Static versus Dynamic Heterogeneities in the $D = 3$ Edwards-Anderson-Ising Spin Glass

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We numerically study the aging properties of the dynamical heterogeneities in the Ising spin glass. We find that a phase transition takes place during the aging process. Statics-dynamics correspondence implies that systems of finite size in equilibrium have static heterogeneities that obey finite-size scaling, thus signaling an analogous phase transition in the thermodynamical limit. We compute the critical exponents and the transition point in the equilibrium setting, and use them to show that aging in dynamic heterogeneities can be described by a finite-time scaling ansatz, with potential implications for experimental work.

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Spin glasses, fragile molecular glasses, polymers, colloids, and many other materials display a dramatic increase of characteristic times when cooled down to their glass temperature, T_g [1]. This is probably due to the collective movements of an increasing number of elements in the system, with a (free) energy barrier growing with the size of the cooperative regions [2] (the cooperative regions become larger as the temperature gets closer to T_g). Experimentally, one can get the fingerprints of these movements by observing dynamical heterogeneities [3] or nonlinear susceptibilities [4].

Below T_g, aging appears [5]. Consider a rapid quench from a high temperature to the working temperature T ($T < T_g$), where the system is left to equilibrate for time t_w and probed at a later time $t + t_w$. One finds that the response functions (e.g., magnetic susceptibility) depend on t/t_w^{μ}, with $\mu \approx 1$ [5–7]. The age of the glass, t_w, remains the relevant time scale even for $t_w \sim$ days.

Dynamical heterogeneities age as well, as found numerically in their characteristic length $\zeta(t, t_w)$ [8,9]. Recent measurements of aging correlation and response functions with space-time resolution [10] suggest that $\zeta(t, t_w)$ will soon be experimentally investigated. Characterizing aging for $\zeta(t, t_w)$ is our main concern here.

We focus on spin glasses, an easier case for a number of reasons: (i) the sluggish dynamics is known to be due to a thermodynamic phase transition at $T_c = T_g$ [11–13]; (ii) the size of the glassy magnetic domains, $\xi(t_w)$, is experimentally accessible [14,15] ($\xi \sim 100$ lattice spacings at $T \sim T_c$ [14], larger than comparable measurements for structural glasses [4]); (iii) $\xi(t_w) \propto t_w^{1/z(T)}$, $z(T) \approx 6.9 T_c/T$ [9] suggests that free-energy barriers grow in spin glasses as $\sim \log \xi(t_w)$, rather than with a power law as in fragile glasses; (iv) equilibrium physics is known to rule nonequilibrium dynamics [16]. A quantitative correspondence exists between equilibrium and nonequilibrium spatial correlation functions [17,18] (equilibrium on systems of size L matches nonequilibrium at time t_w) [19]. Finally, the Janus dedicated computer [20] allows us to simulate nonequilibrium dynamics from picoseconds to a tenth of a second [9,17], and to compute equilibrium correlation functions on lattices as large as $L = 32$, and temperatures as low as $0.64 T_c$ [18].

In this Letter we show that a phase transition occurs in the aging dynamic heterogeneities. As time t proceeds, when the spin correlation function $C(t, t_w)$ (see below) becomes smaller than the spin-glass order parameter q_{EA}, the length scale of the dynamic heterogeneities $\zeta(t, t_w)$ diverges in the limit of large t_w. We use the statics-dynamics correspondence to investigate this phase transition in the equilibrium setting, focusing on spatial correlation functions (static heterogeneities). Finite-size scaling (FSS) yields an accurate estimate of q_{EA} (something never achieved before for a spin glass) as well as of

the relevant critical exponents. Back to nonequilibrium, aging turns out to be amazingly well described by a finite-time scaling ansatz, with critical parameters taken verbatim from the equilibrium computation.

We consider the Edwards-Anderson model on a cubic lattice of size L (volume $V = L^3$), with periodic boundary conditions, at $T = 0.64T_c$. We use Ising spins, $s_{\boldsymbol{x}} = \pm 1$, and binary nearest-neighbor couplings. The average over the quenched disorder, denoted by an overline, is taken after the thermal average $\langle \cdots \rangle$. We consider two clones of the system, $\{s_{\boldsymbol{x}}^{(1)}, s_{\boldsymbol{x}}^{(2)}\}$ evolving independently under the same set of coupling constants, and taken at the same time t_w. The replica field is $q_{\boldsymbol{x}} = s_{\boldsymbol{x}}^{(1)} s_{\boldsymbol{x}}^{(2)}$ and the spin overlap is its spatial average $q = \sum_{\boldsymbol{x}} q_{\boldsymbol{x}}/V$. See Refs. [18,20] for full details of our equilibrium and nonequilibrium simulations.

