Spreading of Damage: An Unexpected Disagreement between the Sequential and Parallel Updatings in Monte Carlo Simulations

F. D. Nobre, A. M. Mariz, and E. S. Sousa
Departamento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, Campus Universitário-CP 1641, 59072-Natal, RN, Brazil
(Received 6 February 1992)

Damage spreading in the Ising model on a triangular lattice, for ferro- and antiferromagnetic interactions, is investigated using Glauber dynamics. Two procedures for updating spins are employed, the sequential and parallel ones. (a) The sequential algorithm leads to a dynamic transition at a temperature very close to the usual static critical temperature T_C in the ferromagnetic case, whereas in the antiferromagnetic problem, no transition is found, suggesting that the equilibrium phase transition and the frozen-chaotic one are strongly correlated. (b) The parallel recipe is not able to distinguish the two interactions, giving a similar dynamic transition for both, at a temperature which is considerably different from T_C.

PACS numbers: 05.50.+q, 75.10.Hk

The study of dynamic critical phenomena [1] has become a very attractive field in statistical mechanics nowadays. Whereas considerable progress has been made in the understanding of static phase transitions throughout the last two decades, much less is known about the dynamic aspects of them. Most of the efforts have made use of Monte Carlo simulations, for which the system, starting from an initial configuration, travels in phase space under the presence of thermal noise; its trajectory follows from application of the specific Monte Carlo rules (heat bath, Glauber, Metropolis, etc.).

A very important question is, for a given temperature, how do small perturbations at time $t=0$ affect the evolution of a given physical system, or in other words, how does the configuration at a time t ($t\rightarrow\infty$) depend on its initial conditions. One way to investigate this is by taking two distinct configurations which are, at the beginning, very close in phase space, and following their dynamics. For the case of Boolean variables, in which we will be interested here, this can be done by studying the time evolution of their "Hamming distance" or "damage" [2], defined by

$$D(t)=\frac{1}{N}\sum_{i=1}^{N}|\sigma_i(t)-\tau_i(t)| \quad (\sigma_i,\tau_i=0,1)\,, \tag{1}$$

where N is the total number of lattice sites and the sum refers to all dynamic variables in each configuration. $\{\sigma_i(t)\}$ and $\{\tau_i(t)\}$ represent two configurations of the system which evolve under the same Monte Carlo rules as well as the same sequence of random numbers. For a given nonzero initial damage $D(0)$, after a long period of time, usually one of the following two distinct regimes can be found, depending on the value of the temperature: a "chaotic" one where the damage propagates, and the two configurations remain apart in phase space, and a "frozen" one where the damage heals and the configurations meet after some time, giving $D(\infty)=0$. The sharp frontier between these two regimes characterizes a phase transition at a given "spreading temperature" T_s.

Some controversy exists concerning the correlation between these transitions and the usual static phase transitions in statistical mechanics models. For the ferromagnetic Ising model on the square lattice, using the Glauber [2,3], heat-bath, and Metropolis dynamics [3], one practically finds a temperature $T_s=T_C$, where T_C is the usual Curie temperature of the system. However, for the same model in the cubic lattice, the Glauber dynamics leads to a small discrepancy (about 4%) between T_s and T_C [4,5]; it has not been investigated up to the moment whether such a difference occurs also within other Monte Carlo rules. More surprising is the persistence of the chaotic-frozen transition in the presence of an external magnetic field; this has been verified for the three-dimensional Ising model within Glauber dynamics [5], and presumably, it may also occur in other systems.

For the $\pm J$ Ising spin glass on a cubic lattice, two characteristic temperatures were found within a heat-bath dynamics [6], which can well be associated, respectively, with the onset of spin-glass ordering (temperature T_2) and a Griffiths phase (temperature T_1, $T_1>T_2$). However, the same approach leads to a qualitatively similar picture in two dimensions, where it is currently believed that there exists no spin-glass phase. The Griffiths phase for the 3D case was shown to present multifractal behavior whereas the corresponding 2D case did not [7], suggesting a possible procedure to single out spin-glass behavior. Nevertheless, the Glauber dynamics was unable to detect the Griffiths phase for the cubic lattice [8].

