Deviations from Full Aging in Numerical Spin Glass Models

Jesper Dall and Paolo Sibani

Fysisk Institut, Syddansk Universitet, Campusvej 55, DK-5230 Odense M, Denmark

(Dated: November 7, 2018)

The deviations from full or pure aging behavior, i.e. perfect $t/t_w$ scaling of the correlation and response functions of aging glassy systems, are not well understood theoretically. Recent experiments of Rodriguez et al. (Phys. Rev. Lett. 91, 037203 (2003)) have shown that full aging applies to the thermoremanent magnetization in the limit of infinite cooling rate during the initial quench. In numerical models, instantaneous thermal quenches can be—and usually are—applied. This has motivated the present numerical investigations of the aging behavior of Edwards-Anderson Ising spin glass models with both short- and long-range Gaussian interactions, respectively. We sample the distribution of residence time $t$ in suitably defined metastable valleys entered at age $t_w$, finding that the deviations from $t/t_w$ scaling are small and decrease systematically as the system size grows and/or the temperature decreases. Finally, the connection between this behavior and the scaling of the correlation function itself is discussed.

PACS numbers: 02.70.Uu ; 05.40.-a ; 75.50.Lk

I. INTRODUCTION

In a typical aging experiment a spin glass sample is quenched below the glass transition temperature in a small magnetic field. At time $t_w$ after the quench, the field is switched off and the subsequent decay of the thermoremanent magnetization is measured. It is well known that linear response functions in spin glasses strongly depend on the age or waiting time $t_w$. In general, the rate of change of macroscopic averages in glassy systems systematically decreases with $t_w$.

Considering the broad variety of aging systems, microscopic time scales are hardly significant, which highlights $t/t_w$ as the obvious choice of scaling variable for aging data. The data collapses obtained in this fashion are fairly good but never perfect: In spin-glass linear response experiments [1, 2] much better scalings are obtained using $t/t_{w}^{\mu}$ with the exponent $\mu$ slightly smaller than one. This situation is referred to as sub-aging, since the apparent age $t_{w}^{\mu}$ is shorter than $t_w$, as opposed to ‘pure’ or ‘full’ $t/t_w$ aging. In gels [3] and colloidal glasses [4], the distribution of the waiting time between pairs of consecutive ‘anomalous fluctuations’ features the opposite deviation, i.e. super- or hyper-aging, where $\mu > 1$. Both sub- and super-aging pose a theoretical challenge as they require the introduction and interpretation of an additional time scale. This remains true even when $\mu$ is very close to unity, as in the present study.

Qualitatively, aging reflects the trapping of trajectories in metastable ‘valleys’ of ever increasing thermal stability [3, 4, 5]: the pseudo-equilibrium fluctuations occur for $t < t_w$ within the valley selected at time $t_w$, while the exploration of new valleys occurs for $t > t_w$ and produces the non-equilibrium part of the aging dynamics. In this picture, the spin rearrangements leading from one valley to the next, ‘quakes’ in our terminology, would appear as anomalous events in a fluctuating background. The waiting time between quakes corresponds to the valley residence time, whose statistical properties have repeatedly been considered in models of complex relaxation [4, 5, 6]. According to a recent description of non-equilibrium dynamics as a log-Poisson process [7], the distribution $R(t \mid t_w)$ of residence time $t$ in valleys entered at time $t_w$ should scale as $t/t_w$ and possess a finite average residence time proportional to $t_w$. The best obtainable data collapse of the corresponding simulational data reveals however a slight super-aging behavior.

On the experimental side, it has recently been shown [10] that sub-aging of the thermoremanent magnetization can be strongly suppressed by increasing the cooling rate of the quench. For the instantaneous quench implied in isothermal numerical simulations with a random initial configuration, this strengthens the expectation that full aging applies, a conclusion which is not unequivocally supported by the existing numerical studies of the correlation function [11, 12].