Out of equilibrium, correlation functions depend either on a single time t_w, or on t and t_w. Let $c_{\boldsymbol{x}}(t, t_w) = s_{\boldsymbol{x}}(t + t_w) s_{\boldsymbol{x}}(t_w)$. The spin correlator, see Fig. 1 (top), is

$$C(t, t_w) = \frac{1}{V} \sum_{\boldsymbol{x}} \overline{\langle c_{\boldsymbol{x}}(t, t_w) \rangle}, \qquad \tilde{C}(t) = C(t, t_w = \infty). \quad (1)$$

Naive aging is approximatively valid: for finite t_w, $C(t, t_w)$ decays for long t, but the decay slows down with increasing t_w. In fact, there is an enveloping curve $\tilde{C}(t)$ with a nonzero limiting value, the order parameter $q_{\rm EA}$. The lack of a reliable parameterization of $\tilde{C}(t)$ precludes a controlled extrapolation of $q_{\rm EA}$, in contrast with the equilibrium computation shown below.

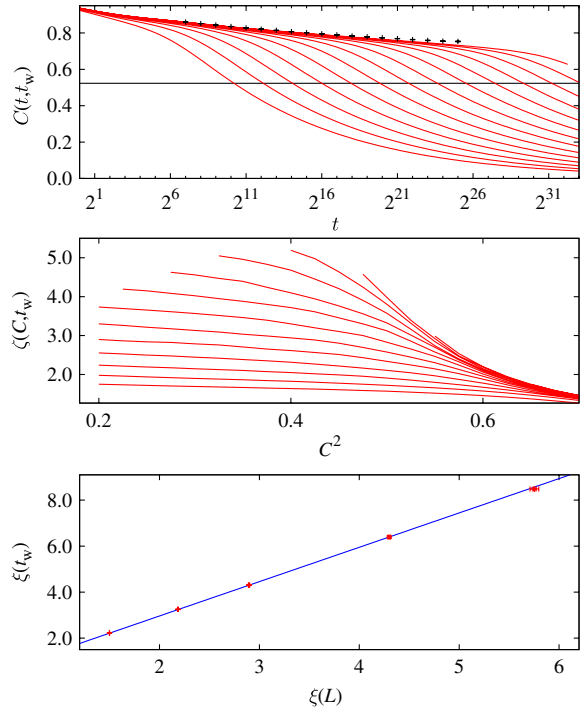

FIG. 1 (color online). Top: $C(t, t_w)$, Eq. (1), as a function of t for $t_w = 4^i$, $i = 3, \ldots, 16$ (lines, t_w grows from bottom to top). We also plot $\tilde{C}(t)$ (points) and our result for $q_{\rm EA}$ from Eq. (9) (horizontal line). Center: Correlation length $\zeta(C, t_w)$ as a function of C^2 (same values of t_w as in the top panel). Bottom: Finite-time coherence length $\xi(t_w)$ against the finite-size coherence length at $q = 0$, $\xi(L)$. The results are compatible with $\xi(t_w) = 1.48\xi(L)$ (straight line).

As for space dependencies, we consider $C_4(\boldsymbol{r}, t_w) = \sum_{\boldsymbol{x}} \overline{\langle q_{\boldsymbol{x}}(t_w) q_{\boldsymbol{x}+\boldsymbol{r}}(t_w) \rangle}/V$. Using integral estimators [9,17] we extract the coherence length $\xi(t_w)$, the size of regions where the two clones of the system are similar. Yet, to learn about heterogeneities on the dynamics probed at time $t + t_w$, at distance $\boldsymbol{r}$, we consider $C_{22}(\boldsymbol{r}, t, t_w) = \sum_{\boldsymbol{x}} \overline{\langle c_{\boldsymbol{x}}(t, t_w) c_{\boldsymbol{x}+\boldsymbol{r}}(t, t_w) \rangle - C^2(t, t_w)}/V$. Using an integral estimator [9], we extract from C_{22} the correlation length $\zeta(t, t_w)$, the characteristic length for heterogeneities, displayed in the central panel of Fig. 1. We replace t with $C(t, t_w)$ [21], as independent variable. For large C, $\zeta(C, t_w)$ reaches a t_w-independent value, which increases when C decreases. On the other hand, for small C, $\zeta(C, t_w)$ grows strongly with t_w. Clearly, something happens when C goes through some special value $q_{\rm EA}$ and we intend to exploit the statics-dynamics correspondence to clarify it.

