

## Monte Carlo studies of Ising spin-glass systems: Aging behavior and crossover between equilibrium and nonequilibrium dynamics

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(Received 14 February 1992)

The crossover between quasiequilibrium and nonequilibrium spin-glass dynamics has been studied in Monte Carlo simulations of two- and three-dimensional short-range Ising spin-glass systems. The spin system was quenched in zero field to a low temperature  $T$ . After equilibrating for a time  $t_w$ , a weak magnetic field was applied and the time dependence of the magnetization  $M(t)$  and the spin autocorrelation function  $q(t)$  was studied. Our results show that the relaxation rate  $S(t) = \partial M(t) / \partial \log_{10}(t)$  exhibits a maximum at  $t \approx t_w$ . If the temperature is lowered or raised, immediately prior to the field application, the apparent age ( $t_a$ ) of the system, as defined by the maximum in relaxation rate, is shifted to longer or shorter time scales, respectively. No significant differences between the aging behavior in two and three dimensions are found. The relation  $\chi(t) = [1 - q(t)] / T$  holds only for short time scales ( $t \ll t_w$ ), clear deviations are found at longer time scales ( $t > t_w$ ). Since this relation should according to the fluctuation-dissipation theorem hold for a system in equilibrium, this result is interpreted as an indication of a crossover between equilibrium and nonequilibrium dynamics. Our results are qualitatively in agreement with experiments as well as with theoretical models for the nonequilibrium spin-glass dynamics.

### I. INTRODUCTION

Results from Monte Carlo (MC) simulations have provided valuable information for the understanding of spin glasses. Furthermore, simulations provide access to quantities and concepts introduced in theory that are not experimentally accessible. The complexity of the problem, however, has made it necessary to use special purpose machines<sup>1</sup> and parallel computers<sup>2</sup> to reach conclusive results. Even with this tremendous computational effort, open questions still remain, such as the controversy on the degeneracy of the ground state in the spin-glass phase.<sup>3,4</sup> Considering this, one might ask if it is possible to gain new insight using only relatively limited computer power. This has to be answered in the affirmative, for the simple reason that the majority of the simulations have been aimed at studying the static and the equilibrium properties of spin glasses. At temperatures below and close to the spin-glass temperature, this is a notoriously difficult problem since, due to the very slow dynamics of spin glasses, it is virtually impossible to reach equilibrium, at best a state that resembles equilibrium relatively closely can be found. Even experimental investigations of spin glasses are plagued with the same kind of problem and a real spin-glass material is effectively never in equilibrium below  $T_g$  on experimental time scales. Only after a sufficiently long equilibration of the spin system, a behavior at short time scales of the spin-glass dynamics almost as in equilibrium can be achieved: This is usually referred to as the spin glass being probed under a quasiequilibrium condition. This fact can be used in simulations of the equilibrium dynamics of spin glasses below the spin-glass temperature. Still it is evident that the equilibration process itself is almost as

interesting as the equilibrium properties, and this part of the problem has mostly been neglected.

Our work considers the equilibration process and more specifically the phenomenon of aging. Aging was found in 1983 in experiments by Lundgren *et al.*<sup>5</sup> and is manifested in the fact that below the spin-glass temperature the magnetic response depends on the time  $t_w$  spent below this temperature or, stated slightly differently, how far the equilibration process has proceeded.

In our simulations, we have tried to find answers to the following questions.

Is it possible to observe the same kind of behavior in simulations as is found in aging experiments?<sup>6-19</sup> Is the simple simulation method capable of capturing the essential features of aging or do we need to use more complicated ones? Does the difference in time scales between simulations and experiments play an important role?

What is the reason for the wait time dependence of the response? This involves finding out what causes the very slow dynamics (by making comparisons to the existing theories<sup>20-23</sup>) and also finding out what causes the maximum in the relaxation rate  $S(t) = \partial M / \partial \ln(t)$  at a time  $t \sim t_w$ .

Are there dimensionality-dependent features? Does the fact that the lower critical dimensionality for an Ising spin glass is  $2 < d_l < 3$  (Refs. 24 and 25) make the aging behavior any different in two dimensions than in three dimensions?

In this paper we present results that answer some of these questions. We are, however, far from being able to present a complete description of the aging behavior in spin glasses. The results are in good qualitative agreement with the experimental findings. One result of our simulations may seem a bit controversial, namely that the

relation  $\chi(t)=[1-q(t)]/T$ , which is a consequence of the fluctuation-dissipation theorem (FDT),<sup>26</sup> does not always hold. However, since the FDT assumes equilibrium conditions, the fact that this equation does not hold simply indicates nonequilibrium conditions. Thus the violation of the equation is not a violation of the FDT, but can rather be used to illustrate the crossover from equilibrium to nonequilibrium dynamics. We have been careful making sure that this result is not caused by finite-size or by nonlinear effects.

The outline of this paper is as follows: In Sec. II, different kinds of experimental procedures and results are reviewed to give the background for the simulations. In Sec. III, the theoretical background needed to interpret our results is given. In Sec. IV, the details of how the simulations were performed are presented. In Secs. V and VI, the results of the simulations are presented.

