Edwards-Anderson spin glasses undergo simple cumulative aging

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(Dated: March 23, 2022)

Abstract

We study and discuss rejuvenation and memory (numerical) experiments in Ising and Heisenberg three and four dimensional spin glasses. We introduce a quantitative procedure to analyze the results of temperature cycling experiments. We also run, compare and discuss “twin” couples of experiments. We find that in our systems aging is always cumulative in nature, and rejuvenation and memory effects are also cumulative: they are very different from the ones observed in experiments on spin glass materials.

PACS numbers: 75.50.Lk,64.70.Pf
Rejuvenation and memory effects (that in the following we will denote by RME) are maybe the most striking features of spin glass materials, and their experimental evidence is very clear (see for example the discussion in [1] and references therein). The simplest experiment showing both rejuvenation and memory in a spin glass is the cycle in temperature, which is based on the following three steps:

1. one lets a spin glass sample relaxing for a time $t_1$ at temperature $T_1$ in the low $T$ phase;

2. then one brings it to a temperature $T_2 < T_1$, where it relaxes for a time $t_2$;

3. finally one heats it back to $T_1$ where relaxation continues.

The relevant experimental observations are mainly the following two:

- independently from the amount of time spent at $T_1$, when the sample is cooled to $T_2$ the relaxation process restarts completely (rejuvenation);

- when the sample is heated back to $T_1$ it seems to remember what happened during time $t_1$ and relaxation continues as if the second step was absent (memory).

We have given here a very simplified description, but it is sufficient for our goal, that is to compare the situation to the results of numerical simulations. Actual experiments show a number of different and subtle effects; we address the interested reader to the experimental results of [1] (and references therein).

RME effects are poorly understood from the theoretical point of view: for example it is still unclear which are the length scales that are relevant in such processes. Unfortunately length scales can not be measured directly in experiments, and numerical simulations could be of great help in this context. At the best of our understanding it is not clear, today, if real RME (of the same nature of the ones observed in experiments) appear in numerical simulation of finite dimensional Edwards-Anderson (EA) models (with either Ising or Heisenberg spins). In this note we clarify this point. We use a phenomenological approach: rather than trying to interpret numerical data within a specific theory in order to validate it we focus on the comparison of numerical and experimental data. Our aim is to check whether RME, as observed in physical experiments, are also present in the EA model. In order to reach
conclusions as general as possible, we consider EA models with different spin types (Ising and Heisenberg) and in $D = 3$ and $D = 4$.

Let us start with a brief review of RME as observed (or not) in numerical simulations of the EA model. A few years ago the work of [2, 3] discussed numerical studies of such effects in the 3D Ising EA model with Gaussian couplings. Unfortunately the lack of a quantitative method for estimating RME brought the authors of these two studies to give different interpretations of the outcome of a “cooling and stop” experiment. While reference [2] states that ”the model exhibits the rejuvenation-like and memory effects within a time-window of the present simulation”, reference [3] says that ”the model does not show, on the time scales we have access to, the strong RME real spin glasses show” (the time scales of the two numerical experiments are of the same order of magnitude, and the spatial volumes of the two systems are comparable).

A couple of years later, two further numerical works on this issue [4, 5] reach again opposite conclusions. Berthier and Bouchaud [4] interpret their data for the 4D Ising EA model as showing strong RME. They also suggest that in 3D such effects are difficult to observe because the spatial correlation function does not change enough when varying the temperature. On the contrary Takayama and Hukushima [5] find the signature of a cumulative aging scenario for small $\Delta T \equiv T_1 - T_2$. The cumulative aging scenario assumes that, as long as the system is in a spin glass phase, temperature changes do not induce a restart of aging, so that effects of relaxations at different temperatures cumulate.

In a recent paper Jimenez et al. [6] find again RME in both 3D and 4D Ising EA models.

