Nonequilibrium spin glass dynamics from picoseconds to 0.1 seconds

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We study numerically the nonequilibrium dynamics of the Ising Spin Glass, for a time that spans eleven orders of magnitude, thus approaching the experimentally relevant scale (i.e., seconds).

We introduce novel analysis techniques that allow to compute the coherence length in a model-independent way. Besides, we present strong evidence for a replicon correlator and for overlap equivalence. The emerging picture is compatible with non-coarsening behavior.

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Spin Glasses1 (SG) exhibit remarkable features, including slow dynamics and a complex space of states: their understanding is a key problem in condensed-matter physics that enjoys a paradigmatic status because of its many applications to glassy behavior, optimization, biology, financial markets, and social dynamics.

Experiments on Spin Glasses2,3 focus on nonequilibrium dynamics. In the simplest experimental protocol, isothermal aging hereafter, the SG is cooled as fast as possible to the working temperature below the critical one, T < Tc. It is let to equilibrate for a waiting time, tw. Its properties are probed at a later time, t + tw. The thermoremanent magnetization is found to be a function of t/tw, for 10⁻³ < t/tw < 10 and tw in the range 50 s — 10⁴ s3,4 (see, however, ref. 4). This lack of any characteristic time scale is named Full-Aging. Also the growing size of the coherent domains, the coherence-length, ξ, can be measured2,5. Two features emerge: (i) the lower T is, the slower the growth of ξ(tw) and (ii) ξ ∼ 100 lattice spacings, even for T ∼ Tc and tw ∼ 10⁴ s5.

The sluggish dynamics arises from a thermodynamic transition at Tc.6,7,8,9. There is a sustained theoretical controversy on the properties of the (unreachable in human times) equilibrium low temperature SG phase, which is nevertheless relevant to (basically nonequilibrium) experiments10. The main scenarios are the droplets11, replica symmetry breaking (RSB)12, and the intermediate Trivial-Non-Trivial (TNT) picture13.

Droplets expects two equilibrium states related by global spin reversal. The SG order parameter, the spin overlap q, takes only two values q = ±qEA. In the RSB scenario an infinite number of pure states influence the dynamics12,14,15, so that all −qEA ≤ q ≤ qEA are reachable. TNT13 describes the SG phase similarly to an antiferromagnet with random boundary conditions: even if q behaves as for RSB systems, TNT agrees with droplets in the vanishing surface-to-volume ratio of the largest thermally activated spin domains (i.e., the link-overlap defined below takes a single value).

Droplets isothermal aging16 is that of a disguised ferromagnet36. A picture of isothermal aging emerges that applies to basically all coarsening systems: superuniversality16. For T < Tc the dynamics consists in the growth of compact domains (inside which the spin overlap coherently takes one of its possible values q = ±qEA). Time dependencies are entirely encoded in the growth law of these domains, ξ(t). The antiferromagnet analogy suggests a similar TNT Aging behavior.

Since in the RSB scenario q = 0 equilibrium states do exist, the nonequilibrium dynamics starts, and remains forever, with a vanishing order parameter. The replicon, a critical mode analogous to magnons in Heisenberg ferromagnets, is present for all T < Tc17. Furthermore, q is not a privileged observable (overlap equivalence14): the link overlap displays equivalent Aging behavior.

These theories need numerics to be quantitative18,19,20,21,22,23,24,25,26 and simulations are too short: one Monte Carlo Step (MCS) corresponds to 10⁻¹² s3. The experimental scale is at 10¹⁴ MCS (∼1008 s), while typical nonequilibrium simulations reach ∼ 10⁻⁵ s. In fact, high-performance computers have been designed for SG simulations27,28,29.

Here we present the results of a large simulation campaign performed on the application-oriented Janus computer30. Janus allows us to simulate the SG instantaneous quench protocol for 10¹¹ MCS (∼0.1 s), enough to reach experimental times by mild extrapolations. Aging is investigated both as a function of time and temper-
nature. We obtain model-independent determinations of the SG coherence length $\xi$. Conclusive evidence is presented for a critical correlator associated with the replica mode. We observe non trivial 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

$$\mathcal{H} = -\sum_{(x,y)} J_{x,y} \sigma_x \sigma_y, \langle \ldots \rangle : \text{nearest neighbors}. \quad (1)$$

The spins $\sigma_x = \pm 1$ are placed on the nodes, $x$, of a cubic lattice of linear size $L$ and periodic boundary conditions. The couplings $J_{x,y} = \pm 1$ are chosen randomly with 50% probability, and are quenched variables. For each choice of the couplings (one sample), we simulate two independent systems, $\{\sigma^{(1)}_x\}$ and $\{\sigma^{(2)}_x\}$. We denote by $\langle \cdots \rangle$ the average over the couplings. Model [1] undergoes a SG transition at $T_c = 1.011(5)$ [30].

