Effective discrete-time dynamics in Monte Carlo simulations

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The effective discrete-time master equation which governs a Monte Carlo simulation is derived. This equation, which takes explicitly into account the type of algorithm used to update the configurations, when specialized for a spin system and sequential updating, coincides with a similar equation recently proposed in the literature. From this effective master equation it is possible to give theoretical support to previous numerical works concerning the validity of different algorithms for spin updating in the study of kinetic processes. All the analytical results are consistently checked through numerical simulations of a simple exactly solvable model.

I. INTRODUCTION

The theoretical basis for the application of Monte Carlo (MC) methods to the study of static and dynamics properties of spin systems has been discussed in the literature many times.[1] However, in most cases, two important questions concerning the validity of the method have been bypassed: first, the discrete nature of time in computer simulations and, second, the influence in dynamical processes of the algorithm used to update the spins.

The first question has been recently discussed by Choi and Huberman,[2] who found that the digital character of time can bring in features which are not encountered in the usual analytical studies using continuous time. To describe the evolution of the sequence of configurations in a MC simulation—which can be thought of as a discrete-time process, rather than a continuous one—these authors proposed[3] a complex discrete-time master equation (DTME). From this equation they conclude that the effective dynamics in numerical experiments is much more complex than continuous-time ones corresponding to real systems.

The second question has also been recently touched upon by Gawlinski *et al.*,[4] in connection with studies of the development of order in rapidly quenched systems. They found that the law for the growth of the average size of magnetized domains depends on the particular updating procedure used. As these authors pointed out, the application of the MC method to dynamics is then somewhat controversial due to the fact that the algorithm one chooses for updating the spins becomes an integral part of the model.

In this work a general DTME associated to a MC simulation is derived. This equation, which takes explicitly into account the influence of the chosen updating algorithm, coincides with the equation of Choi and Huberman[3] when a sequential updating of the spins is considered. It also gives theoretical support to the numerical evidence found by Gawlinski *et al.*[4] concerning the validity of different updating procedures. All the analytical results obtained here are consistently checked in the last section through numerical simulations of a simple exactly solvable model, the Ising spin chain with Glauber's transition probability.[5]

II. DISCRETE-TIME MASTER EQUATION

Consider a system whose dynamical evolution can be described by the continuous-time master equation

$$\frac{d}{dt}P(\sigma,t)=\sum_{\sigma'\neq\sigma}W(\sigma'\rightarrow\sigma;t)P(\sigma',t) -P(\sigma,t)\sum_{\sigma'\neq\sigma}W(\sigma\rightarrow\sigma';t)\ , \tag{1}$$

where $P(\sigma,t)$ is the probability that the system can be found in the configuration $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_N)$ at time t and $W(\sigma'\rightarrow\sigma;t)$ is the transition rate from σ' to $\sigma\neq\sigma'$ at this time. If one sets the time scale for the relaxation process by taking

$$W(\sigma'\rightarrow\sigma;t)=\frac{1}{\tau}\omega\left[\sigma'\rightarrow\sigma;\frac{t}{\tau}\right]\ ,$$

then, for $\Delta t\ll\tau$, it is likely to approximate (1) by the discrete-time equation

$$P(\sigma,t+\Delta t)-P(\sigma,t)=\sum_{\sigma'\neq\sigma}\frac{\Delta t}{\tau}\omega\left[\sigma'\rightarrow\sigma;\frac{t}{\tau}\right]P(\sigma',t) -P(\sigma,t)\sum_{\sigma'\neq\sigma}\frac{\Delta t}{\tau}\omega\left[\sigma\rightarrow\sigma';\frac{t}{\tau}\right]\ . \tag{2}$$