Besides all the elements mentioned above which characterize the dynamic evolution of a given magnetic system, i.e., the interactions (ferromagnetic, antiferromagnetic, spin glass, etc.), the Monte Carlo rules (heat bath, Glauber, Metropolis, etc.), the lattice geometry, and the symmetry of the spin variables, another important feature concerns the particular way in which the spins are updated. Usually two prescriptions are employed for updating spins, namely, the sequential and parallel ones. In the former case, spins are updated one at a time (like a typewriter or in random order), whereas in the latter, all spins are updated at once. The advantage of the parallel algorithm is that the updating operation can be easily vectorized, resulting in a gain of computer speed. It has been shown, within heat-bath dynamics for a non-Hamiltonian system with nonsymmetric interactions, that such recipes lead in the long-time limit to similar results [9,10], whereas for the case of symmetric interactions they give different equilibrium distributions (the sequential method converges to the usual Boltzmann distribution, while the parallel one does not [11]). However, it has been argued in the literature that, although being different, such equilibrium distributions should present many properties in common; e.g., the critical temperature and correlation length should be identical in both cases [12,13]. The main result presented here addresses this point; we show evidence that strongly suggests important physical differences between the sequential and parallel updatings, in particular, in the critical temperature evaluation.

In this Letter we investigate the relation between the chaotic-frozen transition and the usual static phase transition, using both typewriter sequential and parallel updating algorithms. We do this within Glauber dynamics for a simple physical system, i.e., the Ising model on the triangular lattice. Such a system is very suitable for this purpose, since it presents very distinct equilibrium properties depending on whether one deals with ferromagnetic or antiferromagnetic interactions. In the former case, a well-defined static phase transition occurs at a finite temperature, whereas for the latter, one gets a fully frustrated lattice, providing only the paramagnetic state for any nonzero temperature. Therefore, by a simple change in the interaction sign, the damage spreading should change radically, if the above-mentioned transitions are correlated in some way.

In order to study the damage $D(t)$ defined in (1), we shall consider two Ising configurations $\{\sigma_i(t)\}$ and $\{\tau_i(t)\}$, which will evolve in time under the same dynamics and sequence of random numbers. For a time t, a given variable at site i feels the presence of a local field,

$$h_i^s(t)=\sum_j K_{ij}[2s_j(t)-1] \quad (s=\sigma,\tau)\,, \tag{2}$$

where $K_{ij}=\beta J_{ij}$ represent first-neighbor interactions and $\sigma_j(t),\tau_j(t)=0,1$ are Boolean variables. Let us define the probability $P_i^s(t)$ $(s=\sigma,\tau)$ associated with site i by

$$P_i^s(t)=\{1+\exp[-2h_i^s(t)]\}^{-1}\,. \tag{3}$$

The Glauber dynamics, which we will use throughout this Letter, consists in selecting a random number for site i at a given time t, $0\le x_i(t)\le 1$, and determining the new state of the variable s_i at a time $t+1$ according to the following rule:

$$s_i(t+1)=\begin{cases}1 \text{ if } x_i(t)\le P_i^s(t),\\ 0 \text{ if } x_i(t)>P_i^s(t),\end{cases} \text{ when } s_i(t)=0, \tag{4a}$$

$$s_i(t+1)=\begin{cases}0 \text{ if } x_i(t)\le 1-P_i^s(t),\\ 1 \text{ if } x_i(t)>1-P_i^s(t),\end{cases} \text{ when } s_i(t)=1. \tag{4b}$$

In order to average $D(t)$ over thermal and numerical fluctuations, we repeated our simulations by generating M samples of the system; from those, one obtains the number of samples such that $\{\sigma_i(t)\}$ and $\{\tau_i(t)\}$ are still different at time t. We define the average distance $\langle D(t)\rangle$ only over those surviving samples.