## II. AGING EXPERIMENTS

The aging phenomenon was reported in 1983 by Lundgren *et al.*,<sup>5</sup> and has since then been the subject of many experimental studies on a variety of spin-glass systems.<sup>6-19</sup> In the great majority of these experiments, the aging phenomenon was studied by time-dependent zero-field-cooled (ZFC) (Ref. 6) or thermoremanent (TRM) (Ref. 7) magnetization measurements. TRM and ZFC experiments yield similar results and we will therefore in the following restrict ourselves to describe the ZFC magnetization. The spin glass is cooled in zero field to a temperature below the spin-glass transition temperature,  $T_g$ . After a waiting time  $t_w$ , a small field is applied and one observes the relaxation of the magnetization. It is found that the time dependence of the magnetization depends on the waiting time  $t_w$ , which implies that the spin system is in a nonequilibrium state during the waiting time even though experimentally one detects no changes of the magnetization. The most striking feature of the time-dependent magnetization is an inflection point in the  $M(t)$  vs  $\log_{10}(t)$  curve and a corresponding maximum in the relaxation rate  $\partial M/\partial \ln(t)$  at an observation time  $t \sim t_w$ .

The  $t_w$  dependence of  $M(t)$  has also been shown to exist at temperatures above  $T_g$ .<sup>6,8</sup> The experimental results show that the  $t_w$  dependence persists until the waiting time is larger than the largest relaxation time of the spin system,  $t_w > \tau_{\max}$ . This implies that since  $\tau_{\max} = \tau_0(1 - T/T_g)^{-z\nu}$  ( $z\nu \sim 10$  and  $\tau_0 \sim 10^{-13}$  sec),  $M(t)$  is found to be  $t_w$  dependent at temperatures below  $T/T_g \sim 1.02$ . In two-dimensional (2D) spin glasses no ordered spin-glass phase exists above zero temperature. The relaxation of the magnetization is, however, due to large-scale spin-glass fluctuations, found to extend to very long time scales at low temperatures. In view of the observation of aging in 3D spin glasses at  $T > T_g$ , it is not surprising that the aging phenomenon has also been experimentally observed in 2D spin glasses.<sup>9-11</sup>

In temperature shift experiments,<sup>12,13</sup> the spin glass is cooled in zero field to a temperature  $T + \Delta T$  below  $T_g$ . After a waiting time  $t_w$  at this temperature, immediately prior to the field application, the temperature is lowered

or raised to  $T$ . The resulting relaxation curves  $M(t)$  vs  $\log_{10}(t)$  will show inflection points [or, equivalently, the  $\partial M/\partial \ln(t)$  vs  $\log_{10}(t)$  curves will show maxima] at observation times different from  $t_w$ . In an undercooling experiment ( $\Delta T$  negative) the apparent age  $t_a$ , as defined by the maximum in the  $\partial M/\partial \ln(t)$  vs  $\log_{10}(t)$  curve, is shifted to shorter times while in an overheating experiment ( $\Delta T$  positive) the apparent age is shifted to longer times. Results from undercooling experiments show that the logarithmic shift of the apparent age  $\log_{10}(t_w/t_a)$  varies linearly with  $\Delta T$ .<sup>12</sup>

In temperature cycling experiments,<sup>14-16</sup> the sample is cooled in zero field to a temperature  $T$  below  $T_g$ . After a waiting time  $t_{w1}$ , the temperature is changed to  $T + \Delta T$ . The sample is then kept at this temperature for a waiting time  $t_{w2}$  and, immediately prior to the field application, the sample temperature is changed back to  $T$ . Both positive<sup>14,15</sup> and negative<sup>16</sup> temperature cycles are possible. Depending on the magnitudes of  $\Delta T$ ,  $t_{w1}$ , and  $t_{w2}$ , the resulting relaxation curves will show different characteristics. In positive temperature cycling experiments,  $t_{w2}$  is generally kept small  $t_{w2} \ll t_{w1}$ . For  $\Delta T$  small,  $\Delta T$  typically smaller than a few percent of  $T_g$ , the aging process will be unaffected by the temperature cycling, i.e., the  $\partial M/\partial \ln(t)$  vs  $\log_{10}(t)$  curves will show maxima at  $t \sim t_{w1}$ . For  $\Delta T$  sufficiently large, the maximum in the  $\partial M/\partial \ln(t)$  curve will be suppressed to much shorter times  $t \sim t_{w2}$ , i.e., the aging process will be "reborn." For temperature cycles of intermediate magnitude, two maxima in the relaxation rate will appear, one at  $t \sim t_{w1}$  and the other one at  $t \sim t_{w2}$ .

It should be noted that aging effects have also been observed in ac susceptibility  $\chi(\omega)$ ,<sup>10,14,17,18</sup> and magnetic noise  $S(\omega)$  (Ref. 19) measurements. For sufficiently low frequencies, following a quench to a temperature below  $T_g$ , both  $\chi(\omega)$  and  $S(\omega)$  are found to decrease with time.

## III. AGING THEORY

Different theoretical models have been proposed to describe the aging phenomenon in spin glasses.<sup>20-23</sup> The models can be divided into (i) hierarchical phase-space models where the dynamics below the transition temperature is coarse grained into a Markov process on a tree structure<sup>20,21</sup> and (ii) real space "droplet" models based on a scaling ansatz for the low-energy, large length scale excitations in the spin-glass phase.<sup>22,23</sup> The hierarchical phase-space picture has been able to reproduce some of the experimental findings, e.g., a maximum in the relaxation rate at an observation time  $t \sim t_w$ ,<sup>20</sup> and a logarithmic shift of the apparent age, studied in undercooling shift experiments, that varies linearly with  $\Delta T$ .<sup>21</sup> Although this model captures some features of the spin-glass relaxation, it is not in its present form capable of explaining results found in, e.g., temperature cycling experiments. Therefore, we have chosen to analyze our MC results in the context of the "droplet" model, even though we do not present any temperature cycling simulations in this paper.