How does all this appear from an equilibrium viewpoint? In the limit of large system size L, the probability density function for q, $P(q) = \overline{P_J(q)}$, has two Dirac's delta contributions of equal weight at $q = \pm q_{\rm EA}$. Replica symmetry breaking (RSB) theory [22] predicts that $P(q)$ has a support for $|q| < q_{\rm EA}$, while droplet theory expects no support in that region [23].

Our approach focuses on the study of equilibrium connected correlation functions [24], regarded as a function of the spin overlap q. Varying q at fixed T a phase transition is encountered for $q = q_{\rm EA}$. As in [18], our conditional correlation function at fixed $q = c$, $C_4(\boldsymbol{r}|c)$, is obtained as a quotient of the convolutions of $\overline{\langle q_{\boldsymbol{x}} q_{\boldsymbol{x}+\boldsymbol{r}} \delta(q - c) \rangle}$ and $\overline{\langle \delta(q - c) \rangle}$ with a Gaussian of width $1/V$. This combines $O(\sqrt{V})$ levels, thus smoothing the comblike $P(q)$ [25].

It has been recently found [17,18] that the equilibrium $C_4(\boldsymbol{r}|q)$, computed in a system of size L, accurately matches the nonequilibrium $C_{22}(\boldsymbol{r}, C, t_w)$ if one chooses time t such that $C(t, t_w) = q$ and time t_w such that $L \approx 3.7\xi(t_w)$ (at least at $T = 0.64T_c$). It is tempting to assume that the correspondence will become exact in the limit of large L and t_w. In Fig. 1 (bottom) we show an example of this correspondence in the limit $C \to 0$.

To proceed with the equilibrium analysis, we observe that $C_4(\boldsymbol{r}|q)$ tends to q^2 for large r. In a finite system, one needs to perform a subtraction that complicates the analysis [24]. We instead consider the Fourier transform at wave vector $\boldsymbol{k}$, $\hat{C}_4(\boldsymbol{k}|q) = \sum_{\boldsymbol{r}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} C_4(\boldsymbol{r}|q)$, blind to a constant subtraction for $\boldsymbol{k} \neq \boldsymbol{0}$. Defining $\boldsymbol{k}_{\rm min} = (2\pi/L, 0, 0)$ (or permutations), we have

$$F_q = \hat{C}_4.(\boldsymbol{k}_{\rm min}|q). \quad (2)$$

For $T < T_c$ and $|q| \leq q_{\rm EA}$, one expects that

$$C_4(\boldsymbol{r}|q) \simeq q^2 + \frac{A_q}{r^{\theta(q)}}, \qquad \hat{C}_4(\boldsymbol{k}|q) \propto k^{\theta(q)-D} + \ldots \quad (3)$$

[scaling in Fourier space holds only if $\theta(q) < D$]. The dots in (3) stand for scaling corrections, subleading in the limit of large r (or small k). On the other hand [24],

$$C_4(\boldsymbol{k}|q^2 > q^2_{\rm EA}) \propto \frac{1}{k^2 + \xi_q^{-2}}. \quad (4)$$

The correlation length ξ_q diverges when $|q| \to q_{\rm EA}$ from above, $\xi_q^{L=\infty} \propto (q^2 - q^2_{\rm EA})^{-\hat{\nu}}$. In principle, $\hat{\nu}$ is different from the thermal critical exponent at T_c. We note as well the scaling law [26]

$$\theta(q_{\rm EA}) = 2/\hat{\nu}. \quad (5)$$

The theories for the spin-glass phase differ in the precise form of $\theta(q)$, but agree that a crossover can be detected in F_q for finite L. Indeed, $F_q \sim L^{D-\theta(q)}$ for $|q| < q_{\rm EA}$, while $F_q \sim 1$ for $|q| > q_{\rm EA}$, see Eqs. (3) and (4). For large L, $\xi_q^{L=\infty} \propto (q^2 - q^2_{\rm EA})^{-\hat{\nu}}$ and the crossover becomes a phase transition. FSS tells us that, see, e.g., [27],

$$F_q = L^{D-\theta(q_{\rm EA})} G(L^{1/\hat{\nu}}(q - q_{\rm EA})), \quad (6)$$

up to scaling corrections. G is a scaling function.