Given such a confusing situation and such a number of different numerical results, we have decided to make very precise measurements with temperature cycle experiments in the EA model in order to try to answer the following three questions:

1. are true RME present in the EA model or is aging cumulative in nature?
2. if we observe cumulative aging, can we try to understand if true RME can be recovered in the limit of very large (relaxing and probing) time scales, i.e. in the limit relevant for experiments?
3. how much these effects depend on space dimension and spin type?

We consider the EA model with Gaussian couplings and both Ising spins (in 3D, I3D, and 4D, I4D) and Heisenberg spins (in 3D, H3D). Typical sizes used are $L = 40$ for I3D, $L = 20$
for I4D and $L = 60$ for H3D. We have checked that our lattices are large enough to avoid any detectable finite size effect; in particular, the choice of a large size for H3D samples is due to the very large length scales involved in the dynamics of Heisenberg spin glasses. We have computed the disorder averages by using 16 samples for H3D, 176 samples for I4D and 256 samples for I3D. The dynamics of Ising spins models has been based on the popular single spin-flip Metropolis algorithm. For Heisenberg spins we use again Metropolis updates but when changing temperature we fix the acceptance ratio, so the amplitude of the trial updates depends on the temperature: in this way we reproduce at best the physical dynamics. Most of the numerical simulations of I3D were performed on the APEmille parallel computer, while I4D and H3D were simulated on a PC cluster.

The choice for $T$-cycle experiments, which are in principle more complicated than $T$-shift experiments, is dictated by two main reasons. First, $T$-cycle experiments allow for the study of both rejuvenation and memory at the same time. Second, the first part of any relaxation process may be affected by large finite time corrections. Thus it is important that, when extracting the effective age of the system (see below), one compares relaxation processes where the initial steps are performed at the same temperature. In other words the effective age must be measured deep into the aging regime and not in the initial part of the relaxation process.

In order to simplify the analysis, especially when taking the large time limit, we introduce in our experimental procedure only one single relevant time scale $t_p$, that corresponds to the period of the measuring field used in real experiments. $t_p$ is the number of MC steps on which we average data: in other words we divide the total number of MC steps in groups of $t_p$ steps over which we compute expectation values. We use $t_p$ also as the time distance for computing time dependent correlations over spin configurations. We perform different runs for each fixed value of $t_p = 200, 500, 1000, 2000, 5000$ (I3D), $t_p = 100, 1000$ (I4D, H3D). All the other time scales will be proportional to $t_p$. In particular, if $t_i$ is the time spent in the phase $i$ of the experiment, we fix $t_1 = t_2 = t_3 = 20t_p$.

Our first aim is to define properly an effective time $t_{\text{eff}}$, such that after a $T$-cycle (i.e. $t_1$ steps at $T_1$, $t_2$ at $T_2$ and $t_3$ at temperature $T_1$ again) the system is in the same state as if it was let relaxing isothermally at $T_1$ during the time $t_1 + t_{\text{eff}} + t_3$. Because of possible transient effects (just after restoring temperature $T_1$) one should avoid to use small values of $t_3$.  

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Checking that two systems are statistically equivalent is not easy. We have done that by comparing a number of observable quantities and checking whether their values coincide in our statistical accuracy. We have considered both one time and two time quantities. As one time quantities we look at the Edwards-Anderson overlap order parameter \( q_{\text{EA}} \) and the spatial correlation function \( G(x, t) \):

\[
q_{\text{EA}}(t) \equiv \frac{1}{N} \sum_{i=1}^{N} m_i(t) \cdot m_i(t) 
\]

\[
G(x, t) \equiv \frac{1}{zN} \sum_{\|i-j\|=x} (S^a_i(t) \cdot S^a_j(t)) (S^b_i(t) \cdot S^b_j(t))
\]

where \( \cdot \) denotes the average over the quenched disordered couplings and thermal histories, \( z \) is the coordination number of the simple cubic \( D \)-dimensional lattice, \( N = L^D \), and \( a, b \) are real replica indexes. The basic fields of the theory take values \( S_i = \pm 1 \) variables for the Ising spin glasses (I3D, I4D), while are vectors on a sphere of unitary radius in the case of the Heisenberg spin glass (H3D). We define the corresponding time-integrated magnetization (over the time \( t_p \)) as

\[
m_i(t) \equiv \frac{1}{t_p} \sum_{\tau=t-t_p+1}^{t} S_i(\tau)
\]

