Monte Carlo simulations of the violation of the fluctuation-dissipation theorem in domain growth processes

A. Barrat
International Center for Theoretical Physics, Strada Costiera 11, P.O. Box 563, 34100 Trieste, Italy
(Received 7 October 1997)

Numerical simulations of various domain growth systems are reported in order to compute the parameter describing the violation of fluctuation-dissipation theorem (FDT) in aging phenomena. We compute two-time correlation and response functions and find that, as expected from the exact solution of a certain mean-field model [equivalent to the $O(N)$ model in three dimensions, in the limit of N going to infinity], this parameter is equal to one (no violation of FDT) in the quasiequilibrium regime (short separation of times), and zero in the aging regime. [S1063-651X(98)05703-1]

PACS number(s): 02.50.Ng

The study of aging phenomena is currently the subject of many efforts, since this kind of behavior, for which a given system remains out of equilibrium at all available times, is present in many systems of interest, like spin glasses or structural glasses [1]. When concerned with the dynamics of a given system, it is usual to study the correlation function of an observable A,

$$C(t,t')=\langle A(t)A(t')\rangle \tag{1}$$

($\langle\ \rangle$ denotes an average over thermal noise) and the conjugated response function

$$R(t,t')=\left\langle \frac{\partial A(t)}{\partial h(t')}\right\rangle, \tag{2}$$

where h is an external field applied at time t'. Then, at equilibrium, these two-time quantities satisfy time translational invariance [TTI: the functions depend only on the difference of the two times $t-t'$] and the fluctuation dissipation theorem (FDT) relating correlation and response by $R(t-t')=(1/T)\partial C(t-t')/\partial t'$. On the other hand, for aging phenomena, since the dynamics is out of equilibrium, such equilibrium properties are not expected to hold. In the context of mean-field spin glasses, Cugliandolo and Kurchan have proposed the general following scenario, in the limit where the times t and t' go to infinity [2]: for small time differences $[(t-t')/t'\ll 1]$, the system is in quasiequilibrium, and the equilibrium properties hold; however, if $t-t'$ is not small with respect to t', the study of two-time quantities reveals that it is not at equilibrium [$C(t,t')$ depend explicitly on t and t']. Moreover, they have proposed to measure the violation of FDT by the function $X(t,t')$ where

$$R(t,t')=\frac{X(t,t')}{T}\,\frac{\partial C(t,t')}{\partial t'}, \tag{3}$$

with the important assumption (afterwards supported by the study of many different cases, see for example [3–7]) that, as t and t' go to infinity, it becomes a function of time only through $C(t,t')$:

$$R(t,t')=\frac{X(C)}{T}\,\frac{\partial C(t,t')}{\partial t'}. \tag{4}$$

This $X(C)$ has moreover received an interpretation in terms of effective temperature [8]. In the high-temperature phase of any system, X is equal to 1 since the system equilibrates and the equilibrium properties hold. In the low-temperature phase where aging phenomena appear, violations of FDT can be quantified by its departure from 1. In simulations or experiments, it is more convenient to look at an integrated response function: the system can be quenched under a magnetic field, which is cut off after a waiting time t_w (the relaxation of the magnetization is then measured, and found to depend on the waiting time), or it is quenched under zero field, and a field is applied after t_w. In this second case, the growth of the zero-field-cooled magnetization

$$M(t+t_w,t_w)=\int_{t_w}^{t+t_w}R(t+t_w,s)h(s)ds \tag{5}$$

is observed. The quasi-FDT relation (3) allows one to then write (for a constant field)

$$\frac{T}{h}M(t+t_w,t_w)=\int_{t_w}^{t+t_w}X(t+t_w,s)\frac{\partial C(t+t_w,s)}{\partial s}ds, \tag{6}$$

which, in the limit of large t_w, gives

$$\frac{T}{h}M(t+t_w,t_w)=\int_{C(t+t_w,t_w)}^{1}X(C)dC. \tag{7}$$

Then, if FDT is satisfied, we obtain a linear relation $(T/h)M(t+t_w,t_w)=1-C(t+t_w,t_w)$, independently of the system, while a deviation from this straight line in an M versus C plot indicates violation of FDT and gives information on X: different systems can have different types of violation of FDT. This kind of M-versus-C plot has been used to compute the value of X in the aging regime, analytically for various mean-field models [2,3,9], and using numerical simulations for the mean-field Sherrington-Kirkpatrick model [6], for the three-dimensional Edwards-Anderson model [4] (a more realistic spin glass), for the p spin in finite dimensions [5]. While, for the $p=2$ spherical p-spin model, equivalent to the $O(N)$ ferromagnetic model in three dimensions, X is zero [9], it is found to be constant for $p\geq 3$, and a nontrivial function of C for the Sherrington-Kirkpatrick and the three-dimensional Edwards-Anderson model. An numerical investigation of a glass forming binary mixture (in three dimensions) has also been made recently [7], with the result of a constant value of X.

