Nonequilibrium Spin-Glass Dynamics from Picoseconds to a Tenth of a Second

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We study numerically the nonequilibrium dynamics of the Ising spin glass, for a time spanning 11 orders of magnitude, thus approaching the experimentally relevant scale (i.e., seconds). We introduce novel analysis techniques to compute the coherence length in a model-independent way. We present strong evidence for a replicon correlator and for overlap equivalence. The emerging picture is compatible with noncoarsening behavior.

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Spin glasses [1] (SG) exhibit remarkable features, including slow dynamics and a complex space of states: they are a paradigmatic problem because of its many applications to glassy behavior, optimization, biology, financial markets, social dynamics, etc.

Experiments on SG [1, 2] focus on nonequilibrium dynamics. In the simplest protocol, isothermal aging, the SG is cooled as fast as possible to a subcritical working temperature, \( T < T_c \), let to equilibrate for a waiting time, \( t_w \), and probed at a later time, \( t + t_w \). The thermoremanent magnetization is found to be a function of \( t/t_w \) (full aging), for \( 10^{-3} < t/t_w < 10 \) and \( 50 \text{ s} < t_w < 10^4 \text{ s} \) [3] (see, however, [4]). The growing size of the coherent domains, the coherence-length \( \xi \), is also measured [5, 6]. Two features emerge: (i) the lower \( T \), the slower the growth of \( \xi(t_w) \) and (ii) \( \xi \sim 100 \) lattice spacings, even for \( T < T_c \) and \( t_w \sim 10^4 \text{ s} \) [5].

The sluggish dynamics arises from a thermodynamic transition at \( T_c \) [7–9]. There is a sustained theoretical debate on the properties of the (unreachable in human times) equilibrium low \( T \) SG phase, which is nevertheless relevant to (basically nonequilibrium) experiments [10]. The main scenarios are the droplets [11], replica symmetry breaking (RSB) [12], and the intermediate trivial-nontrivial (TNT) picture [13].

Droplets expects two equilibrium states related by global spin reversal. The SG order parameter, the spin magnetization is found to be a function of \( t = t_w \) times (equilibrium low \( T < T_c \) transition at \( \tilde{T} = T_c \)). In the RSB scenario an infinite number of pure states influence the dynamics [12, 14, 15], so all \( \bar{q}_{EA} \leq q \leq q_{EA} \) are reachable. In TNT the SG phase is similar to an antiferromagnet with random boundary conditions: \( q \) behaves as for RSB systems but, similar to droplets, the surface-to-volume ratio of the largest thermally activated domains vanishes (i.e., the link overlap defined below takes a single value).

Because of superuniversality [16], the isothermal aging of basically all coarsening systems is qualitatively the same (droplets being analogous to a disguised ferromagnet [17]). For \( T < T_c \), the dynamics consists in the growth of compact domains, where the spin overlap takes one of the values \( q = \pm q_{EA} \). The corresponding growth law, \( \xi(t) \), completely encodes all time dependencies. The antiferromagnet analogy suggests a similar TNT aging.

Since in the RSB scenario \( q = 0 \) equilibrium states do exist, the nonequilibrium dynamics starts with a vanishing order parameter and remains there forever. The replicon, a critical mode analogous to magnons in Heisenberg ferromagnets, is present for all \( T < T_c \) [18]. Furthermore, \( q \) is not a privileged observable (overlap equivalence [14]): the link overlap displays equivalent aging behavior.

These theories need numerics to be quantitative [19–27]. Simulations so far have been too short: experimental scales are at \( \approx 100 \text{ s} \), while typical nonequilibrium simulations reach \( \approx 10^{-5} \text{ s} \) (one Monte Carlo step, MCS, corresponds to \( 10^{-12} \text{ s} \) [1]).

