

Heterogeneous Aging in Spin Glasses

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(Received 13 December 2001; published 20 May 2002)

We introduce a set of theoretical ideas that form the basis for an analytical framework capable of describing nonequilibrium dynamics in glassy systems. We test the resulting scenario by comparing its predictions with numerical simulations of short-range spin glasses. Local fluctuations and responses are shown to be connected by a generalized local out-of-equilibrium fluctuation-dissipation relation. Scaling relationships are uncovered for the slow evolution of heterogeneities at all time scales.

DOI: 10.1103/PhysRevLett.88.237201

PACS numbers: 75.10.Nr, 75.10.Hk, 75.10.Jm, 75.50.Lk

Very slow equilibration and sluggish dynamics are characteristics shared by disordered spin systems and by other glassy systems such as structural and polymeric glasses. The origin of this dynamic arrest near and below the glass transition is currently poorly understood. Studies of the time evolution of many quantities, such as the remanent magnetization, the dielectric constant, or the incoherent correlation function, have shown that below the glass transition the system falls out of equilibrium [1,2]. This is evidenced by the presence of aging, i.e., the dependence of physical properties on the time since the quench into the glassy state, and also by the breakdown of the equilibrium relations dictated by the fluctuation-dissipation theorem (FDT) [3,4].

Most analytical progress in understanding nonequilibrium glassy dynamics has been achieved in mean-field fully connected spin models [3], while numerical simulations have addressed both structural glasses [5] and short-range spin glass models [6]. Until recently, however, experimental, numerical, and analytical studies have mainly focused on global quantities, such as global correlations and responses, which do not directly probe local relaxation mechanisms. Local regions that behave differently from the bulk, or dynamic heterogeneities, could be crucial to understand the full temporal evolution, and have received considerable experimental [7–9] and numerical [10] attention lately. However, no clear theoretical picture has yet emerged to describe the local nonequilibrium dynamics of the glassy phase.

Here we introduce such a theoretical framework, and test its predictions via numerical simulations of a short-range spin glass model. We show that local correlations and responses are linked, and we find scaling properties for the heterogeneities that connect the evolution of the system at different times. This universality may provide a general basis for a realistic physical understanding of glassy dynamics in a wide range of systems.

The framework that we propose is motivated by an analogy [11] between aging dynamics and the well-known

statics of Heisenberg magnets. For concreteness, we test its predictions against Monte Carlo simulations on the prototypical spin glass model, the three-dimensional Edwards-Anderson (3DEA) model, $H = \sum_{\langle ij \rangle} J_{ij} s_i s_j$, where $s_i = \pm 1$ and the nearest-neighbor couplings are $J_{ij} = \pm 1$ with equal probability. We argue that two dynamical *local* quantities, the coarse-grained local correlation $C_r(t, t_w) \equiv \frac{1}{V} \sum_{i \in V_r} \bar{s}_i(t) \bar{s}_i(t_w)$ and integrated response $\chi_r(t, t_w) \equiv \frac{1}{N_f} \sum_{k=1}^{N_f} \frac{1}{V} \sum_{i \in V_r} \frac{\bar{s}_i(t) |_{h_i^{(k)}} - \bar{s}_i(t_w)}{h_i^{(k)}}$, are essential to understand the mechanisms controlling the dynamics of glassy systems. The spins are represented by s_i in the absence of an applied field and by $s_i |_{h_i^{(k)}}$ in the presence of an applied field. $\bar{s}_i(t) \equiv \frac{1}{\tau} \sum_{t'=t-\tau}^{t-1} s_i(t')$ is the result of coarse graining the spin over a small time window [typically, $\tau = 1000$ Monte Carlo steps (MCS)]. V_r is a cubic box with volume V centered at the point r . By taking V to be the volume of the whole system, the bulk or global correlation $C(t, t_w)$ and response $\chi(t, t_w)$ are recovered. Two generic times after preparation are represented by t_w and t , with $t_w \leq t$. When the system is not in equilibrium, time dependences *do not* reduce to a dependence on the time difference $t - t_w$. We measure a staggered local integrated linear response by applying a bimodal random field on each site $h_i^{(k)} = \pm h$ during the time interval $[t_w, t]$. Linear response holds for the values of h that we use. The index $k = 1, \dots, N_f$ labels different realizations of the perturbing field. We use random initial conditions. The thermal histories, i.e., the sequences of spins and random numbers used in the MC test, are the same with and without a perturbing field.