In the droplet model, at fixed temperature below the spin-glass transition temperature, only two pure states ex-

ist related by a global spin reversal. The dominant excitations are large-scale coherent spin-glass fluctuations, droplets, which occur on a length scale  $L$ . The dynamics of these droplets is governed by thermal activation over barriers of characteristic magnitude  $\Delta(T)L^\Psi$ , where  $\Delta(T)$  sets the free-energy scale of the barriers and  $\Psi$  is the barrier exponent.  $\Delta(T)$  is expected to go to zero as  $\sim(1-T/T_g)^\nu$ , where  $\nu$  is the correlation length exponent, and  $\Delta(T)$  is also expected to be weakly temperature dependent for  $T \ll T_g$ . After a temperature quench to a temperature below  $T_g$ , the spin system will be out of equilibrium and the spin configuration can be divided into spin-glass domains. The spin system will lower its energy by the growth of larger and larger domains, a process which is logarithmically slow in time,  $R(t) \sim [T \ln(t/\tau_0)/\Delta(T)]^{1/\Psi}$  ( $\tau_0$  is a microscopic spin-flip time). Recent MC simulation results support such a growth law.<sup>27</sup> If the system is equilibrated for a waiting time  $t_w$  and then probed in a ZFC magnetization measurement, the response to the field application can be divided into different time regimes. At times  $t \ll t_w$ , the magnetization grows through the polarization of active droplets of size  $L(t) \sim [T \ln(t/\tau_0)/\Delta(T)]^{1/\Psi}$ . Since the droplet size in this case is much smaller than the characteristic domain size  $R(t_w+t)$ , the droplet excitations will, apart from a small fraction close to domain walls, be those of the pure states. In this time regime, quasiequilibrium dynamics will be probed. For times  $t \gg t_w$ , the magnetization cannot grow through the polarization of droplets of size smaller than  $R(t_w+t)$ , instead the magnetization will increase with the growth of  $R(t_w+t)$  and the dynamics can be described as nonequilibrium dynamics. At times  $t \sim t_w$ ,  $L(t) \sim R(t+t_w)$ , there is a crossover from equilibrium to nonequilibrium dynamics. In experiments, this crossover is visible as a maximum in  $\partial M/\partial \ln(t)$ . While the droplet theory can account for the fact that there is a crossover, there is no explanation given for the maximum in  $\partial M/\partial \ln(t)$ .

Results from temperature cycling experiments can in the droplet model be explained using the overlap correlation function

$$\Xi(i, j, T, T + \Delta T) = \overline{\langle S_i S_j \rangle_T \langle S_i S_j \rangle_{T + \Delta T}},$$

which will decay with increasing distance  $r_{ij} = |i - j|$  with the characteristic length scale  $L_{\Delta T}(T)$ . This correlation function tells us that the positions of large-scale active droplets will differ from any one temperature to another and thus that the equilibrium states at the temperatures  $T$  and  $T + \Delta T$  will differ at length scales larger than  $L_{\Delta T}(T)$ . The interpretation of temperature cycling experiments is given in Ref. 23.

In temperature shift experiments, as long as the overlap length  $L_{\Delta T}$  is larger than the domain size  $R$ , the crossover between equilibrium and nonequilibrium dynamics [indicated by a maximum in the relaxation rate  $\partial \chi/\partial \ln(t)$  at a time  $t = t_a$ ] will occur when  $L(t_a, T) \sim R(t_w, T + \Delta T)$ , which can be written

$$\frac{T_1 \ln(t_w/\tau_0)}{\Delta(T_1)} = \frac{T_2 \ln(t_a/\tau_0)}{\Delta(T_2)}. \quad (1)$$

In the case of  $T_1 = T + \Delta T$  and  $T_2 = T$ , this expression can be rewritten as

$$\ln \left[ \frac{t_a}{t_w} \right] = \left[ \frac{T + \Delta T}{T} \frac{\Delta(T)}{\Delta(T + \Delta T)} - 1 \right] \ln \left[ \frac{t_w}{\tau_0} \right]. \quad (2)$$

If  $\Delta(T)$  is weakly temperature dependent, the logarithmic shift of the apparent age will simply be given by

$$\ln \left[ \frac{t_a}{t_w} \right] \approx \frac{\Delta T}{T} \ln \left[ \frac{t_w}{\tau_0} \right]. \quad (3)$$

#### IV. MODEL AND METHOD OF SIMULATION

We have used the standard model of a spin glass,<sup>28</sup> with the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} S_i S_j - h \sum_i S_i, \quad (4)$$

where the exchange interactions  $J_{ij}$  between the spins were chosen randomly from a Gaussian distribution with zero mean and width  $J$ . Only nearest-neighbor interactions were considered. Helical boundary conditions were used and the spins were updated according to the standard kinetic Ising Monte Carlo algorithm.<sup>29</sup> The starting configuration was chosen randomly. This corresponds to a quench from infinite temperature to a low temperature  $T$ . Since we are interested in the nonequilibrium properties, the spin system was equilibrated only for a relatively short time, the equilibration time  $t_w$ . After this equilibration time a small magnetic field  $H$  was applied. The magnetization  $M(t) = N^{-1} \sum S_i(t)$  and the autocorrelation function  $q(t) = N^{-1} \sum S_i(t) S_i(0)$  were then studied for different equilibration times  $t_w$ . For each partially equilibrated configuration, phase-space trajectories were obtained for both positive and negative field  $H$ . This removes effects that are not caused by the application of the field, but are rather caused by the particular choice of bond configuration and initial configuration. The magnetization and the autocorrelation function were calculated continuously. The results at each Monte Carlo step were used to get average values at logarithmically spaced times. The simulation procedure was repeated for  $N_{tr}$  statistically independent trajectories, originating from different starting configurations. Depending on system size  $N^d$ ,  $N_{tr}$  was varied to keep  $N_{tr} N^d$  approximately constant. In some cases, averages were also taken over different bond configurations. Bond averaging did not alter the characteristics of the quantities studied, merely improved the accuracy in the simulations.