Here we report on a large simulation (\( 10^{11} \text{ MCS} \sim 0.1 \text{ s} \)) of an instantaneous SG quench protocol performed on the Janus computer [30], which allows us to reach experimental times by mild extrapolations. Aging is investigated as a function of time and temperature. We obtain model-independent determinations of the SG coherence length \( \xi \). Conclusive evidence is presented for a critical correlator associated with the replicon mode. We observe nontrivial aging in the link correlation (a nonequilibrium test of overlap equivalence [14]). We conclude that, up to experimental scales, SG dynamics is not coarsening like.
The $D = 3$ Edwards-Anderson Hamiltonian is

$$\mathcal{H} = -\sum_{(x,y)} J_{x,y} \sigma_x \sigma_y,$$

(\cdot \cdot \cdot) denote nearest neighbors). Spins $\sigma_x = \pm 1$ sit at the
nodes, $x$, of a cubic lattice of size $L$ and periodic boundary
conditions. The couplings (quenched variables) $J_{x,y} = \pm 1$ are chosen randomly with 50% probability. For each set of
couplings (a sample), we simulate two independent systems,
$\{\sigma_x^{(1)}\}$ and $\{\sigma_x^{(2)}\}$. We denote by (\cdot \cdot \cdot) the average
over the couplings. Model (1) has a SG transition at
$T_c = 1.101(5)$ [31].

Our $L = 80$ systems evolve with Heat-Bath dynamics
[32], which is in the Universality Class of physical evolution.
Fully disordered spin configurations are placed at the working temperature (96 samples at $T = 0.8 = 0.73T_c$ and at $T = 0.6 = 0.54T_c$; 64 at $T = 0.7 = 0.64T_c$). We also perform shorter simulations (32 samples) at $T_c$, and $L = 40$ and $L = 24$ runs to check for finite-size
effects.

A crucial quantity is the two-times correlation function
[19,20,23]:

$$C(t, t_w) \equiv \sigma_x(t + t_w)\sigma_x(t_w)$$

(2)

linearly related to the real part of the a.c. susceptibility at
waiting time $t_w$ and frequency $\omega = \pi/t$.

To check for full aging [3] in a systematic way, we fit
$C(t, t_w)$ as $A(t_w)/(1 + t/t_w)^{-\alpha(t_w)}$ in the range $t_w \leq t \leq 10t_w$ [33], obtaining a fit for all $t_w > 10^3$; see Fig. 1. To
be consistent with the experimental claim of full-aging behavior for $10^{14} < t_w < 10^{16}$ [3], $\alpha(t_w)$ should be constant
in this $t_w$ range. Although $\alpha(t_w)$ grows keeping for
our largest times (with the large errors in [23]) it seemed
constant for $t_w > 10^4$, its growth slows down. The
behavior at $t_w = 10^{16}$ seems beyond reasonable extrapolation.

The coherence length is studied from the correlations of the
 replica field $q_x(t_w) \equiv \sigma_x^{(1)}(t_w)\sigma_x^{(2)}(t_w)$,

$$C_q(r, t_w) = L^{-3} \sum_{x} q_x(t_w) q_{x+r}(t_w).$$

(3)

For $T < T_c$, it is well described by [12,21]

$$C_q(r, t_w) \sim r^{-a} e^{-\gamma(t_w) r^b},$$

(4)

The actual value of $a$ is relevant. For coarsening dynamics
$a = 0$, while in a RSB scenario $a = \frac{1}{2}$ and $C_q(r, t_w)$ vanishes at long times for fixed $r/\xi(t_w)$. At $T_c$, the latest estimate is $a = 1 + \eta = 0.616(9)$ [31].

To study $a$ independently of a particular Ansatz as (4) we consider the integrals

$$I_k(t_w) = \int_0^\infty d r r^k C_q(r, t_w),$$

(5)

(e.g., the SG susceptibility is $\chi^{SG}(t_w) = 4\pi I_2(t_w)$). As
we assume $L \gg \xi(t_w)$ we safely reduce the upper limit to
$L/2$. If a scaling form $C_q(r, t_w) \sim r^{-a} e^{-\gamma(t_w) r^b}$ is
adequate at large $r$, then $I_k(t_w) \propto (\xi(t_w))^{3+2a}$. It follows that $\xi_{k+1} = (I_{k+1}/I_k)$ is $a$ and $I_k(t_w) \propto \xi_{k+1}^{3+2a}$.

We find $\xi_{12}(t_w) = 0.88_2(2)$, where $\xi_{12}$ is the noisy second-moment estimate [9]. Furthermore, for $\xi_{12} > 3$, we find $\xi_{01}(t_w) = 0.46_5(12)$, and $\xi_{12}(t_w) = 1.06_5(12)$, where $\xi_{01}$ is from a fit to (4) with $a = 0.4$.

Note that, when $\xi \ll L$, irrelevant distances $r \gg \xi$
 largely increase statistical errors for $I_k$. Fortunately, the
very same problem was encountered in the analysis of
correlated time series [34], and we may borrow the cure
[35].