Now, from its very definition,

$$W(\sigma'\rightarrow\sigma;t)=\lim_{\Delta t\rightarrow 0}\frac{P(\sigma,t+\Delta t\mid\sigma',t)}{\Delta t}\quad(\sigma\neq\sigma')\ ,$$

where $P(\sigma,t\mid\sigma',t')$ is the conditional probability for the system to be found in the configuration σ at time $t>t'$ given that it was in σ' at t'. Then, to the same order of accuracy, Eq. (2) can be rewritten as

$$P(\sigma,t+\Delta t)-P(\sigma,t)=\sum_{\sigma'\neq\sigma}P(\sigma,t+\Delta t\mid\sigma',t)P(\sigma',t) -P(\sigma,t)\sum_{\sigma'\neq\sigma}P(\sigma',t+\Delta t\mid\sigma,t)\ . \tag{3}$$

This last equation is, in fact, the one which is simulated in usual MC studies of the dynamics of a system: as Choi and Huberman assert,[2] in a computer, time can only be implemented by discrete processes which correspond to steps of a program.

Besides this discrete nature of time, a computer simulation also incorporates as an integral part of the model the algorithm one chooses for updating the configurations of the system. In the course of the simulation one actually has

$$P(\sigma,t+\delta t\mid\sigma',t)=\frac{\delta t}{\tau_{\rm MC}}\omega\left[\sigma'\to\sigma;\frac{t}{\tau_{\rm MC}}\right]\Omega\left[\sigma'\to\sigma;\frac{t}{\tau_{\rm MC}}\right] \tag{4}$$

where $\Omega(\sigma'\to\sigma;t/\tau_{\rm MC})$ is the probability that in the MC step between t and $t+\delta t$ the updating of the configuration σ' was attempted in the (configuration-space) direction which leads from σ' to σ. A different time scale, $\tau_{\rm MC}$, is used to adjust the evolution of the system so that $\delta t\lesssim\tau_{\rm MC}$, where δt is the time wasted for the real system to evolve according to the algorithm in a MC step, i.e., the evolution is retarded (or accelerated) in such a way that it can be adequately followed by the computer (this will become clear in the example below).

From Eqs. (3) and (4), in a MC simulation the dynamics is then governed by the effective DTME:

$$P(\sigma,t+\delta t)-P(\sigma,t)=\sum_{\sigma'\neq\sigma}\frac{\delta t}{\tau_{\rm MC}}\omega\left[\sigma'\to\sigma;\frac{t}{\tau_{\rm MC}}\right]\Omega\left[\sigma'\to\sigma;\frac{t}{\tau_{\rm MC}}\right]P(\sigma',t)-P(\sigma,t)\sum_{\sigma'\neq\sigma}\frac{\delta t}{\tau_{\rm MC}}\omega\left[\sigma\to\sigma';\frac{t}{\tau_{\rm MC}}\right]\Omega\left[\sigma\to\sigma';\frac{t}{\tau_{\rm MC}}\right], \tag{5}$$

which is supposed to approximate (2) [and also (1)]. This equation clearly shows the importance of choosing an adequate updating algorithm in the study of kinetic processes, a point which has been previously stressed by Gawlinski *et al.*[4] However, these authors give only numerical evidence to favor or discard different algorithms for a particular system, without attempting any general proof.

III. MONTE CARLO DYNAMICS OF SPIN SYSTEMS

For a general Ising spin system which can only flip a single spin during a MC step, one has

$$\Omega\left[\sigma'\to\sigma;\frac{t}{\tau_{\rm MC}}\right]=\sum_{k=1}^{N}\Omega\left[-\sigma_k,\frac{t}{\tau_{\rm MC}}\right]\prod_{i\neq k}\delta_{\sigma_i\sigma_i'} \tag{6}$$

where $\Omega(\sigma_k,t/\tau_{\rm MC})$ is the probability of choosing the kth spin for a spin-flip trial at time t.