In this paper, we report numerical simulations of various domain-growth systems (for a review on such systems, see [10]), for which it is expected [8] that X is zero in the aging regime. We examine Ising ferromagnetic systems in two and three dimensions at various temperatures, and with conserved or nonconserved order parameter. We also make a simulation of the Edwards-Anderson model in three dimensions, to show the striking difference of behavior.

We consider Ising spins s_i on a square or cubic lattice of linear size L, with ferromagnetic interactions. Starting from a random configuration, we quench the system at time 0 to temperature T and let it evolve according to Glauber dynamics, with a single-spin-flip algorithm (we will also consider later soft spins evolving through a Langevin equation). We then measure the spin-spin correlation function

$$C(t,t')=\frac{1}{N}\sum_{i=1}^{N}\langle s_i(t)s_i(t')\rangle \tag{8}$$

for an unperturbed system. It is known that this correlation function exhibits two time regimes: for $t-t'\ll t'$ (for simplicity we take $t'<t$), it decays rapidly from $1=C(t',t')$ to $q_{\rm EA}=m^2$, m being the magnetization at temperature T; then, for more separated times, it scales like $L(t)/L(t')$, where $L(t)$ is the characteristic size of the domains at time t. We also check that the domain sizes remain much less than L, thus ensuring that finite size effects are not significant. At a certain waiting time t_w, we take a copy of the system, to which a small, constant magnetic field is applied. We then measure the staggered magnetization

$$M(t+t_w,t_w)=\frac{1}{N}\sum_{i=1}^{N}\overline{\langle s_i(t_w+t)h_i\rangle}. \tag{9}$$

For spin glasses, the applied field can equivalently be taken uniform or random, since the interactions between spins are random. Taking a uniform field allows one to avoid averaging over the realizations of the field. On the other hand, for a ferromagnetic system, the action of a uniform field is to favor one of the phases, which will grow faster. The correct quantity to measure is therefore the response to a random field: the staggered magnetization (9). [In two dimensions, a random field destroys the long range order (see [11] for a review on the random field Ising model); however, the instability destroying it appears only for domain sizes growing exponentially with $1/h$ [12], so that this effect is not important as long as we work with small enough fields and at times not to long]. For simplicity, the random h_i are taken from a bimodal distribution ($h_i=\pm h$). The staggered magnetization is averaged over the realizations of h_i, and we checked linear response using various values of h (typically from 0.01 to 0.2). The sizes used are $L=600$ in two dimensions, and $L=80$ in three dimensions.

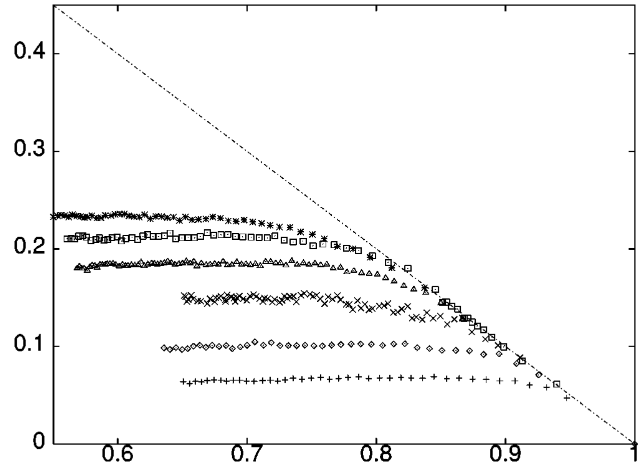

FIG. 1. $TM(t+t_w,t_w)/h$ vs $C(t+t_w,t_w)$ for two-dimensional domain growth ($T_c=2.27$), at temperatures (from top to bottom) $T=1.7$ and $t_w=200$, 400, 800, 2000, $T=1.3$ and $t_w=800$, $T=1$ and $t_w=800$. The straight line is $M=1-C$: we see that FDT holds at short times t, and the violation of FDT with $X=0$ at longer time separation.