The simulations were performed for two-dimensional lattices of size up to  $200^2$  and three-dimensional lattices were of size up to  $60^3$ . All results presented in this paper are for sizes  $200^2$  and  $60^3$ , respectively, and  $N_{tr} = 10$ , unless stated otherwise. All temperatures and fields are given in terms of  $J$  (the width of the Gaussian distribution of interactions). The simulations were performed on Digital DECstation work stations.

## V. RESULTS OF NORMAL AGING SIMULATIONS

In the simplest kind of aging simulation the equilibration temperature and the measurement temperatures are equal. In Fig. 1 the susceptibility  $\chi(t)=M(t)/H$  ( $H=0.03J$ ) and the relaxation rate  $S(t)=\partial\chi(t)/\partial\log_{10}(t)$  are shown for different equilibration times  $t_w$  for a three-dimensional system at the temperatures  $T=0.10J$  and  $T=0.30J$ . There is a characteristic inflection point in  $\chi(t)$  and a corresponding maximum in  $S(t)$  at  $t \approx t_w$ , in accordance with experimental findings. Most of our results have been obtained at the temperature  $T=0.10J$ , but the same characteristic be-

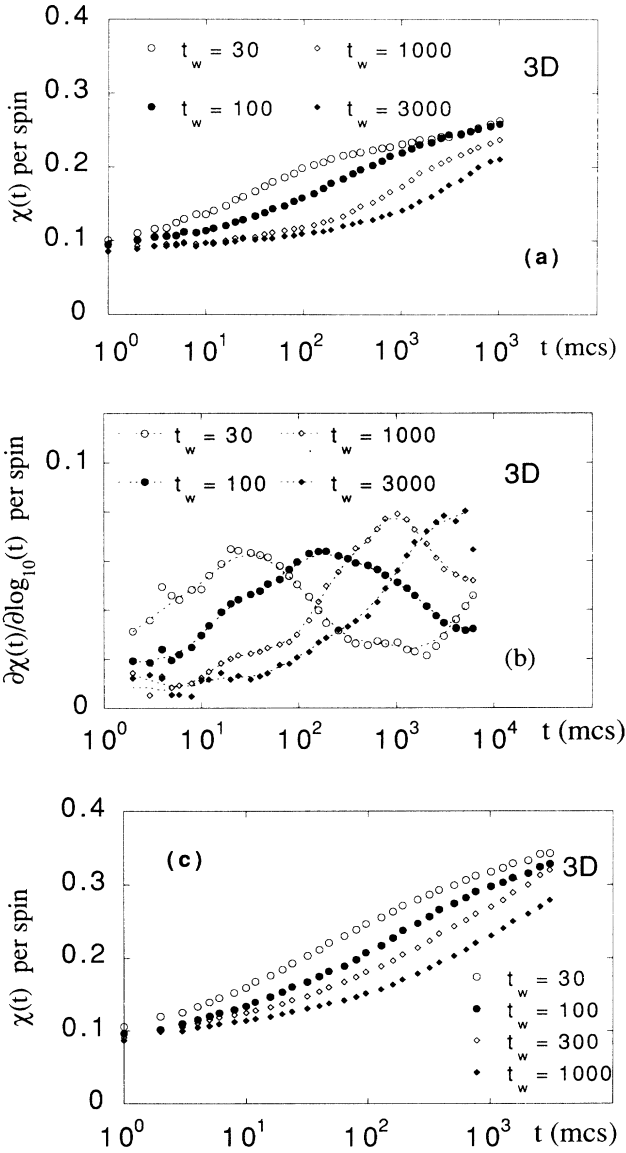


FIG. 1. (a) Susceptibility  $\chi(t)=M(t)/H$  ( $H=0.03J$ ) for different wait times  $t_w$  at the temperature  $T=0.1J$  for a 3D system of size  $60^3$ . (b) The corresponding relaxation rate  $S(t)=\partial\chi(t)/\log_{10}(t)$ . (c) The susceptibility  $\chi(t)=M(t)/H$  ( $H=0.03J$ ) for different wait times  $t_w$  at the temperature  $T=0.3J$  for a 3D system of size  $60^3$ .

havior of  $\chi(t)$  was observed for all temperatures investigated  $0.02 \leq T/J \leq 0.6$ . The only significant temperature-dependent feature of  $\chi(t)$  is an increase with temperature of the relaxation rate at short time scales.

In most of our simulations we have used the field  $H=0.03J$ . The basis for this choice is, on the one hand, to be in the linear response regime and, on the other hand, to keep a reasonable signal-to-noise ratio in the quantities studied. In Fig. 2  $\chi(t;H)$  is shown for different fields  $H$  for a 3D system at the temperature  $T=0.10J$  and for the equilibration time  $t_w=1000$  MC steps per spin (mcs).  $\chi(t;H)$  is independent of  $H$  within the accuracy of the simulations for  $H \leq 0.05J$  and the differences are not too large even for fields up to  $H=0.10J$ . Furthermore, for fields  $H \leq 0.03J$  we find that  $q(t;H)=q(t;H=0)$ . Based on these results,  $H=0.03J$  is well within the linear response regime.