The paper is organized as follows: In Section [11] we summarize the exploration method used to identify the metastable valleys and describe the procedures followed. In Section [11] we present our numerical findings for the scaling of the residence time distribution in these valleys for spin glass models defined on Euclidean lattices with nearest neighbor interactions as well as on random regular graphs. In particular, we focus on the system size and temperature dependence of $\mu$. Section [14] compares the empirical properties of this distribution with the prediction of the idealized log-Poisson theory of Ref. [8]. We show that the theoretical description becomes gradually better in the sense that full aging is slowly approached as the temperature decreases or the system size increases. Finally, the implications for the correlation function are discussed, and tentative conclusions are drawn regarding the geometrical origin of the deviations from pure aging behavior.

*Corresponding author paolo@planck.fys.sdu.dk
behavior.

II. METHOD AND MODELS

While the fluctuation dynamics of glassy systems within metastable valleys is uncontroversially determined by the local free energy, a similarly well established theoretical framework for the irreversible quakes interrupting the pseudo-equilibrium regime is lacking. Surprisingly, there has not been much focus on how these jumps or quakes should be identified and characterized. This question is subtle since the first occurrence of a certain rearrangement could well have a non-equilibrium character, while subsequent rearrangements of similar nature might represent pseudo-equilibrium fluctuations within a larger valley.

The classic analysis of energy landscapes \[13\,14\] samples local energy minima using e.g. downhill search algorithms as thermal quenches, and is not overly concerned with how attractors are dynamically selected in the course of unperturbed isothermal aging. An empirical procedure to identify the quakes \[15\] distinguishes ‘first’ and ‘subsequent’ occurrences of certain events by keeping track of the sequence of energies visited while aging. Within this sequence, states of energy lower than all previously visited states, together with barriers \[20\] higher than all previously surmounted barriers, define a quake as a rearrangement which overcomes a barrier of record height and leads to a state of energy lower than the lowest energy seen so far. A valley is then simply the set of states visited between two subsequent quakes, where onset of the latter is marked by the barrier records. Very restrictive by construction, this procedure yields no output if the dynamics is time translationally invariant, and is therefore not available to analyze e.g. the diffusive regime of supercooled glass formers. Within the aging regime, it produces a highly non-trivial yet relatively simple picture of the energy landscape of spin glasses \[16\].

The Edwards-Anderson \[17\] model considered below is an archetypal glassy system which possesses a complex dynamics while remaining relatively easy to simulate. The energy of a configuration in this model is given by

\[
E\left\{s_1, \ldots, s_N \right\} = - \frac{1}{2} \sum_{i,j} J_{ij} s_i s_j, \tag{1}
\]

The couplings \(J_{ij}\) are symmetric, independent Gaussian variables of unit variance. We used standard cubic lattices with periodic boundary conditions, where \(J_{ij}\) is non-zero if and only if \(i\) and \(j\) are nearest neighbors. To investigate more general networks as well, we additionally explored \(k\)-regular random graphs, i.e. where each spin interacts with exactly \(k\) other spins chosen at random. This is similar to the Viana-Bray model \[18\], except that the number of links emanating from each spin was fixed to \(k = 6\) for better comparison with the Euclidean 3d case.

The systems considered contain up to \(N = 40^3\) spins in 3d, and \(N = 16000\) spins in the regular random graph case. The dynamics is simulated using the Waiting Time Method (WTM) \[19\]. This rejectionless method is equivalent to the Metropolis algorithm, but much faster at low \(T\) for simulations of glassy systems. The intrinsic, size independent time variable \(t\) of the WTM corresponds to the number of Monte Carlo (lattice) sweeps in the Metropolis algorithm as well as to the physical time of a real experiment.