Our $L = 80$ systems evolve with a Heat-Bath dynamics [31], which is in the Universality Class of the physical evolution. The fully disordered starting spin configurations are instantaneously placed at the working temperature (96 samples at $T = 0.8 \approx 0.73 T_c$, 64 at $T = 0.7 \approx 0.64 T_c$ and 96 at $T = 0.6 \approx 0.54 T_c$). We also perform shorter simulations (32 samples) at $T_c$, as well as $L = 40$ and $L = 24$ runs to check for Finite-Size effects.

A crucial quantity in non equilibrium dynamics is the two-times correlation function (defined in terms of the field $c_x(t, t_w) = \sigma_x(t + t_w)\sigma_x(t)$) [18, 19, 22]:

$$C(t, t_w) = L^{-3} \sum_x c_x(t, t_w), \quad (2)$$

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

$$C(t, t_w) \sim A(t_w)(1 + t/t_w)^{-1/\alpha(t_w)}$$

in the range $t_w \leq t \leq 10 t_w$ [32], obtaining fair fits for all $t_w > 10^3$. To be consistent with the experimental claim of Full-Aging behavior for $10^3 < t_w < 10^6$, $\alpha(t_w)$ should be constant in this $t_w$ range. Although $\alpha(t)$ keeps growing for our largest times (with the large errors in [22]) it seemed constant for $t_w > 10^4$, its growth slows down. The behavior at $t_w = 10^6$ seems beyond reasonable extrapolation.

The coherence length is studied from the correlations of the replica field $q_x(t_w) = \sigma^{(1)}_x(t_w)\sigma^{(2)}_x(t_w)$

$$C_4(r, t_w) = L^{-3} \sum_x q_x(t_w)q_{x+r}(t_w). \quad (3)$$

For $T < T_c$, it is well described by [12, 20]

$$C_4(r, t_w) \sim r^{-a} e^{-(r/\xi(t_w))^\eta}, \quad a \approx 0.5, \: b \approx 1.5. \quad (4)$$

The actual value of $a$ is relevant. For coarsening dynamics $a = 0$, while in a RSB scenario $a > 0$ and $C_4(r, t_w)$ vanishes at long times for fixed $r/\xi(t_w)$. At $T_c$, the latest estimate is $a = 1 + \eta = 0.616(9)$ [30].

To study $a$ independently of a particular Ansatz as [1], we consider the integrals

$$I_k(t_w) = \int_0^\infty dr \: r^k C_4(r, t_w), \quad (5)$$

(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 $C_4(r, t_w) \sim r^{-a} f(r/\xi(t_w))$ is adequate at large $r$, then $I_k(t_w) \propto [\xi(t_w)]^{k-1-a}$. It follows that $\xi_{k, k+1}(t_w) \approx I_{k+1}(t_w)/I_k(t_w)$ is proportional to $\xi(t_w)$ and $I_1(t_w) \propto \xi_{\infty, 2}^{-2-a}$. We find $\xi^{(2)}(t_w) \approx 0.8 \xi_{1,2}(t_w)$, where $\xi^{(2)}$ is the noisy second-moment estimate[9]. Furthermore, for $\xi_{1,2} > 3$, we find $\xi_{0,1}(t_w) \approx 0.46 \xi_{1,2}(t_w)$, and $\xi^{(fit)}(t_w) = 1.06 \xi_{1,2}(t_w)$, $(\xi^{(fit)}$ from a fit to [11] 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 [53], and we may borrow the cure [38].

The largest $t_w$ where $L = 80$ still represents $L = \infty$ physics follows from Finite Size Scaling [31]: for a given numerical accuracy, one should have $L \geq k \xi_{1,2}(t_w)$. To compute $k$, we compare $\xi_{1,2}$ for $L = 24, 40$ and $80$ with $\xi_{1,2}$ 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 $\xi(t_w) = A(T) t_w^{1/2(T)}$: $z(T_c) = 6.86(16)$, $z(0.8) = 9.42(15)$, $z(0.7) = 11.8(2)$ and $z(0.6) = 14.1(3)$, in good agreement with previous numerical and experimental findings $z(T) = z(T_c) T_c / T$ [20]. We restricted the fitting range to $3 \leq \xi \leq 10$, to avoid both Finite-Size and lattice discretization effects. Extrapolating to experimental times ($t_w = 10^{14} \approx 100 s$), 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 $T = 1.1 = T_c$, respectively, which seem fairly sensible compared with experimental data [5, 6].

In Fig. 2 we also explore the scaling of $I_1$ as a function of $\xi_{1,2}$ ($I_1 \propto \xi^{2\zeta}$). The nonequilibrium data for $T = 1.1$ scales with $a = 0.585(12)$. The deviation from the equilibrium estimate $a = 0.616(9)$ [30] is at the limit of statistical significance (if present, it would be due to scaling corrections). For $T = 0.8, 0.7$ and $0.6$, we find $a = 0.442(1), 0.355(15)$ 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 $a(T = 0) \approx 0.43[33]$. These numbers differ both from critical and coarsening dynamics ($a = 0$).