We have also measured and used some two time quantities: the in-phase and out-of-phase susceptibilities. Provided that we are in the quasi-equilibrium regime (so that FDT holds) they can be estimated via the spin autocorrelation function

\[
C(t, t') \equiv \frac{1}{N} \sum_{i=1}^{N} S_i(t) \cdot S_i(t')
\]

In order to improve the signal-to-noise ratio we have integrated the above autocorrelation function over short times, \( \tau < t_p \), and defined

\[
\tilde{C}(t, t') \equiv \frac{1}{N} \sum_{i=1}^{N} m_i(t) \cdot m_i(t')
\]

The in-phase and out-of-phase susceptibilities are then expressed as a function of this time-integrated correlation function

\[
\tilde{\chi}'(t, t + t_p) \equiv \frac{\tilde{C}(t, t) - \tilde{C}(t, t + t_p)}{T},
\]

\[
\tilde{\chi}''(t, t + t_p) \equiv \frac{1}{T} \left[ \tilde{C}(t, t) + \tilde{C}(t-t_p, t + t_p) - \tilde{C}(t - t_p, t) - \tilde{C}(t, t + t_p) \right].
\]
Since $\tilde{\chi}''$ showed too small excursions upon $T$ changes, we preferred to use the out-of-phase susceptibility defined via the spin-spin autocorrelation (4)

$$\chi''(t, t + t_p) \equiv \frac{1}{T} [1 + C(t - t_p, t + t_p) - C(t - t_p, t) - C(t, t + t_p)]$$

Notice that relations (7) and (8) hold apart from an overall multiplicative factor $2$.

For each period $t_p$ we measure one-time quantities only at the end of period, and we integrate measurements of two-time quantities over the period, in close analogy with real experiments. This observation can be relevant since the only data which have been interpreted as a rejuvenation effect in [4] have been measured before the end of the first period after the $T$-shift: this is not done in real experiments. A possibility that we consider plausible is indeed that the RME showed in [4] are not related to the experimental RME effects, but to the fact that right after the temperature change the system is (for a very short time) strongly out of equilibrium. In such a situation the response measured in [4] with the expression $\chi(t) \equiv \frac{1-C(t,t+t_p)}{T}$ may overestimate the true susceptibility, giving rise to a signal which looks like a stronger rejuvenation. A deeper analysis of this effect has been done in [6].

Figures 1 and 2 show how our method for estimating $t_{eff}$ works. In Fig. 1 we show $G(1)$ and $\chi''$ for I3D in a $T_1 = 0.7$, $T_2 = 0.6$ cycle (remember that here $T_c \simeq 0.95$), while in Fig. 2 we show $G(1)$ and $\chi'$ for I4D in a $T_1 = 1.3$, $T_2 = 0.9$ cycle (here $T_c \simeq 1.8$). For clarity only half of the data points are presented in the figures. In each plot we show raw data measured during the $T$-cycle ($\bullet$). Isothermal aging data, from very long ($300t_p$) simulations at fixed $T = T_1$, are fitted on a simple smooth function $f(t)$ (that fits perfectly the data and is only used as a book keeping device for the matching procedure) that we represent with a solid line. $t_{eff}$ is calculated by shifting horizontally $f(t)$ to fit the data from the third stage of the $T$-cycle, and adding the needed time shift $t_s$ to the time $t_2$. $t_s$ enters the procedure as a fitting parameter, allowing a fully automatized estimation of $t_{eff} = 20t_p + t_s$, so we do not introduce any systematic error due to human perception of collapsing goodness.