We have exploited Eq. (6) in the following nonstandard way. We focus on quantities depending on the continuous parameter y ($\epsilon = D - \theta(q_{\rm EA})$):

$$F_q/L^y = L^{\epsilon - y} G(L^{1/\hat{\nu}}(q - q_{\rm EA})). \quad (7)$$

When y is smaller than $D - \theta(0)$, F_q/L^y vanishes in the large-L limit for $|q| > q_{\rm EA}$, while it diverges for $|q| < q_{\rm EA}$. Hence, fixing y, the curves for pairs of lattices $(L, 2L)$ will cross at a point $q_{L,y}$, see Fig. 2. To leading order in L^{-1}, the crossing point approaches $q_{\rm EA}$ for large L as

$$q_{L,y} = q_{\rm EA} + A_y L^{-1/\hat{\nu}}, \qquad A_y = \frac{G(0)}{G'(0)} \frac{2^{\epsilon - y} - 1}{2^{1/\hat{\nu}} - 2^{\epsilon - y}}. \quad (8)$$

Note that the amplitude A_y changes sign at $y = \epsilon$.

We could use a fit to Eq. (8) in order to obtain the order parameter, but, for a fixed y, there are only three crossing points ($L = 8, 12, 16$) for three parameters (zero degrees of freedom). Fortunately, one can extract more information from the data by computing the crossings for several y values and performing a joint fit, sharing $q_{\rm EA}$ and $1/\hat{\nu}$. Since these additional crossing points are not statistically independent, this procedure requires a proper consideration of the cross correlations. This can be achieved by computing the fit goodness estimator χ^2 with the full covariance matrix for the $q_{L,y}$. The number of y values considered is a compromise between adding more degrees of freedom and keeping the covariance matrix invertible. We have chosen

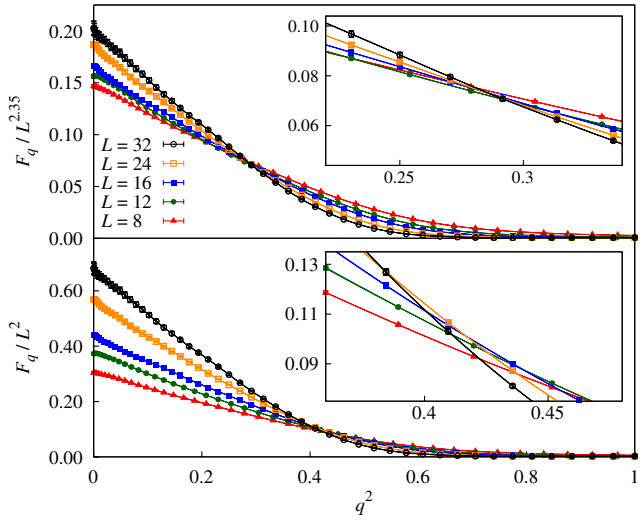

FIG. 2 (color online). F_q/L^y, Eq. (7), against q^2 for all our L values at $T = 0.703 \approx 0.64 T_c$, both for the free-field scaling [$F_q(\boldsymbol{k}) \propto 1/k^2$, i.e., $y = 2$] and for $y = 2.35 \approx D - \theta(q_{\rm EA})$. The insets are closeups of the crossing region.

9 values of y obtaining $\chi^2 = 18.9$, reasonable for a fit with 16 degrees of freedom (see Fig. 3). The result is

$$q_{\rm EA} = 0.52(3), \qquad 1/\hat{\nu} = 0.39(5). \quad (9)$$

These numbers are remarkably stable to variations in the set of y values. Also, removing the $L = 8$ data for $y = 2.3, 2.4$ (the outliers in Fig. 3) shifts our results by one fifth of the error bars. Note as well that the slope A_y changes sign at $y \approx 2.35$. Hence, $\theta(q_{\rm EA}) \approx 0.65$, in reasonable agreement with Eq. (5).