Calling $\omega(\sigma_k)/\tau_{\rm MC}$ the (t independent) flipping transition rate for the spin σ_k, from Eqs. (5) and (6) the effective DTME is

$$P(\sigma,t+\delta t)-P(\sigma,t)=\sum_{k=1}^{N}\frac{\delta t}{\tau_{\rm MC}}\omega(-\sigma_k)\Omega\left[-\sigma_k,\frac{t}{\tau_{\rm MC}}\right]P(\sigma_1,\ldots,-\sigma_k,\ldots,\sigma_N,t)-P(\sigma,t)\sum_{k=1}^{N}\frac{\delta t}{\tau_{\rm MC}}\omega(\sigma_k)\Omega\left[\sigma_k,\frac{t}{\tau_{\rm MC}}\right]. \tag{7}$$

The selection of the active site in a given MC step may be made randomly or by proceeding through the lattice in a regular fashion. In the first case, in which

$$\Omega\left[\sigma_k,\frac{t}{\tau_{\rm MC}}\right]=\frac{1}{N}\ , \tag{8}$$

Eq. (7), with $\delta t/(N\tau_{\rm MC})=\Delta t/\tau$, shows that the MC simulation with random updating is a faithful realization of (at least) the discrete-time dynamics (2) of the real system.

For the sequential updating, one has instead

$$\Omega\left[\sigma_k,\frac{t+(n-1)\delta t}{\tau_{\rm MC}}\right]=\delta_{kn},\quad n=1,2,\ldots,N \tag{9}$$

and Eq. (7) gives

$$P(\sigma,t+n\delta t)-P(\sigma,t+(n-1)\delta t)=\frac{\delta t}{\tau_{\rm MC}}\omega(-\sigma_n)P(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N,t+(n-1)\delta t)-\frac{\delta t}{\tau_{\rm MC}}\omega(\sigma_n)P(\sigma,t+(n-1)\delta t)\ . \tag{10}$$

Summing these N equations one obtains

$$P(\sigma,t+N\delta t)-P(\sigma,t)=\sum_{n=1}^{N}\frac{\delta t}{\tau_{\mathrm{MC}}}\omega(-\sigma_n)P(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N,t+(n-1)\delta t)-\sum_{n=1}^{N}\frac{\delta t}{\tau_{\mathrm{MC}}}\omega(\sigma_n)P(\sigma,t+(n-1)\delta t)\ ,$$

which coincides with the DTME discussed (regardless of the updating algorithm) by Choi and Huberman.[3] As these authors pointed out, although one could set $N\delta t/\tau_{\mathrm{MC}}=\Delta t/\tau$, the Eqs. (2) and (10) would still differ in the time arguments of their right-hand sides, which leads them to conclude that the dynamics in a MC simulation of a many-body system is in fact much more complex than that corresponding to a discrete-time evolution, and, of course, also much more complex than the continuous-time dynamics. This remains true for sequential updating, and explains why in Ref. 4, using this procedure for updating spins, a behavior not in accordance with the Allen-Cahn[6] law for the growth of domains in rapidly quenched systems was found. It must be stressed that a random updating gives the correct behavior, in agreement with the conclusion following Eq. (8).[7]

It is also possible to consider a simultaneous (within a MC step) upgrading of all the spins, in such a way that the same initial configuration is used for computing all the transition probabilities. This procedure has been proposed in Ref. 2 as likely to be much closer to the true dynamics than other algorithms because it closely resembles Eq. (2). In that case, instead of (4) one has

$$P(\sigma,t+\delta t\mid\sigma',t)=\prod_{\{i=\}}\left[1-\omega(\sigma_i)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]\prod_{\{j\neq\}}\left[\omega(-\sigma_j)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]\ ,$$

where the symbols $\prod_{\{i=\}}$ and $\prod_{\{j\neq\}}$ indicate products over sites i and j for which $\sigma_i=\sigma_i'$ and $\sigma_j=-\sigma_j'$, respectively. The following DTME is then obtained from (3):

$$\begin{aligned}P(\sigma,t+\delta t)-P(\sigma,t)=&\sum_{\sigma'\neq\sigma}\prod_{\{i=\}}\left[1-\omega(\sigma_i)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]\prod_{\{j\neq\}}\left[\omega(-\sigma_j)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]P(\sigma',t)\\&-\sum_{\sigma'\neq\sigma}\prod_{\{i=\}}\left[1-\omega(\sigma_i)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]\prod_{\{j\neq\}}\left[\omega(\sigma_j)\frac{\delta t}{\tau_{\mathrm{MC}}}\right]P(\sigma,t)\ .\end{aligned}\tag{11}$$