The largest $t_w$ where $L = 80$ still represents $L = \infty$
physics follows from finite-size scaling [32]: for a given

FIG. 1 (color online). Fit parameters, $A$ and $\alpha$ ($C(t, t_w) = A(t_w)(1 + t/t_w)^{-\alpha(t_w)}$) vs $t_w$ for temperatures below $T_c$ ($T = 0.6$ line): fit for $t_w > 10^3$, to $\alpha(t_w) = \alpha_0 + \alpha_1 \log(t_w) + \alpha_2 \log^2(t_w)$, $\alpha_0 = 6.35795$, $\alpha_1 = 0.18605$, $\alpha_2 = -0.00351835$, diagonal $\chi^2$/d.o.f. = $66.26/63$. Oscillations are due to strong correlations of $\alpha(t_w)$ at neighboring times (the fit and $\chi^2$/d.o.f. do not change if we bin data in blocks of 5 consecutive $t_w$).

FIG. 2 (color online). Left: SG coherence length $\xi_{12}$ vs waiting time, for $T \approx T_c$. Right: $\xi_{12}$ vs $I_1$, ($\xi_{12} \propto I_1^{(3+2a)}$). Also shown data for the site-diluted Ising model ($\xi_{12}$ and $I_1$ rescaled by 2). Full lines: Ising (coarsening, $a = 0$) and SG, $a(T_c) = 0.616$ [31]. Inset: $[\xi_{12}^2(t_w) - \xi_{12}^2(t_w)]/L$ vs $\xi_{12}^2(t_w)/L$ for $T = 0.8$ and $L = 24, 40$ and $80$ ($\xi_{12}^2(t_w)$ from a fit $\xi_{12}(t_w) = A(T) t_w^{(2-\delta)}$ for $L = 80$ in the range $3 < \xi_{12} < 10$).

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numerical accuracy, one should have \( L \geq k\xi_{1,2}(t_w) \). To compute \( k \), we compare \( \xi_{1,2}^0 \) for \( L = 24, 40 \) and 80 with \( \xi_{1,2}^\infty \), estimated with the power law described below (Fig. 2, inset). It is clear that the safe range is \( L \geq 7\xi_{1,2}(t_w) \) at \( T = 0.8 \) (at \( T_c \) the safety bound is \( L \geq 6\xi_{1,2}(t_w) \)).

Our results for \( \xi_{1,2} \) are shown in Fig. 2. Note for \( T = 0.8 \) the finite-size change of regime at \( t_w = 10^9(\xi_{1,2} \sim 11) \). We find fair fits to \( \xi(t_w) = A(T)t_w^z(T) \); \( z(T) = 6.86(16) \), \( z(0.8) = 9.42(15) \), \( z(0.7) = 11.8(2) \) and \( z(0.6) = 14.1(3) \), in good agreement with previous numerical and experimental findings \( z(T) = z(T_c)T_c/T \) [5,21]. Our fits are for \( 3 \leq \xi \leq 10 \), to avoid both finite-size and lattice discretization effects. Extrapolating to experimental times \( t_w = 10^{14} \sim 100 \) s, we find \( \xi = 14.0(3), 21.2(6), 37.0(14), \) and 119(9) for \( T = 0.6 \), \( T = 0.7 \), \( T = 0.8 \) and \( T = 1.1 \approx T_c \), respectively, which nicely compares with experiments [5,6].

In Fig. 2, we also explore the scaling of \( I_1 \) as a function of \( \xi_{1,2} \) (\( I_1 \approx \xi^{2-a} \)). The nonequilibrium data for \( T = 1.1 \) scales with \( a = 0.585(12) \). The deviation from the equilibrium estimate \( a = 0.616(9) \) [31] is at the limit of statistical significance (if due to be scaling corrections). For \( T = 0.8, 0.7, \) and 0.6, we find \( a = 0.442(11), 0.355(15), \) and 0.359(13), respectively (the residual \( T \)-dependence is probably due to critical effects still felt at \( T = 0.8 \)). Note that ground state computations for \( L \leq 14 \) yielded \( a(T = 0) = 0.4 \) [37]. These numbers differ both from critical and coarsening dynamics (\( a = 0 \)).

