Digital dynamics and chaotic behavior in Monte Carlo simulations of magnetic systems

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Recently, it has been shown that the discrete nature of time in numerical simulations can bring in features which are not encountered in the usual analytical studies using continuous time. This was illustrated with the study of the discrete dynamics of simple magnetic systems with competing interactions, where a complex behavior characterized by broken symmetries, oscillations, and chaos was found. In this work it is shown that, in the case of Monte Carlo simulations with random updating of spins, such an anomalous behavior can be viewed as a sort of finite-size effect, which should not appear in actual simulations of systems large enough to be of interest.

Recently, Choi and Huberman[1] (CH) have pointed out that the digital (discrete) character of time in numerical simulations can have serious consequences on the dynamical behavior of the system being simulated. These authors showed that for simple magnetic systems with competing interactions, whereas continuous dynamics as derived from the usual master-equation (ME) 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. They also suggest these results might provide a dynamical explanation for the breakdown of ergodicity reported in Monte Carlo (MC) studies of spin glasses.[2,3] Later, this suggestion was supported by the study of the effective dynamics associated with MC simulations with sequential updating of spins.[4]

However, in most relevant MC studies (especially on spin glasses), a random updating of spins is considered. Then, it is worthwhile to see if the results of Ref. 1 also apply in this case.

In order to do so, two main points which these results rely on must be discussed further. First, the ME considered by CH is the discrete-time version of the true continuous ME, with a basic time step Δt of fixed length τ, equal to the bare relaxation time. This is not a good approximation to the effective discrete-time dynamics in MC simulations with random updating, because in this case the larger the system size N, the smaller is the time Δt in which a single spin flip occurs ($\Delta t \sim 1/N$).[5]

The second point referred to above concerns the approximation implied by the use, in Ref. 1, of the mean field with local corrections approach to obtain explicit recursion relations for the magnetization and susceptibility. Although one can argue that this must be a good approximation, at least far enough from critical lines, inside the disordered phase, a subtle point related to the discrete nature of time must be carefully taken into account in defining the local susceptibility [see the discussion following Eq. (9)].

In this work I discuss the effects of the discreteness of time in MC simulations with random spin updating. To this purpose I use a ME which has been previously shown[5] to reproduce faithfully the effective digital dynamics associated to these simulations. From this more appropriate ME—and essentially with the same procedure followed in Ref. 1—it is shown that the anomalous behavior reported there can be viewed, in this case, as a sort of (extreme) finite-size effect, which manifests itself for parameter values beyond their range of validity. Then, it should not appear in actual simulations of systems large enough to be of interest.

Consider a spin system whose dynamical evolution is described by the following ME:

$$\frac{d}{dt}P(\sigma;t)=\sum_k\left[\frac{1}{\tau}\omega(-\sigma_k)P(\sigma_1,\ldots-\sigma_k,\ldots\sigma_N;t)-\frac{1}{\tau}\omega(\sigma_k)P(\sigma_1,\ldots\sigma_k,\ldots\sigma_N;t)\right], \quad (1)$$

where $P(\sigma;t)$ is the probability of finding the system in the configuration $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_N)$ and $\omega(\sigma_k)$ is the Glauber[6] transition probability:

$$\omega(\sigma_k)=\tfrac{1}{2}[1-\tanh(\beta E_k)], \quad (2a)$$

$$E_k=\sum_j J_{kj}\sigma_j+h_k . \quad (2b)$$

In Eq. (1), τ sets the bare time scale for the relaxation process. As in Ref. 1, the coupling constants J_{ij} are given by

$$J_{ij}=\begin{cases} J_1 \text{ for } p \text{ neighbors} \\ -J_2 \text{ for } r=z-p \text{ neighbors.}\end{cases} \quad (3)$$

In the course of a MC simulation of Eq. (1) with transition probability given by (2), for random updating of spins the dynamics is effectively governed by the discrete-time ME:[5]

$$P_{n+1}(\sigma)-P_n(\sigma)=\frac{1}{N}\sum_k[\omega(-\sigma_k)P_n(\sigma_1\ldots-\sigma_k\ldots\sigma_N)-\omega(\sigma_k)P_n(\sigma_1\ldots\sigma_k\ldots\sigma_N)] . \quad (4)$$

