y. Choi and B. A. Huberman, Phys. Rev. A 28, 1204 (1983).

[23]See, for example, D. Bedeaux, S. Milosevic, and G. Paul, J. Stat. Phys. 3, 39 (1971).