We studied both ferromagnetic $(J_{ij}=J>0)$ and antiferromagnetic $(J_{ij}=J<0)$ cases and the updating of spins was either sequential or parallel. We simulated systems with a number of samples $M=40$ outside the critical region, going up to $M=250$ near criticality; sizes were taken up to $L=40$ $(N=L^2)$. The time averagings were taken over periods $t_2\approx\frac{1}{2}L^2$, after waiting for an equilibration transient $t_1\approx\frac{1}{2}L^2$. The initial condition was always $D(0)=1/N$; this is the smallest possible damage and with such a choice the results obtained are the most insensitive to the particular initial site(s) to be damaged.

Within the sequential updating we found strong evidence of correlation between the dynamic chaotic-frozen transition at a temperature T_s and the usual static phase transition at a temperature T_C. For the ferromagnetic case, T_s and T_C are indeed very close (essentially indistinguishable) as can be seen in Fig. 1, for $L=40$. For the antiferromagnetic case, we found only the chaotic regime for any finite temperature (see Fig. 1); this supports the argument of correlation between the above-mentioned transitions, since it is well known that the antiferromagnetic Ising model on the triangular lattice exhibits no static phase transition at a finite temperature.

However, for the parallel algorithm a very different

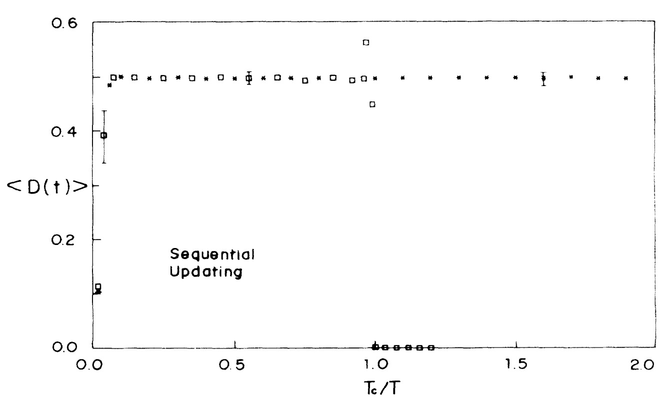

FIG. 1. The averaged damage $\langle D(t)\rangle$ for the sequential updating as a function of T_C/T, where T_C is defined as the Curie temperature of the ferromagnetic Ising model on the triangular lattice ($T_C=3.64096J$, in units of the Boltzmann constant). For the ferromagnetic case (□), the temperatures T_s and T_C are essentially the same, whereas for the antiferromagnetic one (∗), no frozen regime was found at any finite temperature. Both cases shown above are for $L=40$.

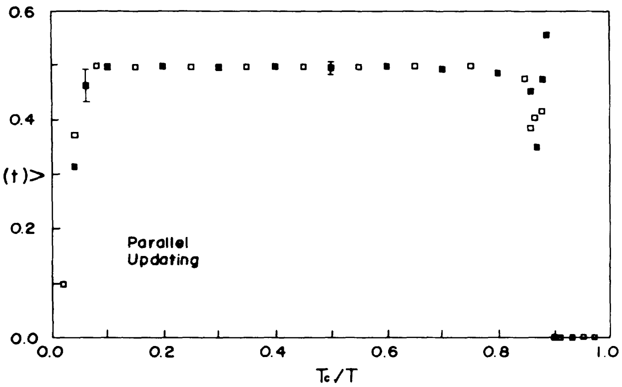

FIG. 2. The averaged damage $\langle D(t)\rangle$ for the ferromagnetic Ising model on the triangular lattice, within the parallel updating algorithm, for the sizes $L=20$ (■) and 40 (□). T_C is defined as in Fig. 1. This shows a significant shift between temperatures T_s and T_C, which is very insensitive to size changes.