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

$$C_{\text{link}}(t, t_w) = \sum_{(x,y)} c_{x}(t, t_w) c_{y}(t, t_w) / (3L^2).$$

Experimentalists have yet to find a way to access $C_{\text{link}}$, which is complementary to $C(t, t_w)$ (it 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 eliminate $t$ as independent variable in favor of $C^2(t, t_w)$, Figs. 3 and 4. Our expectation for a coarsening dynamics is that, for $C^2 < q_{\text{EA}}$ and large $t_w$, $C_{\text{link}}$ will be $C$-independent (the relevant system excitations are the spin-reversal of compact droplets not affecting $C_{\text{link}}$). Conversely, in a RSB system new states are continuously found as time goes by, so we expect a non constant $C^2$ dependence even if $C < q_{\text{EA}}$.

General arguments tell us that the nonequilibrium $C_{\text{link}}$ at finite times coincides with equilibrium correlation functions for systems of finite size [10]. Fig. 3 ($Q_{\text{link}}$ is just $C_4(r = 1)$, while $q$ is the spatial average of $q_{\text{EA}}, Eq. (2)$). Therefore, see caption to Fig. 3 we predict the $q^2$ dependence of the equilibrium conditional expectation $Q_{\text{link}}/q$ for lattices as large as $L = 33$.

As for the shape of the curve $C_{\text{link}} = f(C^2, t_w)$, Fig. 4—bottom, $t_w$ dependency is residual. Within our time window, $C_{\text{link}}$ is not constant for $C < q_{\text{EA}}$. For comparison (inset) we show the, qualitatively different, curves for a coarsening dynamics. Therefore, a major difference between a coarsening and a SG dynamics is in the derivative $dC_{\text{link}} / dC^2$, for $C^2 < q_{\text{EA}}$, Fig. 3—top. We first smooth the curves by fitting $C_{\text{link}} = f(C^2)$ to the lowest order polynomial that provides a fair fit (seventh order for $t_w \leq 2^{25}$, sixth for larger $t_w$), whose derivative was taken afterwards (Jackknife’s statistical errors)

Furthermore, we have extrapolated both $C_{\text{link}}(t = t_w, t_w)$ and $C(t = t_w, t_w)$ to $t_w \approx 10^{14}$ ($\approx 100s$), for
growth of the coherence length sensibly extrapolates to $t_w = 10^{14}$ fall on a straight line whose slope is plotted in the upper panel (thick line). The derivative is non vanishing for $C^2 < C_{EA}^2$, for the experimental time scale.

In summary, Janus\textsuperscript{[29]} halves the (logarithmic) time-gap between simulations and nonequilibrium Spin Glass experiments. We analyzed the simplest temperature quench, finding numerical evidence for a non-coarsening dynamics, at least up to experimental times (see also\textsuperscript{[26]}). Let us highlight: nonequilibrium overlap equivalence (Figs. 3,4); nonequilibrium scaling functions reproducing equilibrium conditional expectations in finite systems (Fig. 3); and a nonequilibrium replicon exponent compatible with equilibrium computations\textsuperscript{[34]}. The growth of the coherence length sensibly extrapolates to $t_w = 100$ s (our analysis of dynamic heterogeneities\textsuperscript{[25, 26]} will appear elsewhere\textsuperscript{[35]}). Exploring with Janus nonequilibrium dynamics up to the \textit{seconds} scale will allow the investigation of many intriguing experiments.

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\[ r = 8, 4, \ldots, 1 \rightarrow 4. \] The extrapolated points for $t_w = 10^{14}$

\[ C(\chi_{EA}) \leq C_{EA}. \]

\[ C_{EA}^2 \leq C^2, \] for the experimental time scale.

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[36] Temperature chaos could spoil the analogy if temperature is varied during the Aging experiment\textsuperscript{[14]}.
[37] Because data at different $t$ and $t_w$ are exceedingly correlated, for all fits in this work we consider the diagonal $\chi^2$ (i.e. we keep only the diagonal terms in the covariance matrix). The effect of time correlations is considered by first forming jackknife blocks\textsuperscript{[31]} (JKB) with the data for different samples (JKB at different $t$ and $t_w$, preserve time correlations), then minimizing $\chi^2$ for each JKB\textsuperscript{[22]}.
[38] We numerically integrate $C_4(r, t_w)$ up to a $t_w$ dependent cutoff, chosen as the smallest integer such that $C_4(r_{cutoff}(t_w), t_w)$ was smaller than three times its own statistical error. We estimate the (small) remaining contribution, by fitting to Eq.\textsuperscript{[31]} then integrating numerically the fitted function from $r_{cutoff}^{-1}$ to $L/2$. Details (including consistency checks) will be given elsewhere\textsuperscript{[25]}.
[39] $C_{\text{link}}=C^2$ in the full-LSB Sherrington-Kirkpatrick model.
[40] For each $r$, both the link and the spin correlation functions are independently fitted to $a_r + b_r t_w^{-w}$ (fits are stable for $t_w > 10^7$ with $c_r \approx 0.5$). These fits are then used to extrapolate the two correlation functions to $t_w = 10^{14}$. 