Multiplying both sides of this equation by σ_k and summing over all the configurations σ one obtains

$$\langle\sigma_k,t+\delta t\rangle-\langle\sigma_k,t\rangle=-2\frac{\delta t}{\tau_{\mathrm{MC}}}\langle\sigma_k\omega(\sigma_k),t\rangle\ ,$$

where $\langle\sigma_k,t\rangle=\sum_\sigma\sigma_k P(\sigma,t)$ is the kth spin magnetization. This is the same result one would have obtained from (2) with $\Delta t/\tau=\delta t/\tau_{\mathrm{MC}}$. However, for the spatial correlation $\langle\sigma_k\sigma_r,t\rangle$, (11) gives

$$\langle\sigma_k\sigma_r,t+\delta t\rangle-\langle\sigma_k\sigma_r,t\rangle=-2\frac{\delta t}{\tau_{\mathrm{MC}}}\langle\sigma_k\sigma_r[\omega(\sigma_k)+\omega(\sigma_r)],t\rangle+\left[\frac{2\delta t}{\tau_{\mathrm{MC}}}\right]^2\langle\sigma_k\sigma_r\omega(\sigma_k)\omega(\sigma_r),t\rangle$$

which differs in the last term of the right-hand side from the corresponding discrete-time result. Thus only the time-evolution of the magnetization is faithfully reproduced for the algorithm in discussion and then it is not clear which could be the practical interest for its implementation.[8]

Finally, it is interesting to point out that Eq. (7) could be interpreted, for a general $\Omega(\sigma_k,t/\tau_{\mathrm{MC}})$, as the DTME associated to the system evolution in contact with an external (spatially and temporal) varying heat bath, with perhaps a small fluctuating local field if $\Omega(\sigma_k,t/\tau_{\mathrm{MC}})\neq\Omega(-\sigma_k,t/\tau_{\mathrm{MC}})$. From this point of view, the sequential updating equation (9) would correspond to a sort of heat wave acting on the spin system.

IV. EXAMPLE: ISING SPIN CHAIN

Consider a linear Ising chain with periodic boundary conditions and Glauber's single spin-flip transition rate:

$$\frac{1}{\tau}\omega(\sigma_k)=\frac{1}{2\tau}\left[1-\frac{\gamma}{2}\sigma_k(\sigma_{k+1}+\sigma_{k-1})\right]\ ,$$

$$k=1,2,\ldots,N\quad(\gamma<1)\ .\tag{12}$$

The dynamics of this model can be exactly solved in its continuum[5] and discrete-time versions, thus providing a complete check by comparison of these analytical results with the corresponding ones in MC simulations with different updating algorithms. Only the relaxation of a single-spin magnetization $\langle\sigma_k,t\rangle$ and the average magnetization $\langle\sigma,t\rangle=\sum_k\langle\sigma_k,t\rangle/N$ from their initial values $\langle\sigma_k,0\rangle=\langle\sigma,0\rangle=1$ will be considered in the following. Note that although periodic boundary conditions are imposed, $\langle\sigma_k,t\rangle$ and $\langle\sigma,t\rangle$ do not agree for the sequential updating.

Glauber's solution[5] for the continuous-time ME gives

$$\langle\sigma_k,t\rangle=\langle\sigma,t\rangle=\exp\left[-(1-\gamma)\frac{t}{\tau}\right]\ .\tag{13}$$

The time scale τ is, in this case, the relaxation time of a single spin in the presence of the heat bath which induces random spin flips. The net effect of the spin interactions in the linear chain is to produce a larger effective relaxation time $\tau/(1-\gamma)$.