III. NUMERICAL RESULTS

Using the valley-identification method outlined in Section III, we examine the distribution of residence time \(t_{res}\) in a valley entered at \(t_w\), i.e.

\[
R(t \mid t_w) = \text{Prob}(t_{res} < t \mid t_w). \tag{2}
\]

The distribution for a 3d system with \(N = 16^3\) spins at temperature \(T = 0.5\) is shown in Fig. 1 for a wide range of \(t_w\) values. To collapse the data shown we used the scaling variable \(t/t_w^0\) with \(\mu = 1.077(6)\). The insert confirms that full aging, \(\mu = 1\), is only a fair approximation. The data collapse thus obtained is closely matched by the graph of the function \(f(x) = 1 - (1 + x)^{-\alpha}\), where \(\alpha \approx 2\). The latter is not shown in order to avoid masking the data—see Fig. 3 of Ref. 7 for a direct comparison.

The present simulations greatly extend our earlier findings \[8\,16\] by probing the size and temperature dependence of the small deviations from unity of the scaling exponent \(\mu\). Numerical investigation of such effects requires the removal of any visible statistical flutter. This has been achieved by averaging over at least 4,000 runs with different realizations of the couplings \(J_{ij}\) for every combination of \(N\) and \(T\). The calculations were performed on a large Linux cluster, with a total run-time equivalent to four years of computation on a single 2GHz processor. The result of these simulations is summed up in Fig. 2.

The high quality of the data collapse in Fig. 1 is representative for all sets of runs at fixed size and temperature on which the data points in Fig. 3 are based. This suggests that the ‘best’ value of \(\mu\) can readily be estimated by eye, as small variations of \(\mu\) immediately produce a visible scatter. To remove any personal bias, we did however utilize a quantitative error measure \(e(\mu)\) gauging the deviation from perfect collapse of a set of scaled exit time distributions: The horizontal standard deviation for a set of \(R(t \mid t_w)\) values chosen equidistantly between 0.2 and 0.8 is calculated for ten values of \(t/t_w^0\) at fixed \(\mu\). The value of \(e(\mu)\) is the sum of these standard deviations, and it attains a minimum within a ‘reasonable’ \(\mu\)-interval.

The uncertainty bracket around the \(\mu\) value producing the least scatter is arbitrarily defined by the two values of \(\mu\) for which \(e(\mu)\) is no more than 20% larger than its minimum value.
Figure 2 provides information on $\mu = \mu(N, T)$ in both 3d lattices (●) and random graphs (□). The data points and error bars are determined as explained above, ensuring that the quality of the data collapse behind the estimate of $\mu$ is near-perfect, i.e. as good as in Fig. 1. In the left panel, $\mu(N, T)$ is shown as a function of $T$ for fixed size $N = 16^3$. There is a clear decreasing trend, which however seems to taper off as the temperature decreases. The diminishing deviation from pure scaling concurs with the results by Kisker et al. [12] regarding the correlation function $C(t_w, t + t)$ in 3d Gaussian spin glasses. The right panel illustrates the behavior of $\mu(N, T)$ for $T = 0.5$ as a function of the logarithm of $N$. Again, as the number of degrees of freedom grows, super-aging is suppressed, albeit in a very slow fashion. Finally, we note the striking similarity between the Euclidean and random networks data in Fig. 2. The scaling of the residence time distribution seems to be indifferent to the topology of the graph considered.

When the system size becomes too small, the quality of the scaling of $R(t | t_w)$ begins to deteriorate. This applies to systems defined on 3d lattices as well as on random graphs. A possible explanation is a finite time (or size) effect: by construction, the valley containing the ground state will never be exited. By the same token, very low lying valleys, which are most likely entered for large $t_w$ and in small systems, are never exited during the simulation time. This flattens the s-shape of the distribution.

Figure 1: The probability distribution of residing at most a time $t$ in a valley entered at time $t_w$ is calculated for a set of 10 waiting times equally spaced on a logarithmic scale in the interval $10^2 \leq t_w \leq 10^5$. Each distribution function is plotted versus the scaled variable $t/t_w$, with $\mu = 1.077$, producing the perfect data collapse shown in the main panel. All data pertain to a 3d spin glass as defined in Section II. The insert shows that choosing $\mu = 1$ gives a visible spread of the curves, the latter being shifted to the right as $t_w$ grows. The apparent age $t^\mu_\nu$ inferred from the scaling plots is thus larger than the actual age, which is super-aging behavior.