In a disordered spin model, the coarse-grained local magnetization typically vanishes, but the local correlation is nontrivial. Averaged over disorder and the thermal history, this correlator defines the Edwards-Anderson parameter q_{EA} when $t_w \rightarrow \infty$, and $t - t_w \rightarrow \infty$ subsequently. Can we detect the growth of local order [12] by analyzing the evolution of the local correlator, as one easily can for a system undergoing ferromagnetic domain growth? In

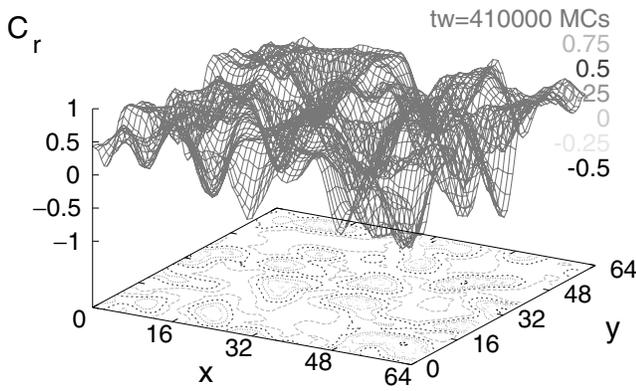


FIG. 1. The local correlations on a 2D cut of the cubic cell. The linear size is $L = 64$. $T = 0.72T_c$, $V = 3^3$, $t_w = 4.1 \times 10^5$ MCS, and $t = 2.8 \times 10^6$ MCS.

Fig. 1 we show the local correlation for fixed t_w and t on a 2D cut of the 3DEA model. Regions with large values of C_r are intertwined with regions with a small value of C_r as shown by the contour levels. This behavior persists for all t_w and t that we can reach with the simulation, and a more sophisticated analysis is necessary to identify a growing order in this system.

It is clear from Fig. 1 that different sites have distinct dynamics. Analysis of the local correlation for fixed t_w as a function of t shows that in general the relaxation is nonexponential; this is often ascribed to the presence of heterogeneous dynamics. How can one characterize the heterogeneous dynamics and determine its origin? We argue that relevant quantities are the probability distribution function (PDF) of the local correlation, $\rho(C_r(t, t_w))$, the PDF of the local integrated response, $\rho(\chi_r(t, t_w))$, and the joint PDF $\rho(C_r(t, t_w), \chi_r(t, t_w))$, and we start by discussing the latter.

The FDT relates the correlation of spontaneous fluctuations to the integrated linear response of a chosen observable [e.g., $C_r(t, t_w)$ and $\chi_r(t, t_w)$ averaged over thermal histories] at equilibrium. Glassy systems modify the FDT in a particular way first obtained analytically for mean-field models [3], later verified numerically in a number of realistic models [13,14], and more recently tested experimentally [15]. A parametric plot of the bulk integrated response, $\chi(t, t_w)$, against the bulk correlation, $C(t, t_w)$, for fixed and long waiting time t_w and using t as a parameter, approaches a nontrivial limit, $\chi(C)$, represented by the crosses in Fig. 2(b). The curve has a straight section, for which $t - t_w \ll t_w$ and the correlation decays from 1 to q_{EA} with a slope $-1/T$ as found with the equilibrium FDT. Beyond this point, as t increases towards infinity, the curve separates from the FDT line. Now, consider each lattice site for fixed times t_w and t . If we plot points for the pairs $[C_r(t, t_w), \chi_r(t, t_w)]$, where will they lie?

When $t_w \rightarrow \infty$ and $t - t_w \ll t_w$, all local correlators satisfy the FDT strictly once averaged over thermal histories, since the magnitude of local deviations from the FDT has an upper bound [16]. We have checked that $C_r(t, t_w)$

and $\chi_r(t, t_w)$ obey the FDT for an individual thermal history apart from small fluctuations [see Fig. 2(b)].

For the regime of widely separated times we propose an analysis similar in spirit to the one that applies to the low energy excitations of the Heisenberg model. There, the free energy for the coarse-grained magnetization $\vec{m}(\vec{r})$ is $F = \int d^d r [(\vec{\nabla}_{\vec{r}} \vec{m}(\vec{r}))^2 + V(|\vec{m}(\vec{r})|)]$. A spontaneous symmetry breaking signals the transition into the ordered phase $\langle \vec{m} \rangle = \vec{m}_0 \neq 0$, in which the order parameter has both a uniform length [the radius of the bottom of the effective potential $V(|\vec{m}|)$], and a uniform direction. F is invariant under uniform rotations $\vec{m}(\vec{r}) \rightarrow \mathcal{R} \vec{m}(\vec{r})$. The lowest energy excitations (spin waves) are obtained from the ground state by leaving the length of the vector invariant and applying a slowly varying rotation to it: $\vec{m}(\vec{r}) = \mathcal{R}(\vec{r}) \vec{m}_0$. These are massless transverse fluctuations (Goldstone modes). In contrast, longitudinal fluctuations, which change the magnitude of the magnetization vector, are massive and energetically costly.