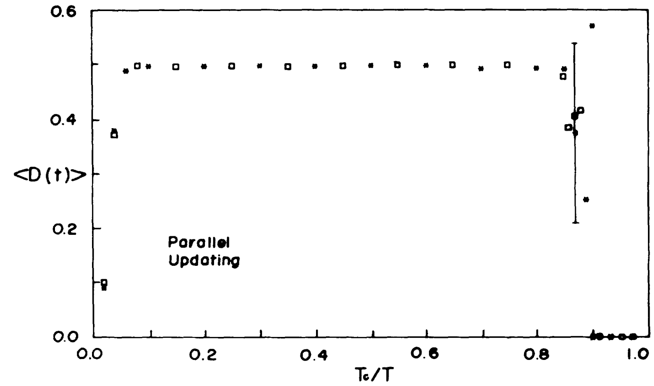

FIG. 3. The averaged damage $\langle D(t)\rangle$ for the ferromagnetic (□) and antiferromagnetic (∗) models, within the parallel updating. In both cases, $L=40$. T_C is defined as in Fig. 1. The points overlap within the error bars, showing that this algorithm is unable to distinguish positive from negative interactions. The temperature T_s is far from T_C (about 9% difference).

picture was observed, in disagreement with earlier arguments [12,13]. For ferromagnetic interactions, T_s and T_C are not as close as in the sequential case, as shown in Fig. 2 (about 9% difference) and this shift is very insensitive to the size L; this was verified for $L=20,40$. It would be desirable to simulate larger systems in order to check if $T_s \rightarrow T_C$, but from the sharpness of the transitions shown in Fig. 2, we believe this difference will persist as $L\rightarrow\infty$. For the antiferromagnetic case, a surprising result was found; a chaotic-frozen transition occurred with basically the same characteristics as the ferromagnetic one (see Fig. 3): essentially the same temperature T_s, which is also very insensitive to changes in the size of the system. Therefore, the parallel updating induced a dynamic transition which has no relation whatsoever with the static case; besides that, within this algorithm the system was not able to distinguish between positive and negative nearest-neighbor interactions.

This striking disagreement between sequential and parallel updating recipes for antiferromagnetic interactions is directly related to frustrations in the lattice [14]. By looking at an elementary triangular plaquette at $T=0$ (see Fig. 4), there are eight possible configurations associated with it: Two of them present higher energy [all spins up ($\sigma_i=1$) or all spins down ($\sigma_i=0$)], with all three bonds unsatisfied; the other six, which are lower in energy, always exhibit a single bond unsatisfied. One can easily see that in this case, $P_i^s(t)=0$ for configuration (a), whereas $P_i^s(t)=1$ for configuration (b) ($s=\sigma,\tau$ and $i=1,2,3$). For configurations (c)-(h), one can have, in this limit, $P_i^s(t)=0,\frac{1}{2},1$. Therefore, at low temperatures, if one starts the simulation in any of the eight configurations, Eqs. (4) give the following: (i) The sequential algorithm converges to the lower-energy states [(c)-(h)], with all of them being visited with equal probability ($p=1/6$). (ii) The parallel recipe leads after some time to one of two higher-energy states [(a) or (b)]; after that, the system jumps only between these two states (i.e., a circle of period 2, which corresponds to the lowest-energy states for the ferromagnetic problem), characterizing an erroneously induced breakdown of ergodicity. This may explain why this prescription does not recognize the sign of the interaction.