IV. DISCUSSION

The residence time analyzed in the previous section appears from the outset conceptually similar to the trapping time introduced in a heuristic trap model by Bouchaud [6] and later considered by Rinn et al. [9] in a development specifically dealing with sub-aging behavior. However, the statistical properties hypothesized in the above models deviate considerably from those presently found. Crucially, the fitting form

$$R(t | t_w) = 1 - (1 + t/t_w^\mu)^{-\alpha}$$

with $\alpha = 2$ yields an average residence time

$$\langle t_{res} \rangle = \int_0^{\infty} R(t | t_w) dt = \frac{t_w^\mu}{\alpha - 1} = t_w^\mu,$$

which is finite, in contrast with the assumption of the trap model [6]. Secondly, the only temperature dependence is the weak increase of $\mu$, while the exponent $\alpha$ remains independent of $T$.

The numerical results of Fig. 2 points to pure aging as the correct limit for small $T$ or large $N$, although the sub-logarithmic size dependence of $N$ prevents us from turning this into a firm conclusion. The possible physical origin of the deviations from $\mu = 1$ for finite $N$ was already hinted to: Eventually, the trajectory enters the valley containing the ground state and never leaves. While this happens at extreme time scales for realistic system
sizes, fewer valleys will in general be available as the trajectories approach the ground state. The residence time for valleys entered at late stages will hence tend to be longer than otherwise expected. In accord with this interpretation, lowering $T$ has an effect on $\mu$ similar to the effect of enlarging $N$. In any case, the deviation from a pure log-Poisson description of quake dynamics becomes very small for large $N$, irrespective of the topology of the system. This supports the generality of log-Poisson statistics, whose prediction for the distribution of the residence time in a valley entered at age $t_w$ coincides with Eq. (3) for $\mu = 1$.

While $R(t | t_w)$ might be directly accessible in some experimental situations, its relationship to correlation functions for spin glasses is indirect and requires further assumptions and/or empirical input. If one assumes with Ref. [9] full decorrelation once a trap is left, and that the system. This supports the generality of log-Poisson statistics, whose prediction for the distribution of the residence time in a valley entered at age $t_w$ coincides with Eq. (3) for $\mu = 1$.

While $R(t | t_w)$ might be directly accessible in some experimental situations, its relationship to correlation functions for spin glasses is indirect and requires further assumptions and/or empirical input. If one assumes with Ref. [9] full decorrelation once a trap is left, and that the age $t_w$ uniquely determines the properties of the 'initial' trap, the correlation function basically coincides with the probability that no events occur from $t_w$ to $t_w + t$. As the latter is again given by Eq. (3), this would allow us to extend the conclusions already drawn for $R$ to the correlation function.

To assess the validity of such reasoning we will use a cartoon picture of the quake dynamics which neglects the internal structure of the valleys. This is a questionable step, as the time spent searching for the bottom state within a valley is of the same order of magnitude as the step, as the time spent searching for the bottom state within a valley is of the same order of magnitude as the time spent searching for the bottom state. With this caveat in mind, we write the non-equilibrium thermal correlation function as an average over the distribution of quakes:

$$C(t_w, t_w + t) = \sum_{m,k} P_m(t_w) P_k(t_w, t_w + t) c(m, m + k), \quad (5)$$

valid in the $t > t_w$ regime. In the above formula, $P_m(t_w)$ is the probability that $m$ quakes are recorded during the aging time $t_w$, $P_k(t_w, t_w + t)$ is the probability that $k$ quakes occurred between $t_w$ and $t + t_w$, and, finally, $c(m, m + k)$ is the configurational overlap between the 'bottom states' of the $m$'th and $(m + k)$'th valley.