Let us now apply the same kind of analysis to the dynamics of the spin glass. Here, the relevant fluctuating quantities are the coarse-grained local correlations C_r and their associated local integrated responses χ_r . In Ref. [11] we derived an effective action for these functions that becomes invariant under a global time reparametrization $t \rightarrow h(t)$ in the aging regime. This symmetry leaves the bulk relation, $\chi(C)$, invariant. A uniform reparametrization is analogous to a global rotation in the Heisenberg magnet, and the curve $\chi(C)$ is analogous to the surface where $V(|\vec{m}|)$ is minimized. Hence, we expect that, for fixed long times t_w and t in the aging regime, the local fluctuations in C_r and χ_r should be given by smooth spatial variations in the time reparametrization, $h_r(t)$, i.e., $C_r(t, t_w) = C_{SP}(h_r(t), h_r(t_w)) \approx C(h_r(t), h_r(t_w))$, where C_{SP} is the global correlation at the saddle-point level which in the numerical studies we approximate by the actual global correlation C , and similarly for χ_r . These transverse fluctuations are soft Goldstone modes. Longitudinal fluctuations, which move away from the $\chi(C)$ curve, are massive and penalized. This implies the first testable prediction of our theoretical framework: the pairs (C_r, χ_r) should follow the curve $\chi(C)$ for the bulk integrated response against the bulk correlation.

In Fig. 2, we test this prediction by plotting the distribution of pairs (C_r, χ_r) . We find, as expected, that for long times the dispersion in the longitudinal direction [i.e., away from the bulk $\chi(C)$ curve] is much weaker than in the transverse direction [i.e., along the bulk $\chi(C)$ curve]. In the coarse-grained aging limit we expect the former to disappear while the latter should remain. (This limit corresponds to the way actual measurements are performed: the thermodynamic limit is taken first to eliminate finite size effects and undesired equilibration; then the large t_w limit is taken to reach the asymptotic regime, and, finally, the limit $V \rightarrow \infty$ serves to eliminate fluctuations through the coarse-graining process; in the figure we used a large volume $V = 13^3$ to approach the latter limit though we found

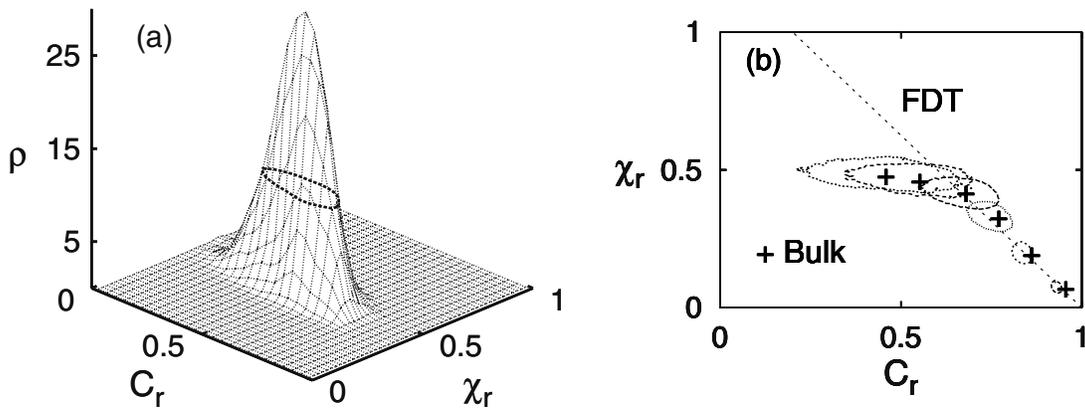


FIG. 2. $L = 64$, $T = 0.72T_c$, $V = 13^3$, $t_w = 4 \times 10^4$. (a) Surface plot of the joint PDF for $t/t_w = 16$. Points within the shown contour account for 2/3 of the total probability. (b) Time evolution of $\rho(C_r(t, t_w), \chi_r(t, t_w))$, for $t/t_w = 1.00005, 1.001, 1.06, 2, 8, 32$ (from right to left). Each contour contains 2/3 of the total probability for the given pair of times. The line marked FDT is the equilibrium relation between χ_r and C_r . The crosses are the bulk $\chi(C)$ for the same pairs of times.

a similar qualitative behavior for smaller V .) Figure 2(a) displays the joint PDF $\rho(C_r, \chi_r)$ for a pair of times (t_w, t) that are far away from each other. Figure 2(b) shows the projection of a set of contour levels for t_w fixed and six values of t . Even though the data for each contour correspond to a single pair of times (t_w, t) , the fluctuations span a range of values that, for the bulk quantities, would require a whole family of pairs (t_w, t) . This reveals that the aging process is nonuniform across a finite-range model.