Finite-size effects should always be considered in simulations. Such effects are known to drastically influence the equilibrium behavior in the spin-glass phase<sup>30</sup> as well as the behavior of  $q(t)$  at long time scales.<sup>1</sup> However, since we are interested in the finite-time nonequilibrium behavior of the spin-glass dynamics and are limited by the available computer power to study the dynamics at relatively modest time scales, we are likely to be less influenced by finite-size effects. Indeed, for the lattice sizes studied, in 2D from  $20^2$  to  $200^2$  and in 3D from  $8^3$  to  $60^3$ , there are no indications of finite-size effects.

While in experiments the usual way to study the system is by observing the susceptibility  $\chi(t)=M(t)/H$  in the zero-field limit, in theory and in most simulations the autocorrelation function  $q(t)$  is normally studied. The reason why the autocorrelation function is used in simulations is that no field  $H$  is needed. By applying a field the system is disturbed. When determining  $M(t)$  the nonlinear effects have to be negligible, while still retaining a reasonable signal-to-noise ratio. The basis for using  $\chi(t)$  and  $q(t)$  interchangeably is that  $\chi$  and  $q$  are related in equilibrium by the fluctuation-dissipation theorem (FDT),<sup>26</sup>

$$\chi=(1-q)/T, \quad (5)$$

where  $q=\lim_{H \rightarrow 0} \lim_{N \rightarrow \infty} [\langle S_i \rangle_T^2]_{av}$ . This relation can

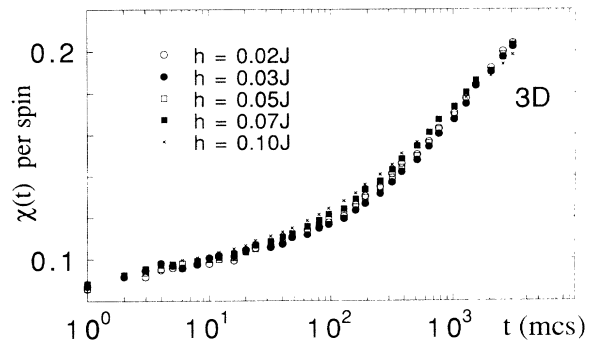


FIG. 2. Susceptibility  $\chi(t)=M(t)/H$  for different fields  $H$  at the temperature  $T=0.1J$  for a 3D system of size  $60^3$ .  $t_w=1000_0$  mcs.

be generalized to the time-dependent quantities  $\chi(t)$  and  $q(t)$ :

$$\chi(t) = [1 - q(t)] / T. \quad (6)$$

A necessary requirement, for this relation to hold, is that the time-dependent quantities are representative of an equilibrium situation. Since spin glasses, at low temperatures, are effectively always out of equilibrium, we cannot assume this relation to be satisfied in general. There is experimental evidence that FDT still holds, based on magnetic noise and ac susceptibility measurements.<sup>19,31,32</sup>

However, such measurements are always performed *in or close to quasiequilibrium conditions*, with the equilibration time longer or even much longer than the measurement time ( $\sim \omega^{-1}$  where  $\omega$  is the angular frequency). Furthermore, the experimental resolution in magnetic noise measurements is relatively poor (unless one averages over many noise spectra), which makes a compar-

ison between time-dependent ac susceptibility and magnetic noise data difficult. Therefore, these measurements can hardly be used as evidence for Eq. (6) being satisfied in a nonequilibrium situation.

Since in most simulations reported hitherto the equilibrating procedure has been dealt with carefully, the use of Eq. (6) is clearly justified. In the kind of simulations we have performed the situation is different. In Fig. 3  $\chi(t)$  and  $[1 - q(t)] / T$  are plotted for a 3D system at the temperature  $T = 0.10J$ . The different curves correspond to different equilibration times  $t_w$ . This figure clearly shows that Eq. (6) is only satisfied for short time scales  $t/t_w \ll 1$ , large deviations are seen at longer time scales  $t/t_w > 1$ . Since equilibrium is assumed in the FDT, the results are not indicative of a violation of the FDT. Rather, a violation of Eq. (6) is an indication of nonequilibrium conditions. Therefore, the results shown in Fig. 3 can be interpreted as a crossover from quasiequilibrium to nonequilibrium dynamics.

Notice that  $1 - q(t)$  behaves in some ways as is expected in the droplet theories: a slow relaxation at short times corresponding to the quasiequilibrium dynamics and a faster relaxation at longer times corresponding to nonequilibrium dynamics. On the other hand,  $M(t)$  behaves in another way, and in fact there is no explanation for this in any of the spin-glass theories. Even though there is a crossover at  $t \approx t_w$  in both  $M(t)$  and  $q(t)$  and the crossover behavior is easily seen in both quantities, it is much easier to determine at which time