To compare the various curves, obtained for various systems, temperatures and waiting times t_w, we look at the plots of $TM(t+t_w,t_w)/h$ versus $C(t_w+t,t_w)$. We first made some runs at high T: in this case, the system reaches quickly equilibrium, with TTI [$C(t_w+t,t_w)=C_{\rm eq}(t)$, $M(t+t_w,t_w)=M_{\rm eq}(t)$] and we checked that FDT holds [$TM_{\rm eq}(T)/h=1-C_{\rm eq}(t)$]. For temperatures below the transition temperature, a dependence on t_w appears in C and M (violation of TTI), corresponding to the growth of domains of the two competing phases. We observe as expected two time regimes [we stress that we are interested in long time limits, since the $X(C)$ function is defined as such; nevertheless, we already can observe two distinct regimes with finite times, and deduce the limit of interest]:

(i) For times t smaller than t_w, the two-times quantities do not depend on t_w, and FDT also holds: $TM(t+t_w,t_w)/h=1-C(t_w+t,t_w)$. This happens at large values of C (close to 1) and small values of M.

(ii) For larger times separation, we observe aging in the correlation function, and also clearly a deviation from FDT.

We show the data in Figs. 1–3 for the various systems, and for various waiting times. In the aging part, we see that the M versus C curves are in fact getting flat, except at small t_w. A closer look at the data for the aging part shows that (i) for larger t_w, the plateau reached by the magnetization is lower, and (ii) for a fixed t_w, the magnetization first grows [like $1-C(t_w+t,t_w)$, this is the nonaging part], then saturates, and eventually goes slowly down again, this last effect becoming less important as t_w grows, with a flattening of the curves (the slope of this part of the curves decreases as t_w increases). We can explain these effects in the following way: after t_w, the domains have reached a certain typical size, and the domain walls have a certain total length. The effect of the random field is then to try to flip some spins; this flipping will be easier at the domain walls, since the spins there are less constrained by their neighbors. Therefore

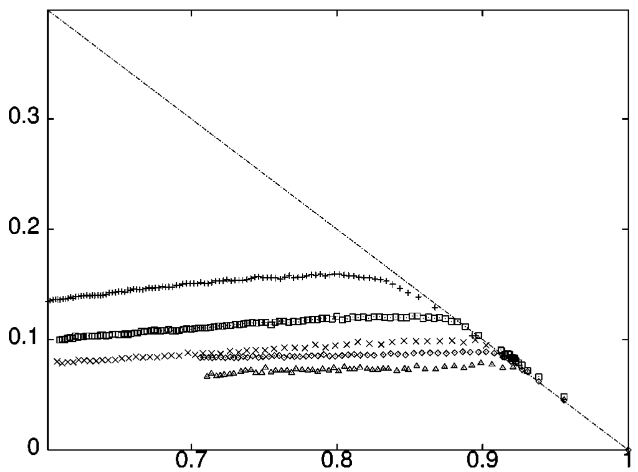

FIG. 2. Same as Fig. 1 for a nonconserved order parameter in three dimensions, $T=2.5$ ($T_c\approx 3.5$), $t_w=100$, 300, 600, 1000, 1500.

we have two contributions to the staggered magnetization: one from the bulk, and one from the domain walls. As time evolves, the domains grow and the total length (or surface, in three dimensions) of the domain walls decreases. Therefore, the contribution from the interfaces decreases. On the other hand, the contribution of the bulk will be rather independent of t_w, since the effect on a random field on a domain of $+$ spins or on a domain of $-$ is the same on average. The total staggered magnetization is thus decreasing when t_w increases, and also, at t_w fixed, as t grows (after the initial growth, when the field is switched on). In the limit of large t_w, the effect of the bulk becomes relatively more important, and we observe the flattening. (We have checked by a direct visualization of the spins that this is indeed what happens: at short times, the majority of the spins flipped by the random field are on the domain walls, this fraction going then down as the domains grow; we will also see that this effect due to the motion of domain walls is not present for the Edwards-Anderson spin glass.)

