Damage spreading in the Ising model with a microcanonical constraint

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We study damage spreading in the ferromagnetic Ising model, on the square lattice, by performing numerical simulations in the microcanonical ensemble. Although the damage spreads for all temperature values, a dynamical critical phenomenon is observed at $T_d = 1.020(2)T_C$ (T_C is the Curie temperature): For $T \geq T_d$ the damage $D(t)$ is insensitive to its initial value $D(0)$, while for $T < T_d$ a weak dependence on $D(0)$ is present in such a way that for each T there are two values of $D(t)$ corresponding to the initial conditions $D(0) < 1/2$ and $D(0) > 1/2$. We have also identified a convenient order parameter to characterize the transition occurring at T_d.

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In the past years, the evolution of computational systems has increased the use of numerical simulations as a convenient method of investigating static and dynamic physical properties of many-body systems, which are described by theoretical models with many degrees of freedom. The time evolution of physical systems can be studied by using suitable dynamic rules, permitting systems (via transitions between their microscopic configurations) to trace trajectories in phase space preserving some physical constraints (e.g., ergodicity) [1].

A useful method that has been employed to investigate how these trajectories are sensitive to small perturbations (chaos) is damage spreading, which consists of investigating the time behavior of the "difference" between two microscopic configurations of the same system. Besides, this approach has proved to be useful in giving information on the energy valley structure of the phase space [2–7].

To be more specific, we will consider a system of N boolean variables $\sigma(i) = 0, 1; i = 1, 2, \ldots, N$ localized on the sites of a square lattice. Two configurations of the system, say $A = \{\sigma_i^A(t)\}$ and $B = \{\sigma_i^B(t)\}$, have damage in a given site, when the corresponding variables are in different states. The total average damage $D(t)$ (or Hamming distance) is defined as the fraction of damaged sites, that is,

$$D(t) = \frac{1}{N} \sum_{i=1}^{N} \left| \sigma_i^A(t) - \sigma_i^B(t) \right| . \tag{1}$$

When the variables $\sigma(i)$ are related to the well-known Ising model, it is usual to employ the $S_i = 2\sigma_i - 1$ variables, interacting through a Hamiltonian (in the absence of external field) given by

$$H = -J \sum_{\langle i,j \rangle} S_i S_j , \tag{2}$$

where $J > 0$ (< 0) is the ferromagnetic (antiferromagnetic) exchange coupling between nearest-neighbor sites.

The damage spreading problem has been exhaustively investigated in the Ising model, and very interesting aspects were observed. To name a few, we have the following: (i) A dynamical phase transition may be present at a temperature T_d, separating the chaotic phase where the damage spreads, from the frozen phase where the damage heals; (ii) the temperature T_d is, in some cases, near (or equal to) the critical temperature T_c and, in other cases, has no apparent correlation with T_c; (iii) the damage spreading transition persists even in the presence of a magnetic field [8], which is not the case for the ferromagnetic-paramagnetic phase transition; (iv) there is a strong damage dependence on the particular dynamics (Glauber, heat-bath, Kawasaki, etc.) ruling the time evolution of the model.

The fact that the damage depends on the particular dynamics is somewhat cumbersome, since different dynamics used to simulate the thermodynamic behavior of the model have been successful (in this case, only one configuration is monitored in time). This has motivated the proposal of an alternative dynamics [9], which takes into account the orientation of the thermal noise in determining the transition probabilities. In fact, recent damage spreading simulations [10] on the Ising model using heat-bath, Glauber, and Metropolis dynamics, and considering explicitly the orientation of the stochastic field acting over the spins, yield the same temperature dependence for the long-time damage behavior.

The overwhelming majority of damage spreading sim-

ulations have been carried out within the context of dynamics defined in the canonical ensemble. As far as we know, the only damage study made in a microcanonical way (for the Ising model), was the work by Stanley *et al.* [3] by using the (nonergodic) Q2R dynamics. They found a qualitative change in the spreading phenomenon, near T_c, despite the fact that damage propagates for all temperatures.

Our main goal in this paper is to investigate the question of whether there is a dynamical critical phenomenon associated with damage spreading, in a microcanonical simulation of the ferromagnetic Ising model. We consider the model on the square lattice, using the dynamic rule for the time evolution of configurations proposed by Creutz [11], which has been shown to be appropriate for simulating critical fluctuations of Ising systems [12].

The Creutz algorithm employs a demon that sets up a walk through the lattice, trying to flip spins. The energy that the demon carries is bounded, and a move is accepted if the demon can supply (absorb) the energy required (released) by the system. Hence the total (system plus demon) energy is held constant during the simulation and, if the energy carried by the demon is small as compared to the system energy, a microcanonical ensemble describes the system evolution. We recall that, in microcanonical simulations, the energy is a control parameter and the temperature is calculated from the energy data of simulation.