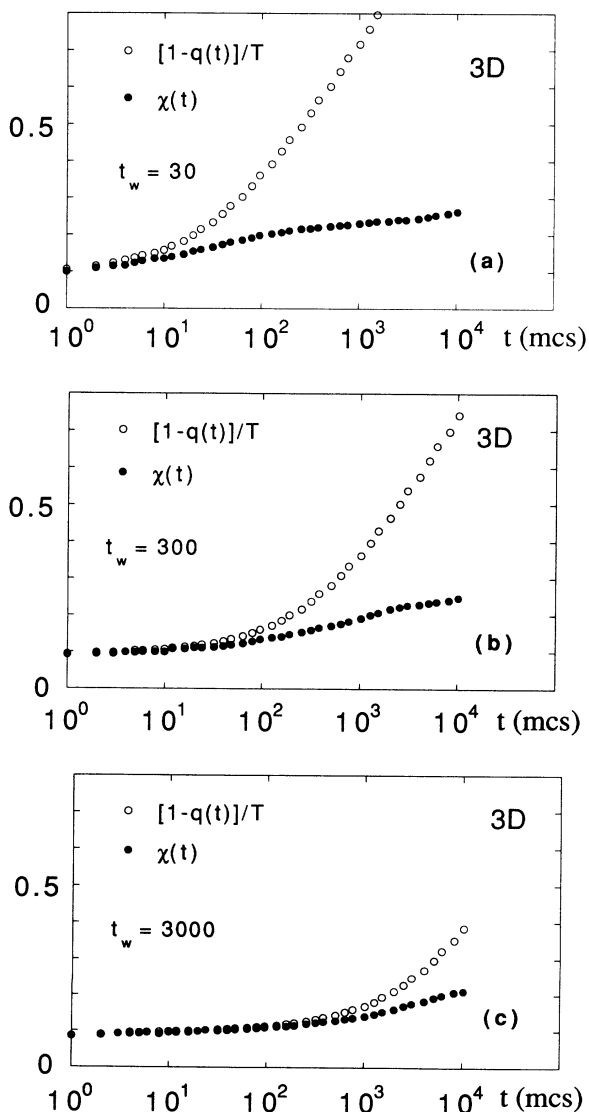


FIG. 3.  $\chi(t)$  and  $[1 - q(t)] / T$ . Size  $60^3$ .  $T = 0.10J$ . (a)  $t_w = 30$  mcs, (b)  $t_w = 300$  mcs, and (c)  $t_w = 3000$  mcs.

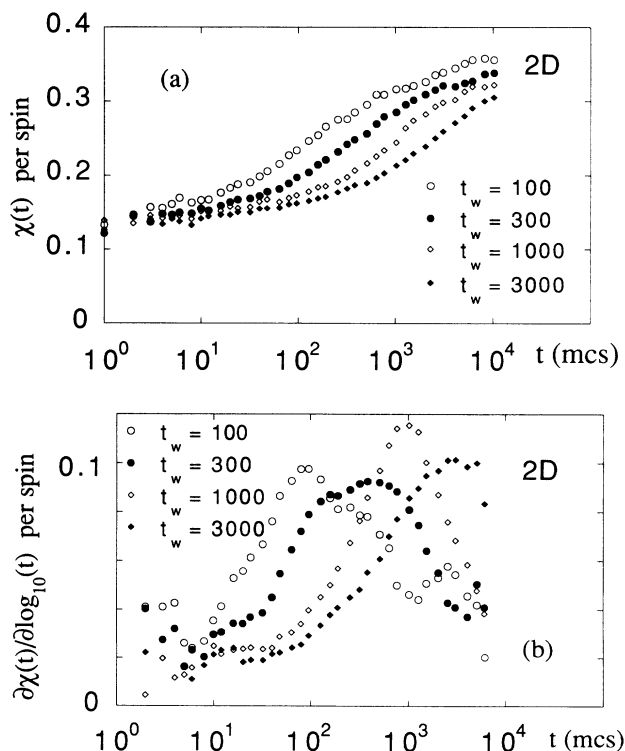


FIG. 4. (a)  $\chi(t)$  for different wait times  $t_w$  for a 2D system of size  $200^2$ .  $H = 0.03J$ .  $T = 0.10J$ . (b) The corresponding relaxation rate  $S(t) = \partial \chi(t) / \partial \log_{10}(t)$ .

this crossover occurs in the magnetization. Especially at higher temperatures it becomes hard to see at what time the crossover in  $q(t)$  takes place.

The behavior in 2D is similar. In Fig. 4 the time dependence of the susceptibility  $\chi(t)$  and the relaxation rate  $\partial\chi(t)/\partial\log_{10}(t)$  are shown for a 2D system at the temperature  $T=0.10J$ . The different curves correspond to different wait times  $t_w$ . As was the case in 3D, there is a characteristic inflection point in  $\chi(t)$  and a corresponding maximum in  $S(t)$  at  $t \approx t_w$ . There is some disagreement in the experimental results on this point. Inflection points were found at times  $t \approx t_w$  for 2D CuMn SG films in Ref. 11, while temperature-dependent inflection points at times  $t \neq t_w$  were found for a 2D short-range Ising SG in Ref. 10. However, the experimental results in Ref. 10 could very well be influenced by the predominance of ferromagnetic couplings. An analysis of  $\chi(t)$  and  $[1-q(t)]/T$  for the 2D system yields similar results to those obtained for the 3D system (see Fig. 3). Comparing the behaviors seen in Figs. 1 and 4, the only significant difference is that the relaxation rate is higher in two dimensions than in three dimensions. Thus, it appears that the aging behavior in spin glasses, at temperatures much lower than the transition temperature for a 3D system  $T_c^{3D} (\approx 0.9J$  for the Gaussian model<sup>30</sup>), is mainly an effect of the slow dynamics. Of course, at temperatures closer to  $T_c^{3D}$  more obvious differences in aging behavior between 2D and 3D spin-glass systems are expected.