We now turn our attention to a more detailed examination of the time dependences in the local dynamics. A good t/t_w scaling that breaks down only for very large values of the subsequent time $t - t_w$ has been obtained for the bulk thermoremanent magnetization experimentally [2] and for the bulk correlation numerically [6] once the stationary ($t - t_w \ll t_w$) part of the relaxation is subtracted, as suggested by the solution to mean-field models [3]. For systems that display this particular dependence on t/t_w for the bulk correlator, a second prediction can be extracted from our theoretical framework: the distribution $\rho(C_r(t, t_w))$ should depend only on the ratio t/t_w . Even further, if the bulk correlator has a simple power law form $C_{SP}(t, t_w) \sim q_{EA}(t/t_w)^{-\rho}$, an approximate treatment of fluctuations leads to a rescaling and collapse of $\rho(C_r(t, t_w))$ even for pairs of times with *different* ratios t/t_w .

Since we are dealing with ratios of times, it is convenient to define $h_r(t) = e^{\varphi_r(t)}$, so that $C_r(t, t_w) = C_{SP}(h_r(t)/h_r(t_w)) = C_{SP}(e^{\varphi_r(t) - \varphi_r(t_w)})$. Therefore the statistics of local correlations are determined from the statistical distribution of distances between two “surfaces,” $\varphi_r(t) - \varphi_r(t_w)$. In this form, a dynamic theory of short-range spin glasses is not different from a theory of fluctuating geometries or elasticity. We propose a simple reparametrization invariant effective action for $\varphi_r(t) = \ln t + \delta\varphi_r(t)$, expanding around $\delta\varphi_r(t) = 0$, with no zeroth or first order term in $\delta\varphi_r(t)$. We ensure that the effective action is reparametrization invariant by taking one time derivative for each time variable. Thus [17]

$$S = \frac{q_{EA}\rho}{2} \int d^d r \int_0^\infty dt \int_0^\infty dt' \nabla \dot{\varphi}_r(t) \nabla \dot{\varphi}_r(t') \times e^{-\rho|\varphi_r(t) - \varphi_r(t')|},$$

where the last factor penalizes fast time variations of φ_r and the ∇ ensures that spatial variations are smooth. Expanding to lowest order in $\delta\varphi_r(t)$ yields $\varphi_r(t) - \varphi_r(t_w) = \ln(t/t_w) + \delta\varphi_r(t) - \delta\varphi_r(t_w) \simeq \ln(t/t_w) + [a + b \ln(t/t_w)]^\alpha X_r(t, t_w)$, where a and b are determined by the magnitude of the fluctuations, and $X_r(t, t_w)$ is a random variable drawn from a time-independent PDF that governs the fluctuations of the surfaces. In our approximation, which describes uncorrelated drift between two surfaces (i.e., a random walk), $\alpha = 1/2$.

Figure 3 displays $\rho(C_r(t, t_w))$ for several choices of the ratio t/t_w . Interestingly enough, all the curves have a noticeable peak at a value of C_r that is independent of t and t_w , with a height that decreases significantly with

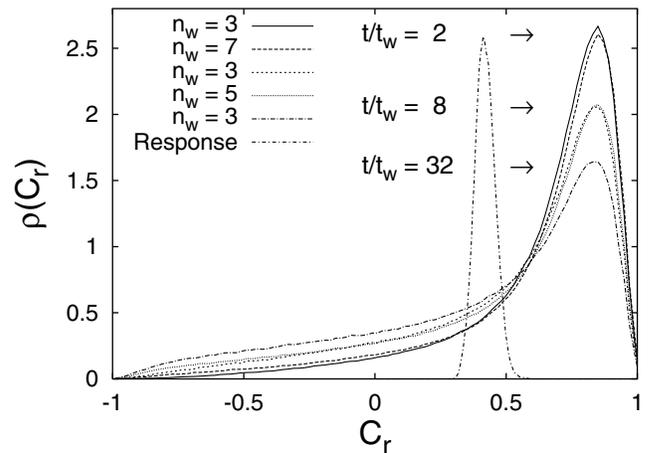


FIG. 3. PDF of the local correlations for the ratios $t/t_w = 2, 8$, and 32 , averaged over 36 realizations of disorder. $L = 32$, $T = 0.72T_c$, and $V = 3^3$. The waiting-times are $t_w = 10^4(2^{n_w-1})$ MCS, with n_w given in the key. We include the PDF of the local integrated responses, $\chi_r(t, t_w)$, for $n_w = 3$ and $t/t_w = 2$. [$\rho(\chi_r)$ is divided by 4 to fit on the figure.]