Finally, we conclude that the particular procedure used

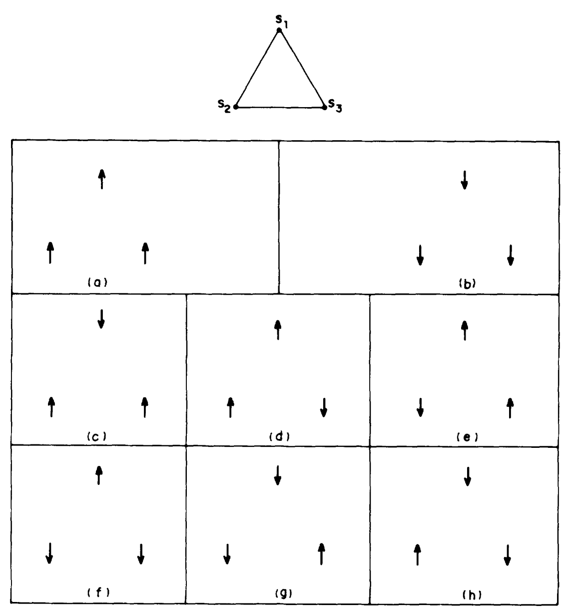

FIG. 4. The eight possible configurations associated with the elementary triangular antiferromagnetic Ising plaquette. In the sequential updating, the plaquette is allowed to visit all eight configurations, and after some time, it will choose the ones with lower energy [(c)-(h)]. In the parallel algorithm, once one of the configurations (a) or (b) is reached, the plaquette will jump only between these two states.

for the updating of spins is physically relevant when one intends to relate dynamic behavior in the long-time limit with pure equilibrium properties: The sequential algorithm seems to be more appropriate than the parallel one for such a purpose. In this Letter, we have shown an example where these two algorithms lead (in contrast with earlier expectations) to very distinct results, namely, the problem of damage spreading in the nearest-neighbor Ising model on a triangular lattice. The former procedure predicted a dynamic transition at a temperature very close to the usual Curie temperature for the ferromagnetic model, whereas in the antiferromagnetic case, no dynamic transition was found; this suggests that the equilibrium phase transition and the frozen-chaotic one are strongly correlated. The latter recipe was not able to discern the sign of the nearest-neighbor interaction, giving a similar dynamic transition for both ferromagnetic and antiferromagnetic cases at a temperature which was significantly different from the ferromagnetic Curie temperature.

Therefore, the use of parallel algorithms for updating spins is very questionable when one wishes to associate dynamic properties in the long-time limit with equilibrium ones: Whereas for ferromagnetic systems it may lead to an error in the estimation of the Curie temperature, for more complex systems where frustration is present, e.g., spin glasses, it may induce nonexistent phase transitions.

Stimulating discussions with C. Tsallis and H. J. Herrmann are gratefully acknowledged. This work was partially supported by CNPq (Brazilian Government).

[1] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
[2] H. E. Stanley, D. Stauffer, J. Kertész, and H. Herrmann, Phys. Rev. Lett. **59**, 2326 (1987).
[3] A. M. Mariz, H. J. Herrmann, and L. de Arcangelis, J. Stat. Phys. **59**, 1043 (1990).
[4] U. M. S. Costa, J. Phys. A **20**, L583 (1987).
[5] G. Le Caër, J. Phys. A **22**, L647 (1989).
[6] B. Derrida and G. Weisbuch, Europhys. Lett. **4**, 657 (1987).
[7] L. de Arcangelis, A. Coniglio, and H. J. Herrmann, Europhys. Lett. **9**, 749 (1989).
[8] H. B. da Cruz, U. M. S. Costa, and E. M. F. Curado, J. Phys. A **22**, L651 (1989).
[9] B. Derrida, J. Phys. A **20**, L721 (1987).
[10] B. Derrida, E. Gardner, and A. Zippelius, Europhys. Lett. **4**, 167 (1987).
[11] J. F. Fontanari and R. Köberle, Phys. Rev. A **36**, 2475 (1987); J. Phys. (Paris) **49**, 13 (1988).
[12] A. U. Neumann and B. Derrida, J. Phys. (Paris) **49**, 1647 (1988).
[13] O. Golinelli and B. Derrida, J. Phys. (Paris) **49**, 1663 (1988).
[14] G. Toulouse, Commun. Phys. **2**, 115 (1977).