Note: the reciprocity relations, which state that, for two

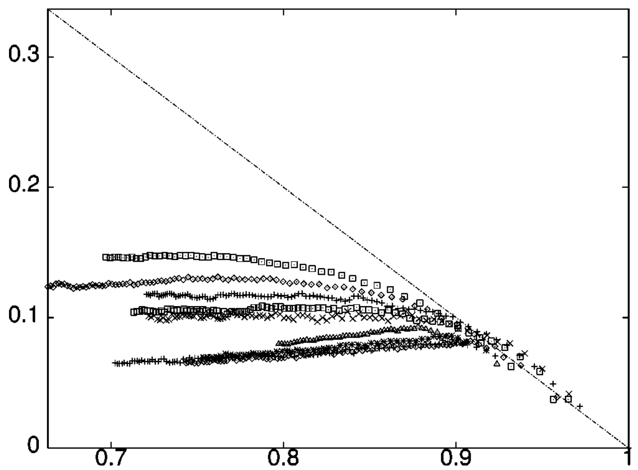

FIG. 3. Same as Fig. 1 for conserved order parameter in two dimensions, $T=0.8$ and from top to bottom $t_w=100$, 200, 400, 600, 800, and in three dimensions (lower symbols), $T=2$, $t_w=100$, 200, 300, 400.

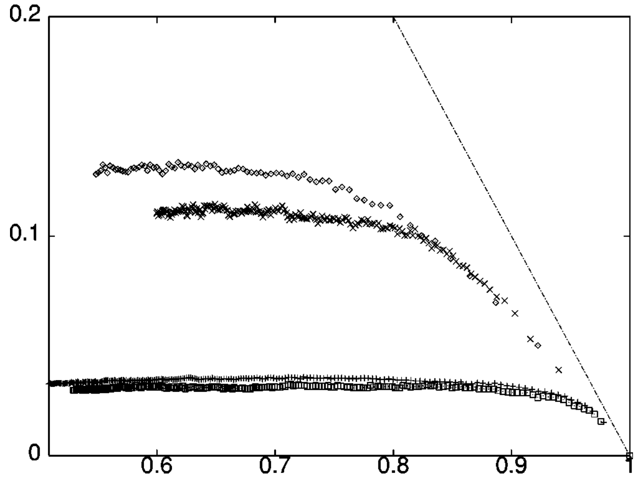

FIG. 4. Same as Fig. 1 for soft spins on a two-dimensional square lattice, evolving through (10), with, from top to bottom, $T=1$ and $t_w=200$, 600, $T=0.33$ and $t_w=200$, 600.

observables A and B, the correlations $C_{AB}(t,t')=\langle A(t)B(t')\rangle$ and $C_{BA}(t,t')$ are equal, are also an equilibrium theorem, and therefore are not expected to hold for aging dynamics. For a field ϕ evolving according to a Langevin equation, where the force at time t is $F(t)$, it can be shown [14] that, even if the asymmetry $\mathcal{A}(t,t')=\langle F(t)\phi(t')-F(t')\phi(t)\rangle$ goes to zero for long times, the integral $\int_0^t\mathcal{A}(t,t')dt'$ has a finite limit as t goes to infinity, if the system is out of equilibrium. Following a suggestion by Franz, and slightly modifying the simulation program, we checked that this fact, derived using the Langevin equation, also holds for a Monte Carlo dynamics, where the field is replaced by the spins, and the role of the force is played by the local field acting on the spins. We therefore mention this integrated quantity, which could also be of interest in the studies of aging phenomena.

Langevin equation: since similar results were obtained independently by Castellano and Sellitto [13] for a system of soft spins evolving through a Langevin equation, we also mention briefly this case, and show in Fig. 4 an example of the results that can be obtained with a system of this type: we simulate soft spins on a square lattice, with a quartic potential confining them to the vicinity of its minima $+1$ and -1, and evolving through the discretized Langevin equation

$$\begin{aligned} s(i,j,t+1)=s(i,j,t)+[&s(i+1,j,t)+s(i-1,j,t)+s(i,j+1,t)+s(i,j-1,t)-4*s(i,j,t)+s(i,j,t)\\ &-s(i,j,t)^3]*h+\eta(i,j,t), \end{aligned} \tag{10}$$

where $s(i,j,t)$ is the value of the spin at the lattice site (i,j) at time t, η is a Gaussian noise with zero mean and variance $2Th$, h being the used time step. We proceed by parallel updating of the field, and, at $t=0$, the $s(i,j)$ are taken as independent random variables uniformly distributed between -1 and 1. Again, at t_w a random field is switched on and the staggered magnetization and the correlation are measured.