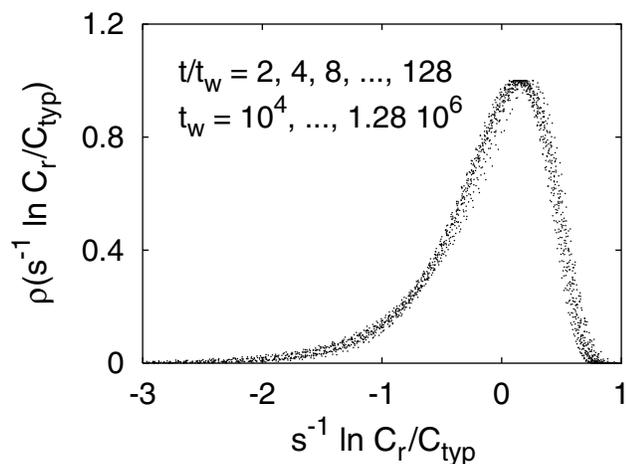


FIG. 4. Scaling of $\rho(C_r(t, t_w))$. $L = 32$, $T = 0.72T_c$, $V = 13^3$, and 28 pairs (t, t_w) , with $t = 10^4(2^{n-1})$ MCS, $n = 1, \dots, 8$, and $t_w = 10^4(2^{n_w-1})$ MCS, $n_w = 1, \dots, n-1$. $C_{\text{typ}} \equiv \exp(\ln C)$, where $\langle \dots \rangle$ denotes an average over the distribution and s rescales the maximum value of each curve. With this choice of V we eliminate the $C_r < 0$; cf. Fig. 3.

increasing ratio t/t_w . The form derived above for $\varphi_r(t) - \varphi_r(t_w)$ explains the approximate collapse of $\rho(C_r(t, t_w))$ for a fixed ratio t/t_w , as shown in Fig. 3 for a small value of V . (Because of mixing with the stationary part, the t/t_w scaling worsens when V increases.) Barely noticeable in Fig. 3 is a slow drift of the curves for increasing values of t_w at fixed ratio t/t_w such that the height of the peak decreases while the area below the tail at lower values of C_r increases. This trend leads to the “subaging” scaling observed for bulk quantities [2,6].

Furthermore, the above expression for $\varphi_r(t) - \varphi_r(t_w)$ implies that the PDFs for all of the 28 pairs of times (t, t_w) should collapse by rescaling with two parameters: $\ln C_{\text{typ}}$ and s , corresponding, respectively, to the nonrandom part in $\varphi_r(t) - \varphi_r(t_w)$ and to the width of the random part (see Fig. 4). The scaling curve itself gives the PDF for $X_r(t, t_w)$. The rather good collapse of the curves should be improved by further knowledge of C_{SP} .

A local separation of time scales leads to a reparametrization invariant action [11] with a soft mode that controls the aging dynamics. Our framework, based on the analogy with Heisenberg magnets, predicts the existence of a local relationship between C_r and χ_r , expressed by $\rho(C_r(t, t_w), \chi_r(t, t_w))$ being sharply concentrated along the global $\chi(C)$ in the (C, χ) plane. Under additional assumptions, we obtained the scaling behavior of $\rho(C_r(t, t_w))$ for all (t, t_w) . Our simulations both confirm these predictions and uncover striking regularities in the geometry of local fluctuations [17]. These results open the way to a systematic study of local dynamic fluctuations in glassy systems and they suggest a number of exciting avenues for future research. On the theoretical side, this framework could be applied to a large variety of glassy models, including those without explicit disorder. More interesting still are the experimental tests suggested

by this work. For instance, the local correlations of colloidal glasses are accessible experimentally with the confocal microscopy technique [8]. Similarly, cantilever measurements of noise spectra [9] allow probing of local fluctuations in the glassy phase of polymer melts. These are just two examples: any experiment that measures local fluctuations in glassy systems is a potential candidate for testing our ideas.

We thank D. Huse and J. Kurchan for useful discussions. This work was supported in part by the NSF Grant No. DMR-98-76208, the NSF-CNRS Grant No. 12931, and the Alfred P. Sloan Foundation. Supercomputing time was allocated by the Boston University SCF.

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