Droplets exist only below  $T_c$ . Still the results for 2D are in agreement with predictions from the droplet model. The free energy of a droplet of linear size  $L$  scales as  $F_L \sim L^\theta$ , with the stiffness exponent  $\theta$ . In 2D,  $\theta < 0$ , implying that large-scale excitations exist with arbitrarily low energy, destroying the long-range spin-glass order at any nonzero temperature. However, for length scales up to  $\xi \sim (k_B T/J)^{-1/|\theta|}$ , the ordering is not completely disrupted by thermal excitations and small ( $L < \xi$ ) droplets may exist.<sup>33</sup> Furthermore, recent theoretical progress<sup>34</sup> has revealed a new critical exponent  $\zeta_c$  which appears in the scaling laws for  $L_{\Delta T}$  close to  $T_g$ . The implication of this exponent is that  $L_{\Delta T}$  becomes smaller than  $\xi$  in the critical region and that “quasidroplets” of size smaller than  $\xi$  will exist close to  $T_g$ .

## VI. TEMPERATURE SHIFT SIMULATIONS: UNDERCOOLING AND OVERHEATING

In temperature shift simulations the apparent age of the spin system, as defined by the maximum in the  $\partial\chi/\partial\ln(t)$  curve, is shifted to shorter or longer times depending on whether the equilibration temperature is lower or higher than the temperature where  $\chi(t)$  is determined. The reason for this shift in apparent age is obvious—the dynamics is governed by thermally activated processes. According to the droplet theory, at temperatures close to  $T_c$ , the dominating temperature dependence in shift simulations will be that of  $\Delta(T)$ , while the low-temperature behavior will simply be governed by the size of the temperature shift.

In Fig. 5(a) the relaxation rate  $S(t)$  is plotted for an undercooling simulation on a 3D system of size  $60^3$ , where

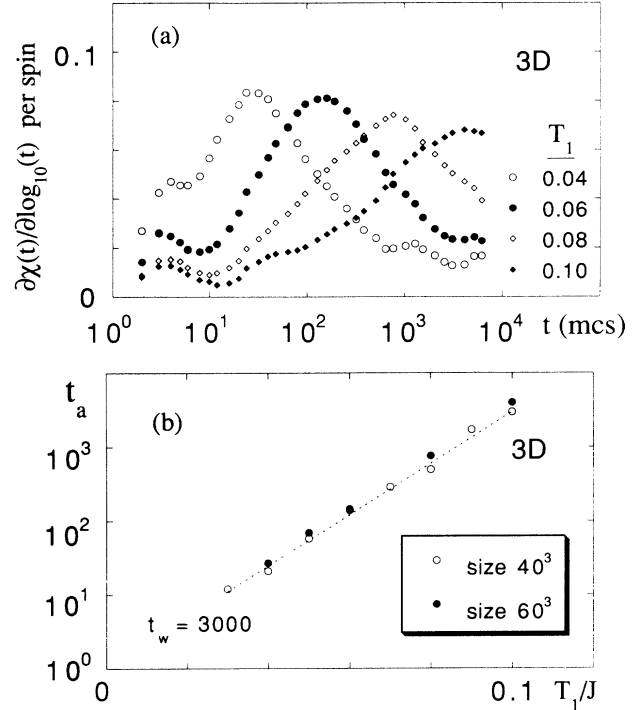


FIG. 5. (a) Relaxation rate  $S(t) = \partial\chi(t)/\partial\log_{10}(t)$  for different equilibration temperatures  $T_1$  in an undercooling simulation on a 3D system of size  $60^3$ .  $T=0.10J$ ,  $H=0.03J$ ,  $t_w=3000$  mcs. (b) The corresponding apparent age  $t_a$  as a function of equilibration temperature  $T_1$ .

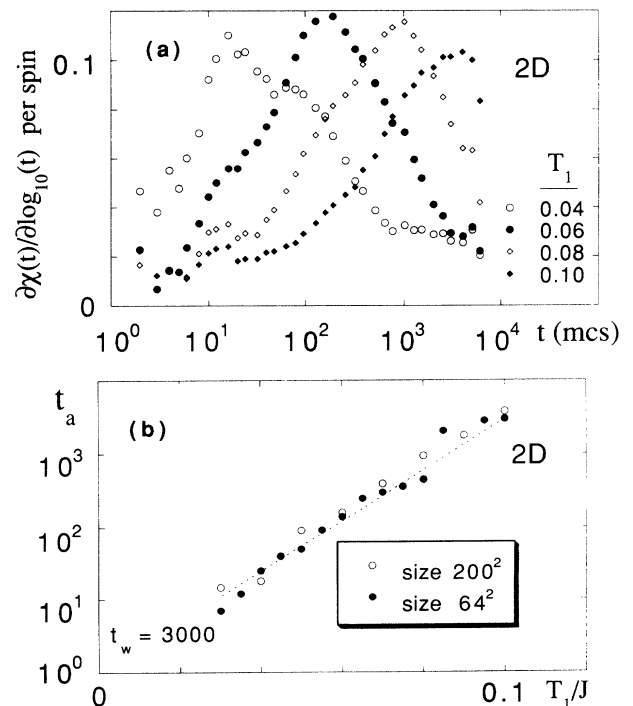


FIG. 6. Relaxation rate  $S(t) = \partial\chi(t)/\partial\log_{10}(t)$  for different equilibration temperatures  $T_1$  in an undercooling simulation on a 2D system of size  $200^2$ .  $T=0.10J$ ,  $H=0.03J$ ,  $t_w=3000$  mcs. (b) The corresponding apparent age  $t_a$  as a function of equilibration temperature  $T_1$ .