We will consider two versions of the demon dynamics: the standard (SD) version proposed by Creutz, and a modified "orientational" (OD) version. The OD dynamics differs from the SD dynamics only with respect to the orientation of the thermal noise acting over the spins, as introduced in Ref. [9]. That is, those spins pointing in the direction of the thermal field are not flipped regardless of the demon state. In both implementations, we use a single demon to evolve the system and apply the multiple energy simulation technique [13], to simultaneously simulate as many systems as the size of the computer word, each one with different energy (temperature). The demon visits sequentially the sites of a square lattice, and the time unit is defined in such a way that each site is visited once.

Starting equilibrium configurations are obtained after 2000 time units, then a damage is created at $t = 0$ by flipping x spins in one of the configurations, corresponding to initial damage $D(0) = x/N$. We assure that both starting configurations have the same energy by hurting sites only if the energy cost is zero. It is worth pointing out that this constraint limits the size of the initial damage, being particularly restrictive for very low energies (temperatures). In the present simulation, we were not able to cause damage at temperatures below half the critical temperature. After allowing the damage to relax over a time of 2000 time units, its spreading is monitored during at least 20000 time units. Each configuration has its own demon, and both demons initiate in the same energy state. Note that the demon introduces a specific dynamics into the system, playing a role that is analogous to the random numbers in Monte Carlo based dynamics.

Figure 1 shows the temperature dependence of the

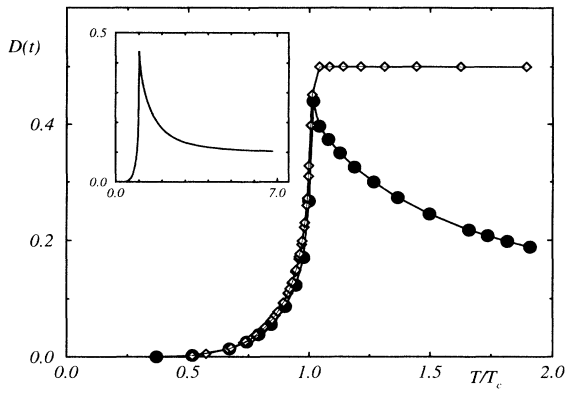

FIG. 1. Average damage $D(t)$ as function of the reduced temperature T/T_c for $D(0) = 1/N$ and 256×256 lattices, obtained from simulations employing the SD (diamonds) and OD (circles) dynamics. Note the very sharp peak (see inset) at $T_d = 2.315(4)$, in the case of OD dynamics.

long-time damage, obtained from simulations on lattices of size 256×256 and for initial damage $D(0) = 1/N$; each point corresponds to averages over at least 40 configurations. For both dynamics, the damage propagates for temperatures above and below the ferromagnetic critical temperature $k_B T_c = 2.2692J$, being almost indistinguishble in the low-temperature region and reaching a maximum at a temperature T_d slightly above T_c. For $T \geq T_d$ the damage obtained using the SD dynamics equals its maximum value of $D = 1/2$, which resembles the well-known result from Glauber dynamics. On the other hand (in contrast behavior for $T < T_d$), the effect of explicitly considering the orientation of the random field (that is, favoring smaller damages) is quite pronounced in the high-temperature region. It should be noticed that in the OD dynamics, the damage presents a very sharp peak very close to T_c (see inset), which, as far as we know, has not yet been observed for any other dynamics.

A better understanding of the problem is achieved by considering various values of the initial damage. For both dynamics we observe that the long-time damage at high temperatures does not depend on the initial conditions. This fact indicates that all possible states occur with equal probability, which might also be seen as an evidence of ergodicity of the demon algorithm.

In the low-temperature region, we have observed a *weak* sensibility on the initial conditions, resulting in only two distinct behaviors of the average damage, namely, $d(T)$ for the case of initial damage $D(0) < 1/2$ and $\tilde{d}(T)$ for $D(0) > 1/2$. The function $d(T)$ $[\tilde{d}(T)]$ is a monotonically nondecreasing (nonincreasing) function of T. In what follows, we shall define the dynamic critical temperature T_d as the temperature above which the average damage does not depend on the initial damage, that is $d(T) = \tilde{d}(T)$ for $T \geq T_d$. An appropriate way to describe the above related behavior is through the use of the quantity $\Psi(T) = \tilde{d}(T) - d(T)$, which acts like an "order parameter" measuring the sensibility (in a general sense) of the damage on the initial value.

Figure 2 illustrates the temperature dependence of the

order parameter Ψ, plotted as a function of the reduced temperature T/T_c, where we show the data from both dynamics on lattices of size 256×256. Typical errors for Ψ are ~ 0.001, being ~ 0.01 at points very close to T_c. In the case of the SD dynamics, where the relation $d(T)+\tilde{d}(T) = 1$ holds, we have numerically calculated the order parameter using both $\Psi = 1 - 2d$ and $\Psi = 2\tilde{d} - 1$. Actually, it can be shown that these relations hold for any dynamics that preserves the symmetrical damage during the time evolution, i.e., $D(t) = 1$ for all $t \geq 0$.