Taking into account Eqs. (8) and (12), for random updating the DTME (7) gives

$$\langle \sigma_k, t+\delta t\rangle = \langle \sigma, t+\delta t\rangle = \left[1-\frac{(1-\gamma)\delta t}{N\tau_{\mathrm{MC}}}\right]\langle \sigma, t\rangle ,$$

i.e.,

$$\langle \sigma_k, m(N\delta t)\rangle = \langle \sigma, m(N\delta t)\rangle = \exp\left\{ m \ln\left[\left[1-\frac{(1-\gamma)\delta t}{N\tau_{\mathrm{MC}}}\right]^N\right]\right\}, \tag{14}$$

which coincides with (13) when

$$-\frac{(1-\gamma)N\delta t}{\tau} = \ln\left[\left[1-\frac{(1-\gamma)\delta t}{N\tau_{\mathrm{MC}}}\right]^N\right] = -\frac{(1-\gamma)\delta t}{\tau_{\mathrm{MC}}} + O(1/N) . \tag{15}$$

This equation gives, regardless of what one takes as a microstep δt, the connection between τ and τ_{MC} as to recover the true continuous dynamics.

For sequential updating, Eqs. (10) and (12) give

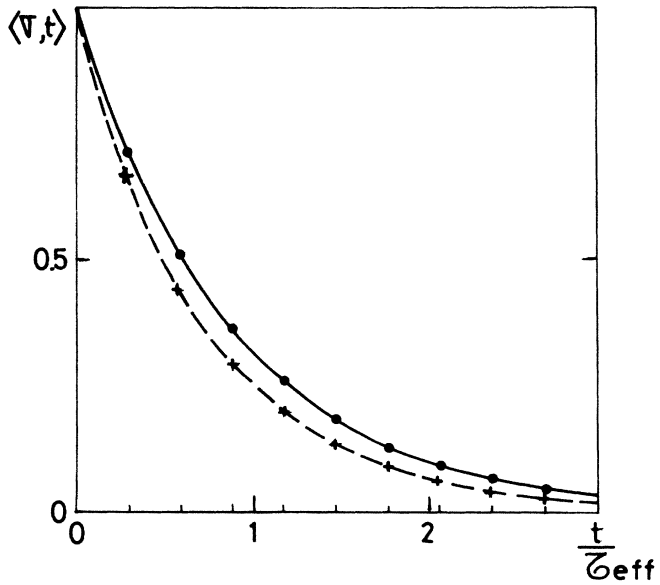

FIG. 1. Average magnetization per spin as a function of time in units of the effective time scale $\tau_{\mathrm{eff}}=\tau/(1-\gamma)$. Dots (crosses) indicate MC results with random (sequential) updating of the spins. The solid line is the exact continuous-time solution of Glauber; the dashed line is merely to guide the eye. In the numerical simulations, $\gamma=0.2$ and $\delta t/\tau_{\mathrm{MC}}=0.4$; Eq. (15) then gives $\delta t\simeq 0.113\tau_{\mathrm{eff}}$, which implies $t/\tau_{\mathrm{eff}}\simeq 0.338 N_{\mathrm{MCs}}$, where N_{MCs} is the number of Monte Carlo steps per spin.

$$\langle \sigma_k, t+N\delta t\rangle - \langle \sigma_k, t\rangle = \frac{\gamma\delta t}{2\tau_{\mathrm{MC}}}[\langle \sigma_{k+1}, t+(k-1)\delta t\rangle + \langle \sigma_{k-1}, t+(k-1)\delta t\rangle] - \frac{\delta t}{\tau_{\mathrm{MC}}}\langle \sigma_k, t+(k-1)\delta t\rangle .$$