This equation with $P_n(\sigma)\equiv P(\sigma;t=n\Delta t)$ and $\Delta t=\tau/N$ approaches (1) up to terms of order $1/N^2$. From it, one

gets the following equations of motion for the magnetization,

$$\left\langle \sigma_k;t=(n+1)\frac{\tau}{N}\right\rangle \equiv m_k(n) = \left(1-\frac{1}{N}\right)m_k(n)+\frac{1}{N}\langle \tanh(\beta E_k);n\rangle \tag{5}$$

and the susceptibility

$$\chi_{ij}(n+1)\equiv \frac{\partial}{\partial h_i}\left\langle \sigma_j;t=(n+1)\frac{\tau}{N}\right\rangle\Bigg|_{h=0} = \left(1-\frac{1}{N}\right)\chi_{ij}(n)+\frac{1}{N}\frac{\partial}{\partial h_i}\langle \tanh(\beta E_j);n\rangle\Bigg|_{h=0} . \tag{6}$$

Following Ref. 1 and according to the scheme proposed by Brout and Thomas,[7] the statistical average of $\tanh(\beta E_k)$ can be approximated by

$$\langle \tanh(\beta E_k);n\rangle \simeq \tanh[\beta h_k^{\rm eff}(n)] , \tag{7}$$

where the effective local field $h_k^{\rm eff}$ is given by

$$h_k^{\rm eff}(n)\equiv \left\langle E_k;t=n\frac{\tau}{N}\right\rangle = \sum_j J_{kj}m_j(n)-\sum_j J_{kj}^2\tilde{\chi}_{kk}(n)m_k(n)+h_k . \tag{8}$$

In this equation $\tilde{\chi}_{kk}$ represents the response of spin k to the average magnetization at site j ($\neq k$):

$$\tilde{\chi}_{kk}(n+1)\equiv N\frac{\partial m_k(n+1)}{\partial[J_{kj}m_j(n)]}\simeq N\frac{\partial m_k(n+1)}{\partial h_k^{\rm eff}(n)} . \tag{9}$$

In the definition of $\tilde{\chi}_{kk}$ it has been assumed that the effective local field $h_k^{\rm eff}$ is felt by the kth spin one MC microstep after it was produced. Note also that with respect to the usual definition of $\tilde{\chi}_{kk}$ an extra factor N has been included in (9). The need for this factor can be explained in the following manner: Consider the time evolution of the magnetization as given by the continuous ME (1) with the approximation (7):

$$\frac{d}{dt}m\left(\frac{t}{\tau}\right)\simeq -\frac{1}{\tau}m_k\left(\frac{t}{\tau}\right)+\frac{1}{\tau}\tanh\left[\beta h_k^{\rm eff}\left(\frac{t}{\tau}\right)\right] .$$

Here, the fact that τ sets the time scale has been made explicit. The formal solution of this equation in terms of $h_k^{\rm eff}$ is

$$m_k\left(\frac{t}{\tau}\right)=e^{-t/\tau}m_k(0)+\frac{1}{\tau}\int_0^t \tanh\left[\beta h_k^{\rm eff}\left(\frac{x}{\tau}\right)\right]e^{(x-t)\tau}dx , \tag{10}$$

from which one obtained $\tilde{\chi}_{kk}$ through the usual definition

$$\tilde{\chi}_{kk}\left(\frac{t}{\tau}\right)\simeq \frac{\partial m_k(t/\tau)}{\partial h_k^{\rm eff}(t/\tau)}=\beta\left\{1-\tanh^2\left[\beta h_k^{\rm eff}\left(\frac{t}{\tau}\right)\right]\right\} . \tag{11}$$

Suppose one now takes the discrete form of (10) with $t=(n+1)\tau/N$ for $N\gg 1$:

$$m_k(n+1)\simeq \left(1-\frac{1}{N}\right)^{n+1}m_k(0)+\frac{1}{N}\sum_{r=0}^{n}\tanh[Bh_k^{\rm eff}(r)]\left(1-\frac{1}{N}\right)^{n-r} ,$$

which is also the formal solution of the recursion relation (5) with the approximation (7). From this equation one gets

$$\frac{\partial m_k(n+1)}{\partial h_k^{\rm eff}(n)}=\frac{\beta}{N}\{1-\tanh^2[\beta h_k^{\rm eff}(n)]\} . \tag{12}$$

The comparison of (11) and (12) justifies the inclusion of the extra factor N in the definition (9) of $\tilde{\chi}_{kk}$.