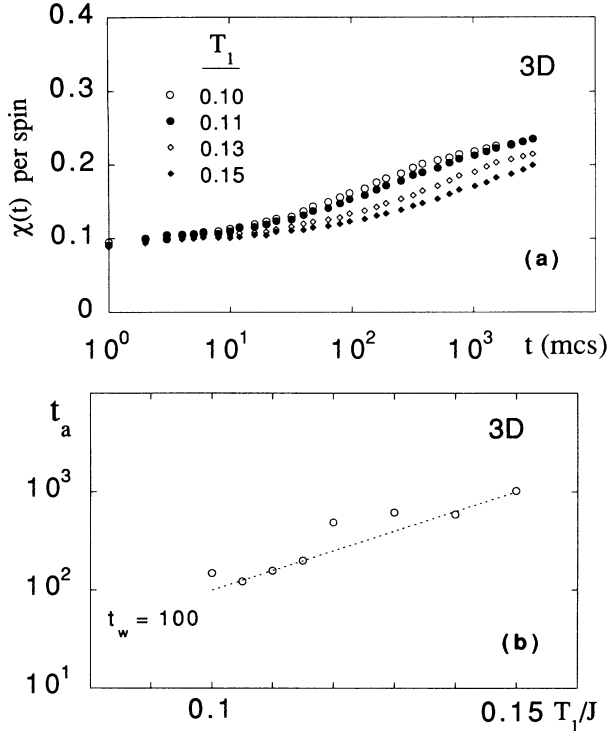


FIG. 7. Susceptibility  $\chi(t)$  for different equilibration temperatures  $T_1$  in an overheating simulation on a 3D system of size  $60^3$ .  $T=0.10J$ ,  $H=0.03J$ ,  $t_w=100$  mcs. (b) The corresponding apparent age  $t_a$  as a function of equilibration temperature  $T_1$ .

after equilibration for a time  $t_w=3000$  mcs at  $T_1(=T-\Delta T)$  the spin system was probed at the temperature  $T=0.10J$ . The different curves correspond to different equilibration temperatures  $T_1$ . In Fig. 5(b) the apparent age  $t_a$  is shown for two different sizes of the spin system ( $40^3$  and  $60^3$ ) as a function of  $T_1$ . The dotted line is the expected behavior

$$\frac{\log_{10}(t_a)}{T_1} = \frac{\log_{10}(t_w)}{T}, \quad (7)$$

where the microscopic time  $\tau_0$  has been set equal to 1 mcs. The agreement between the expected behavior and the simulation results is satisfactory. The spread in the plotted data gives some indication of the error involved when estimating the apparent age  $t_a$ .

In Fig. 6 the corresponding results for an undercooling simulation on a 2D system of size  $200^2$  is shown. The dotted line in Fig. 6(b) marks the expected behavior according to Eq. (7). As was argued in the previous section, the results must in 2D be interpreted in terms of

quasidroplets. Therefore it is not obvious that Eq. (7) should hold. Still the agreement is satisfactory and the fact that the spread in the estimated apparent age  $t_a$  is slightly larger than for the 3D case can be attributed to the difference in size  $N^d$  of the systems.

Comparing these results with the experimental results, the linear dependence of the shift in apparent age,  $\Delta \log_{10}(t) = \log_{10}(t_w) - \log_{10}(t_a)$ , on the temperature shift  $\Delta T$  is clearly seen. However, in experiments  $\Delta \log_{10}(t) \sim \Delta T$  only for small  $\Delta T$ . In our simulations we do not observe any limitations of this linear behavior. It is not clear what causes this difference. The large difference in the order of magnitude of time scales involved could be one reason. Clearly this requires further investigations.

In Fig. 7 the results of an overheating simulation is shown for a 3D system of size  $60^3$ , where after equilibration for a time  $t_w=100$  mcs at  $T_1(=T+\Delta T)$  the spin system was probed at the temperature  $T=0.10J$ . We have chosen to use a smaller  $t_w$  as compared to the undercooling case to keep  $t_a$  within the observation time, since in the overheating case  $t_a > t_w$ . In Fig. 7(a), the susceptibility  $\chi(t)$  vs  $\log_{10}(t)$  is shown for different  $T_1$ . In Fig. 7(b), the apparent age  $t_a$  is shown as a function of  $T_1$ . The dotted line corresponds to the expected behavior according to Eq. (7). We see no indications of a different behavior in overheating simulations as compared to undercooling simulations. This is in accordance with the droplet theory<sup>22</sup> and experimental results by Granberg *et al.*,<sup>2</sup> but in contrast to experimental results by Lederman *et al.*<sup>13</sup>

## VII. CONCLUSIONS

Monte Carlo simulations have been used to study the aging behavior of spin glasses. The results are qualitatively in good agreement with experimental results. The crossover from equilibrium to nonequilibrium dynamics is nicely illustrated by the fact that the fluctuation-dissipation theorem does not hold in the nonequilibrium regime. In the temperature shift simulations, the logarithmic shift of the apparent age varies linearly with  $\Delta T$  in accordance with both experimental results and the "droplet" theory. There are no obvious differences between the results of the undercooling and the overheating simulations.

## ACKNOWLEDGMENT

Financial support from the Swedish Natural Science Research Council is gratefully acknowledged.

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