This equation, together with the conditions

$$\langle \sigma_k, t+n\delta t\rangle = \begin{cases} \langle \sigma_k, t+N\delta t\rangle, & k\le n \\ \langle \sigma_k, t\rangle, & k>n \end{cases}$$

leads to

$$\langle \sigma_1, t+N\delta t\rangle = (1-a)\langle \sigma_1, t\rangle + b\{\langle \sigma_2, t\rangle + \langle \sigma_N, t\rangle\} , \tag{16a}$$

$$\langle \sigma_k, t+N\delta t\rangle = (1-a+b^2)\left[\langle \sigma_k, t\rangle + \sum_{n=1}^{k-2} b^n \langle \sigma_{k-n}, t\rangle\right] + (1-a)b^{k-1}\langle \sigma_1, t\rangle + b\langle \sigma_{k+1}, t\rangle + b^k\langle \sigma_N, t\rangle \quad (2\le k\le N-1) , \tag{16b}$$

$$\langle \sigma_N, t+N\delta t\rangle = (1-a)b(1+b^{N-2})\langle \sigma_1, t\rangle + b^2\langle \sigma_2, t\rangle + (1-a+b^2)\sum_{n=1}^{N-2} b^n\langle \sigma_{N-n}, t\rangle + (1-a+2b^2+b^N)\langle \sigma_N, t\rangle , \tag{16c}$$

where $a=\delta t/\tau_{\mathrm{MC}}$ and $b=\gamma\delta t/(2\tau_{\mathrm{MC}})$. These recursion relations are overly complicated to have $\langle \sigma, m(N\delta t)\rangle$ solved as a function of $\langle \sigma, 0\rangle$ and m. Nevertheless, from its structure it is clear that many different time scales are competing so as to produce a complex behavior that in any case reproduces the simple exponential decay (13).

To give numerical support to the above results, MC simulations have been performed with random and sequential updatings for a "triangle" of interacting spins, which correspond to $N=3$ in Eqs. (14) and (16). Taking $\delta t/\tau_{\mathrm{MC}}=0.4$ and $\gamma=0.2$, averages over 10^5–10^6 runs, from the initial ordered configuration, give, for both algorithms, values near three digits in agreement with those obtained, respectively, from (14) and (16). Figure 1 shows a plot of these results together with Glauber's continuous-time solution (solid line). The time scales are related by taking $\delta t/\tau=0.141$, as given by (15). Note that the results for random and sequential updatings do not

agree over many times the relevant time scale for the effective relaxation process $\tau_{\text{eff}}=\tau(1-\gamma)$. For the small system considered even the gross features of its evolution—such as the average magnetization decay—are sensitive to the updating procedure. For larger systems one expects these gross features to be less modified by the algorithm used but, certainly, fine details of the physics involved may be affected by it.[4]

As a final remark, note also that from Eq. (12), $\eta=\delta t/(2\tau_{\text{MC}})$ ($=0.2$ in this case) is the transition probability for a spin σ_k with its neighboring spins antiparallel ($\sigma_{k+1}=-\sigma_{k-1}$). More generally, for an arbitrary spin system with Glauber's transition probability, η is the transition probability for spin with no nearest-neighbor interaction energy. So this value is an indicator for the acceptation rate of spin flippings and it is convenient, as a practical rule, taking it near 0.5. Then, remembering the relation following Eq. (8), it can be seen that for this value MC simulations with random updating approach the continuous-time dynamics up to terms of order $\Delta t/\tau=2\eta/N=1/N$, which is the general belief.

Of course, the above discussion does not take into account the problems encountered near critical points of a system ($\gamma\simeq 1$ for the linear chain), where its dynamical evolution is very slow (critical slowing down).[1]

V. CONCLUSIONS

In this work I have derived the DTME which governs the dynamics in a MC simulation. This equation clearly shows the importance of choosing an adequate updating algorithm in the study of kinetic processes.

By specializing this DTME for a general Ising spin system, it has been shown that a similar equation recently proposed by Choi and Huberman[3] is only valid for sequential updating of the spins. It also provides a theoretical explanation for the different rates of domain growth in rapidly quenched systems, recently observed by Gawlinski *et al.*[4] in MC simulations with distinct updating algorithms. All the analytical results obtained here have been consistently checked by the numerical study of an Ising spin chain with Glauber's transition probability and random and sequential updating algorithms.

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[8]From the point of view of its technical implementation, this algorithm could be considered as a limit case of a multispin coding updating. As such, it is more extensively discussed in the work cited in Ref. 7.