Now, if all the spins of the system have the same amount of ferromagnetic and antiferromagnetic couplings [as given by (3)], all the physically relevant quantities must be translational invariants. Then the Eqs. (5) and (6) together with the approximation (7) give the following recursion relations for the magnetization,

$$m_k(n+1)\equiv m(n+1) = \left(1-\frac{1}{N}\right)m(n)+\frac{1}{N}\tanh(\beta h_{(n)}^{\rm eff}) , \tag{13}$$

and the susceptibility

$$\chi_{kk}(n+1)\equiv \chi(n+1)=\left(1-\frac{1}{N}\right)\chi(n)+\frac{1}{N}\tilde{\chi}(n+1)[1-J_+^2\chi(n)\tilde{\chi}(n)] . \tag{14}$$

From the definitions (8) and (9) one also gets

$$h_{(n)}^{\rm eff}=[J_- -J_+^2\tilde{\chi}(n)]m(n) , \tag{15a}$$

and

$$\tilde{\chi}(n)=\beta\left\{1-N^2\left[m(n)-\left(1-\frac{1}{N}\right)m(n-1)\right]^2\right\} . \tag{15b}$$

In the above equations it has been called $J_-=pJ_1-rJ_2$ and $J_+^2=pJ_1^2+rJ_2^2$; following CH it has been assumed also that $\sum_k J_{ik}\chi_{ik}\ll 1$ in deriving (14).

The recursion relations (13)–(15) have physical sense only when

$$J_+^2\geq \begin{cases} J_-^2/p, & J_->0,\\ J_-^2/r, & J_-<0,\end{cases} \tag{16}$$

or, for $p\sim r\sim O(z)$, $J_+^2\gtrsim J_-^2/z\ \forall J_-$. The relative strength $\eta=J_-^2/(zJ_+^2)$ gives an idea of the amount of competition present in the system. Whereas for $\eta\to 1$ one has a predominance of ferromagnetic or antiferromagnetic couplings, for $\eta\to 0$ the interactions are strongly competing.

At this point it is worth noting that for $N\to 1$, Eqs. (13)–(15) reproduce the corresponding Eq. (3.3) of Ref. 1. This supports the idea that the anomalous behavior of m and χ found there corresponds to a sort of (extreme) finite-size effect.

Before the numerical study of (13) it is interesting to consider its linearized version for $m(0)\simeq 0$ in the disor-

dered phase

$$m(n) \simeq \left[1 - \frac{1}{N}(1 + K_{\mp}^2 - K_-)\right]^n m(0) \ , \qquad (17)$$

where $K_- = \beta J_-$ and $K_{\mp}^2 = \beta^2 J_{\mp}^2$. From this equation, one can see that the system has a critical slowing down of the magnetization at $(K_{\mp}^2)_c = K_- - 1$, which coincides—as it must be—with the critical line in the plane (J_1, J_2) of the static model.[8] Equation (17) also provides an upper bound for the meaningful values of $K_{\mp}^2$. In fact, for

$$(K_{\mp}^2)_{\max} = K_- + N - 1 \ , \qquad (18)$$

after the first recursion m reaches its equilibrium value $m(1) = 0$, which can be interpreted as a too fast evolution of the system to be followed by the finite time-step recursion (13). Hence, the results this equation gives for $K_{\mp}^2$ greater than $(K_{\mp}^2)_{\max}$ have no physical sense, which is actually a nonserious restriction for those values of N of interest.

I have studied numerically the recursion relations (13)–(15) for fixed arbitrary values of K_- and $K_{\mp}^2$ ranging, according to (16)–(18), from $K_{\mp}^2/z$ (with $z \lesssim 10$) to $(K_- + N - 1)$. Within this range,[9] any initial magnetization relaxes to a simple fixed point, which is (up to nearly five digits) given by

$$m^* = \tanh[K_- - (1 - m^{*2})K_{\mp}^2]m^* \ .$$

This equation is obtained from (13)–(15) with $m(n+1) = m(n-1) = m^*$. Note m^* is independent of N, as usual when approximations of the mean-field type are considered.

In conclusion, I have shown that, for parameter values within their range of validity, no anomalous behavior of the type reported in Ref. 1 should be found in MC simulations with random spin updating. Moreover, the restriction posed on the meaningful values of the coupling constants [Eq. (18)] is not important for systems of the size usually considered in actual simulations.

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[8]Note that to obtain this result it has been essential to include the extra factor N in Eq. (9).

[9]From the numerical values $K_- = 2$, $N = 1$ considered by CH, one can see that $K_{\mp}^2$ must be less than or equal to 2. Up to this value of $K_{\mp}^2$ these authors found no anomalous behavior of m (see Fig. 1 in Ref. 1).