One can see that $\Psi(T)$ does exhibit a small dependence on the orientational noise, only in the critical region. Figure 2 also shows that the dynamic critical temperature T_d is about 2% above the ferromagnetic Ising critical temperature T_c. We obtained $T_d/T_c = 1.020(2)$ and results for $\Psi(T)$ calculated from simulations on square lattices of size up to 1024×1024 presented no dependence, at least within our estimated precision, with the system size. We have also noticed that $\Psi(T)$ has an inflection point at a temperature very close to T_c. In fact, the numerical derivative of $\Psi(T)$ shown a sharp peak at $T/T_c = 1.002(2)$, which is a very good estimate for T_c. Recall that within the context of the demon algorithm, the temperature is calculated from the data of simulation. In the neighborhood of T_c, the system temperature was determined within a precision of less than 1 part in 1000.

For $T < T_c$ the ferromagnetic Ising phase space has two attraction basins, corresponding to free-energy minima at opposite values of magnetization. Two microscopic configurations in the same (different) basins have damage less (greater) than 1/2. In our simulation we observe that for initial damage $D(0) < 1/2$ ($> 1/2$) the final long-time damage, namely, $d(T)$ [$\tilde{d}(T)$] preserves its initial condition; i.e., we obtain $d(T) < 1/2$ and $\tilde{d}(T) > 1/2$. This behavior can be interpreted as the absence of tunneling between the two attraction basins (at least for the present simulation times), which is further evidence to favor the use of the Creutz algorithm in studying thermal properties of the Ising model [14].

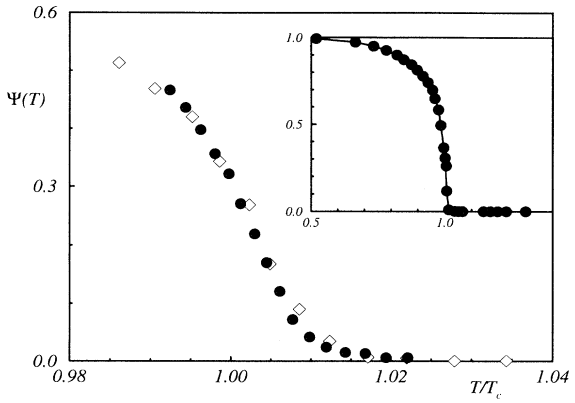

FIG. 2. The "order parameter" $\Psi(T)$, for the SD (diamonds) and OD (circles) dynamics. This quantity equals one for $T/T_c < 0.5$ (see inset) and goes to zero at the dynamic transition temperature T_d.

An additional comment should be made about the difference between the dynamic critical temperature T_d, and the equilibrium ferromagnetic critical temperature T_c. As already mentioned, we have found from simulations on lattices of size up to 1024×1024 that T_d remains about 2% above T_c. It would be of interest to make simulations on systems even larger than those we have worked with, in order to see whether such a discrepancy is a finite-size effect of very slow convergence or is it an intrinsic aspect of this phenomenon.

To conclude, we have observed a dynamical critical phenomenon in the damage spreading problem on a two-dimensional ferromagnetic Ising system, by performing simulations in the microcanonical ensemble. As compared with the canonical case (using single spin flipping rules like heat-bath and Glauber dynamics), where usually a frozen-chaotic transition is found, we have obtained a dynamical phase transition separating two chaotic regions.

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[1] *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1986).
[2] B. Derrida and G. Weisbuch, Europhys. Lett. **4**, 657 (1987); A.U. Neumann and B. Derrida, J. Phys. (France) **49**, 1647 (1988).
[3] H.E. Stanley, D. Stauffer, J. Kertész, and H.J. Herrmann, Phys. Rev. Lett. **59**, 2326 (1987).
[4] A. Coniglio, L. de Arcangelis, H.J. Herrmann, and N. Jan, Europhys. Lett. **8**, 315 (1988); L. de Arcangelis, A. Coniglio, and H.J. Herrmann, Europhys. Lett. **9**, 749 (1989).
[5] U.M.S. Costa, J. Phys A **20**, L583 (1987).
[6] A.M. Mariz, H.J. Herrmann, and L. de Arcangelis, J. Stat. Phys. **59**, 1043 (1990).
[7] F.D. Nobre, A.M. Mariz, and E.S. Sousa, Phys. Rev. Lett. **69**, 13 (1992).
[8] G. Le Caer, J. Phys. A **22**, L647 (1989).
[9] R.M.C. de Almeida, J. Phys. (France) I **3**, 951 (1993).
[10] M.F.A. Bibiano and F.G.B. Moreira (to be published).
[11] M. Creutz, Phys. Rev. Lett. **50**, 1411 (1983).
[12] A.J.F. de Souza and F.G.B. Moreira, Phys. Lett. A **167**, 387 (1992).
[13] A.J.F. de Souza and F.G.B. Moreira, Phys. Rev. B **48**, 9586 (1993).
[14] F.G.B. Moreira, A.J.F. de Souza, and A.M. Mariz (to be published).