All these simulations clearly show that the parameter X is zero for these domain-growth systems. This flattening of the integrated response shows that the long-term memory of

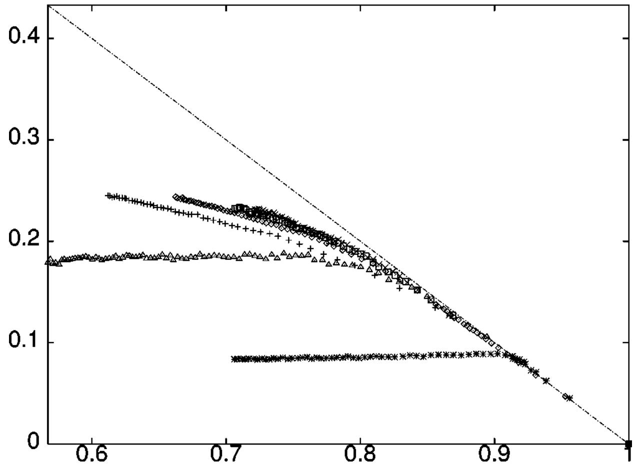

FIG. 5. Same as in Fig. 1 for the Edwards-Anderson model, $T=0.7$, from top to bottom $t_w=1000$, 600, 300, 100, compared to the data for the domain growth in two dimensions at $T=1.7$, $t_w=1000$ (highest plateau), and in three dimensions at $T=2.5$, $t_w=1000$ (lowest plateau).

such systems is in fact weak [8]: the aging phenomena are essentially in the correlations, while it is also important for the response in spin-glasses.

In Fig. 5, we indeed show the obtained data for an Edwards-Anderson system in three dimensions, with Hamiltonian

$$H=\sum_{\langle ij\rangle} J_{ij}s_is_j\,, \tag{11}$$

where the sum is over nearest neighbors, the spins s_i are Ising spins, and the couplings J_{ij} are quenched random variables, taking values $+1$ or -1 with equal probability.

We simulated a system of linear size $L=80$ at $T=0.7$. Although no precise conclusion can be drawn as to the form of the function $X(C)$, since the obtained curves still show a dependence on t_w, it is quite clear (as was shown in [4]) that they tend to a certain nontrivial curve, very different from the case of domain growth systems, like the comparison of Fig. 5 shows. Let us remark that curves similar to the ones obtained for the EA spin glass have also been obtained for the p-spin model in three dimensions in [5] and for the mean-field version of Eq. (11), the Sherrington-Kirkpatrick model [6].

To conclude, we have reported measurements of the violation of the fluctuation-dissipation theorem in some systems exhibiting domain growth, and found that, as expected but shown only in one particular case, the parameter X describing it is equal to zero in the aging phase (and of course to 1 in the quasiequilibrium regime, where FDT holds). In the interpretation of [8], this means that the effective temperature is the temperature of the heat bath in the quasiequilibrium regime (corresponding to the fast relaxation of the spins in the bulk of the domains), while it is infinite in the coarsening regime, which corresponds to the dynamics of the domains themselves (see [8], Sec. IV-C for a detailed discussion). It should also be noted that this behavior shows a tendency of the long-term memory to disappear, in contrast with spin glasses or glasses.

It is a pleasure to thank C. Castellano and S. Franz for interesting discussions. This work was motivated by discussions with L. Cugliandolo and J. Kurchan.

[1] See, for example J.-P. Bouchaud, L. F. Cugliandolo, J. Kurchan, and M. Mézard, Spin Glasses and Random Fields, edited by A. P. Young (World Scientific, Singapore, in press), e-print cond-mat/9702070.

[2] L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. **71**, 173 (1993); J. Phys. A **27**, 5749 (1994).

[3] L. F. Cugliandolo, J. Kurchan, and P. Le Doussal, Phys. Rev. E **53**, 1525 (1996).

[4] S. Franz and H. Rieger, J. Stat. Phys. **79**, 749 (1995).

[5] D. Alvarez, S. Franz, and F. Ritort, Phys. Rev. B **54**, 9756 (1996).

[6] H. Takayama, H. Yoshino, and K. Hukushima (unpublished).

[7] G. Parisi, Phys. Rev. Lett. **79**, 3660 (1997).

[8] L. F. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E **55**, 3898 (1997).

[9] L. F. Cugliandolo and D. S. Dean, J. Phys. A **28**, 4213 (1995).

[10] A. J. Bray, Adv. Phys. **43**, 357 (1994).

[11] T. Nattermann, *Spin Glasses and Random Fields* (Ref. [1]), cond-mat 9705295.

[12] K. Binder, Z. Phys. B **50**, 343 (1983).

[13] C. Castellano (private communication).

[14] S. Franz (private communication).