We finally address the aging properties of \( C_{\text{link}}(t, t_w) \)

\[
C_{\text{link}}(t, t_w) = \sum_{(x,y)} c_x(t, t_w)c_y(t, t_w)/(3L^3).
\]

\( C_{\text{link}} \), still experimentally inaccessible, does not vanish if the configurations at \( t + t_w \) and \( t_w \) differ by the spin inversion of a compact region of half the system size.

It is illuminating to replace \( t \) with \( C^2(t, t_w) \) as an independent variable; Figs. 3 and 4. For a coarsening dynamics \( C_{\text{link}} \) will be \( C \) independent for \( C^2 < q_{\text{EA}}^2 \) and large \( t_w \) (relevant system excitations are the spin reversal of compact droplets not affecting \( C_{\text{link}} \)), while in a RSB system new states are continuously found as time goes by; we expect a non constant \( C^2 \) dependence even if \( C < q_{\text{EA}}^2 \) [38].

By general arguments, the nonequilibrium \( C_{\text{link}} \) at finite times coincides with equilibrium correlation functions for systems of finite size [10]; see Fig. 3. We also predict the \( q^2 \) dependency of the equilibrium conditional expectation \( Q_{\text{link}, q} \) up to \( T = 33 \) [\( Q_{\text{link}} \) is just \( C_4(r = 1) \), while \( q \) is the spatial average of \( q_r \); Eq. (3)].

As for the shape of the curve \( C_{\text{link}} = f(C^2, t_w) \), Fig. 4 bottom, the \( t_w \) dependency is residual. Within our time window, \( C_{\text{link}} \) is not constant for \( C < q_{\text{EA}}^2 \). For comparison (inset) we show the qualitatively different curves for a coarsening dynamics. We studied the derivative \( dC_{\text{link}}/dC^2 \), for \( C^2 < q_{\text{EA}}^2 \), Fig. 4 top. We first smooth the curves by fitting \( C_{\text{link}} = f(C^2) \) to the lowest order polynomial allowing a fair fit (seventh order for \( t_w \approx 2^{25} \), sixth for larger \( t_w \)), whose derivative was taken afterwards (jackknife statistical errors).

Furthermore, we extrapolated both \( C_{\text{link}}(t = rt_w, t_w) \) and \( C(t = rt_w, t_w) \) to \( t_w = 10^{14} \sim 100 \) s, for \( r = 8, 4, \ldots, 1/16 \) [39]. The extrapolated points for \( t_w = 10^{14} \) fall on a straight line whose slope is plotted in the upper panel (thick line). The derivative is nonvanishing for \( C^2 < q_{\text{EA}}^2 \) for the experimental time scale.

In summary, Janus [30] halves the (logarithmic) time gap between simulations and nonequilibrium spin-glass experiments. We analyzed the simplest temperature quench, finding numerical evidence for a noncoarsening dynamics, at least up to experimental times (see also [27]). Let us highlight: nonequilibrium overlap equivalence (Figs. 3 and 4); nonequilibrium scaling functions reproducing equilibrium conditional expectations in finite systems
elsewhere (our analysis of dynamic heterogeneities will appear elsewhere [36]). Exploring with Janus nonequilibrium dy-
analysis of dynamic heterogeneities [26,27] will appear.

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17] Temperature chaos could still spoil the analogy [16].
33] Data at different $t$ and $t_w$ are correlated, so we consider only diagonal terms in the covariance matrix. Time correlations are considered by first forming jackknife blocks [32] (JKB) with the data for different samples, then minimizing this diagonal $\chi^2$ for each JKB [23].
35] We integrate $C_4(r,t_w)$ up to $r_{\text{cutoff}}(t_w)$, where $C_4(r_{\text{cutoff}}(t_w), t_w)$ becomes less than thrice its statistical error. We estimate the (small) remaining contribution, by fitting to (4) then integrating the fitted function from $r_{\text{cutoff}} - 1$ to $L/2$. Details will be given elsewhere [36].
36] (Janus Collaboration) (to be published).
38] $C_{\text{link}} = C^2$ in the full-RSB Sherrington-Kirkpatrick model.
39] For each $r$, both the link and the spin correlation functions are independently fitted to $a_r + b_r t_w^{-\zeta}$ (fits are stable for $t_w > 10^3$ with $c_r = 0.5$). These fits are then used to extrapolate the two correlation functions to $t_w = 10^{14}$.