The value of $q_{\rm EA}$ computed above should be the same as the large-L extrapolation of the position of the peak in $P(q)$: a fit $q_{\rm EA}(L) = q_{\rm EA} + AL^{-1/\hat{\nu}}$, with $\hat{\nu}$ from (9), yields $q_{\rm EA} = 0.54(3)$ [18].

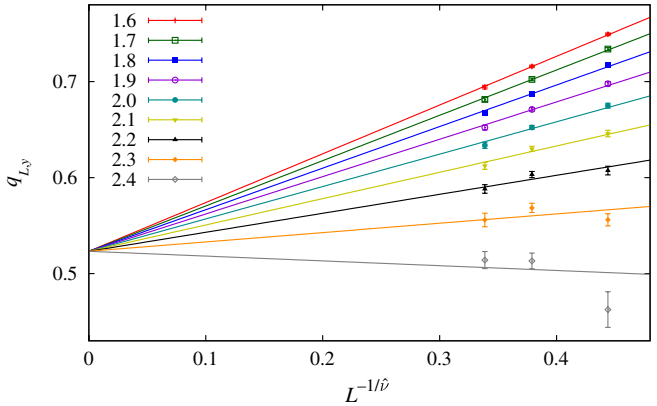

FIG. 3 (color online). Crossing points $q_{L,y}$ for F_q/L^y computed from pairs of lattices $(L, 2L)$, versus $L^{-1/\hat{\nu}}$, for different y values at $T = 0.703$. The continuous lines are fits to Eq. (8), constrained to yield common values for $q_{\rm EA}$ and $1/\hat{\nu}$.

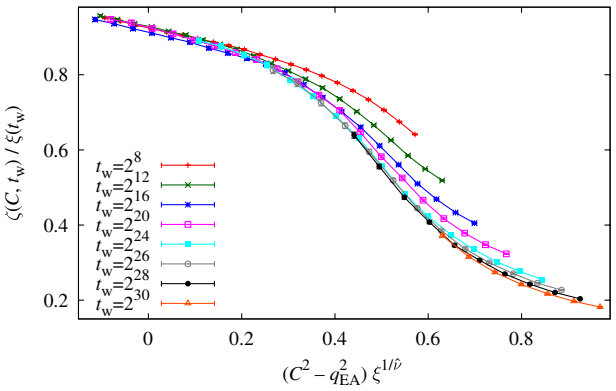

FIG. 4 (color online). Dimensionless ratio $\zeta(C, t_w)/\xi(t_w)$ against the scaling variable $(C^2 - q_{EA}^2)\xi(t_w)^{1/\hat{\nu}}$.

We are finally ready to discuss aging in the dynamic heterogeneities. The statics-dynamics correspondence suggests that it will take the form of a finite-time scaling (FTS) ansatz, similar to Eq. (6), in which $\xi(t_w)$ plays the role of L. Since it is a length, $\zeta(C, t_w)$ should have the same scaling dimensions of $\xi(t_w)$. Setting short-time corrections aside, Fig. 4 shows indeed that $\zeta(C, t_w)/\xi(t_w)$ behaves as a function of $(C^2 - q_{EA}^2)\xi(t_w)^{1/\hat{\nu}}$. FTS also provides a natural explanation for the extremely small exponents found in t-extrapolations for $\tilde{C}(t)$ [28].

In summary, we have studied aging properties in glassy dynamic heterogeneities for the Ising spin glass, characterized through their characteristic length $\zeta(t, t_w)$. Aging takes the form of a finite-time scaling ansatz, which describes the crossover from a regime where $\zeta(t, t_w)$ is of order one, to a regime where it is of order $\xi(t_w)$, the coherence length yielding the size of the glassy magnetic domains. In the limit of an infinite waiting time, the crossover evolves into a phase transition. We have profited from the statics-dynamics correspondence [17,18] to study this phase transition via equilibrium spatial correlation functions, thus obtaining the critical exponents and, for the first time, the spin-glass order parameter. These critical parameters, taken verbatim, describe our nonequilibrium data. For a discussion of the mode-coupling transition in glass-forming liquids in a similar vein see [29].

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