The log-Poisson statistics prescribes the form of both $P_m(t_w)$ and $P_k(t_w, t_w + t)$. While the latter scales with $t/t_w$, the former depends on $t_w$ alone. This ruins pure aging for $C(t_w, t_w + t)$ unless the sum of $P_m(t_w)$ over $m$ happens to factor out. This can only occur if the overlap $c(m, m + k)$ does not depend on $m$. Perfect invariance of $c(m, m + k)$ with respect to the index $m$ must fail at some stage, since, again, the quake-induced rearrangements are likely to change as the ground state is approached. Numerical investigations presented elsewhere show that $c(m, m + k)$ has a small but systematic $m$ dependence already for small $m$ values. This excludes the possibility of 'perfect' pure aging of the correlation function for the numerical models studied, even though pure aging is well fulfilled for the waiting time distribution itself.

As the experimental results of Rodriguez et al. clearly support pure aging of the correlation function, it is possible that a description more refined than what Eq. (5) provides would modify our conclusion. In view of the smallness of the effects involved, it is also possible that some subtle dynamical feature of the experimental systems is missed by the computer models in the size range considered. A final possibility, which we regard as the most likely, is that $c(m, m + k)$ is indeed independent of $m$ for systems in the macroscopic limit. This would emphasize the extreme non-equilibrium nature of the observed low $T$ dynamics in spin glasses.

**Acknowledgments:** The Danish Center for Scientific Computing has provided generous time on the Horseshoe Linux cluster in Odense. The authors are also indebted to Greg Kenning and Stefan Boettcher for discussions. This project has been supported by Statens Naturvidenskabelige Forskningsråd.

[1] E. Vincent, J. Hammann, M. Ocjo, J.-P. Bouchaud, and L. F. Cugliandolo, in *Lecture notes in physics: Complex Behaviour of Glassy Systems*, edited by M. Rubi and C. Pérez-Vicente (Springer, 1997), vol. 492, pp. 184–219.
[2] J.-P. Bouchaud, in *Soft and Fragile Matter*, edited by M. E. Cates and M. R. Evans (1999), pp. 285–304.
[3] H. Bissig, S. Romer, L. Cipelletti, V. Trappe, and P. Schurtenberger, PhysChemComm 6, 21 (2003).
[4] V. Viasnoff and F. Lequeux, Phys. Rev. Lett. 89, 065701 (2002).
[5] P. Sibani and K. H. Hoffmann, Phys. Rev. Lett. 63, 2853 (1989).
[6] J. Bouchaud, J. Phys. I France 2, 1705 (1992).
[7] P. Sibani and J. Dall, Europhys. Lett. 64, 8 (2003).
[8] P. Sibani, Phys. Rev. B 35, 8572 (1987).
[9] B. Rinn, P. Maass, and J.-P. Bouchaud, Phys. Rev. Lett. 84, 5403 (2000).
[10] G. F. Rodriguez, G. G. Kenning, and R. Orbach, Phys. Rev. Lett. 91, 037203 (2003).
[11] L. Berthier and J.-P. Bouchaud, Phys. Rev. B 66, 054404 (2002).
[12] J. Kisker, L. Santen, M. Schreckenberg, and H. Rieger, Phys. Rev. B 53, 6418 (1996).
[13] F. H. Stillinger and T. A. Weber, Science 225, 983 (1984).
[14] B. Doliwa and A. Heuer, Phys. Rev. E 67, 030501(R) (2003).
[15] P. Sibani and J. Dall, cond-mat/0310286 (2003), submitted to EuroPhys. Lett.
[16] J. Dall and P. Sibani, cond-mat/0302575 (2003), submitted to Eur. Phys. J. B.
[17] S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).
[18] L. Viana and A. J. Bray, J. Phys. C: Solid State Physics...
18, 3037 (1985).
[19] J. Dall and P. Sibani, Comp. Phys. Comm. 141, 260 (2001).

[20] Barriers are defined as energy differences with respect to the current lowest energy state.