In these plots we do not see a real and complete rejuvenation as in experiments, where the susceptibility decays in the second stage as if the first stage was absent (at least for a large $\Delta T$ as the one we are using here). This is clear especially if we compare the second part of the $T$-cycle with a direct quench at $T_2$ ($\triangle$). The authors of [4] suggested that in real
FIG. 1: Spatial correlation function at distance one (that coincides with the link overlap) and out-of-phase susceptibility (as defined in the text) in a temperature cycle of Ising 3D. The time evolution of $G(1,t)$ and $\chi''$ are compared with the evolution coming from a direct quench at $T_2$. The continuous line is a fit on data from a long isothermal run at $T_1$.

experiments even the fastest quench always corresponds to a cooling, so that the starting configuration of any relaxation process is never completely random. In order to check how much this fact could affect our hypothesis that the relaxation at $T_2$ strongly depends on the time spent at $T_1$, we have computed a new direct quench curve, starting this time not from a completely random configuration ($T = \infty$), but from a configuration thermalized at temperature $T = 2T_c$. Again we find substantial differences in the observables decays between these softer direct quenches and the relaxation in the second stages of the $T$-cycles: the two decays are not the same, and the discrepancy is not too different than the one from a direct quench (see Figures 1 and 2). This shows that even starting from a slightly correlated spin configuration, that is what could be happening in real experiments, we do not recover
the behavior of the temperature cycle.

Having estimated $t_{\text{eff}}$ for different values of $T_2$, we summarize our results in figure 4. As already noticed for example in [3] (see also [4, 5]), positive $\Delta T$ cycles do not reinitialize aging as in real experiments. On the contrary the time spent at $T_2 > T_1$ strongly increases the relaxation rate: for $\Delta T > 0$, $t_{\text{eff}}$ is larger than $t_2$. Full and dashed lines in figure 4 correspond to predictions obtained in a fully cumulative aging scenario (see below). $t_{\text{eff}}$ values are very far from experimental observations, which predict $t_{\text{eff}} = 0$ for $\Delta T < 0$ and $t_{\text{eff}} = -t_1$ for $\Delta T > 0$. Moreover the experimental behavior does not seem to be approached when we let the simulation time scales grow. We show in the left frame of figure 4 the data for $t_{\text{eff}}$ obtained with $t_p = 1000$ and $t_p = 200$. Both of them are well described by the cumulative hypothesis: this suggests that the cumulative aging scenario remains valid for very long ages of the system. In other words this “cumulative” behavior does not change when changing the total duration of the experiment by modifying the value of $t_p$. In the
FIG. 3: Comparison between the ratio $t_{\text{eff}}/t_2$ and the cumulative hypothesis, for I3D. Measurements of $t_{\text{eff}}/t_2$ are from cycle measurements of $G(x,t)$ with $x = 1, 2$ (left frame) and of the susceptibilities (right frame). In the left frame filled symbols are from measurements in cycles with $t_p = 1000$, while empty symbols come from cycles with $t_p = 200$. These plots are representative of the behavior of one-time and two-times quantities. Full and dashed lines are the theoretical prediction in the cumulative hypothesis with $\gamma = 0.85$ and $\gamma = 1$ respectively (on the right part of the plot higher lines have a larger $t_p$ value).

Let us discuss how we have obtained the analytical predictions shown in figure 3. We assume that the off-equilibrium correlation length grows as $\xi_T(t)$ (a $T$ dependent functional
dependence over time). In this case the cumulative aging prediction for $t_{\text{eff}}$ is that

$$
\xi_{T_1}(t_1 + t_{\text{eff}}) = \xi_{T_2} \left( \xi_{T_2}^{-1}(\xi_{T_1}(t_1)) + t_2 \right).
$$

(9)

The correlation length in Ising EA models is believed to grow as \[ \xi_T(t) \propto t^A, \] with $A = aT$ (with $a \sim 0.17$ in 3D). Using this functional dependence we obtain the dashed line in figure \( \text{A} \). We also explore the possibility of a more general dependence \[ \text{B} \] by assuming that $A = aT^\gamma$ (the usual dependence assumes $\gamma = 1$). The best fit to new high-precision data \[ \text{C} \] gives $\gamma = 0.85 \pm 0.04$. With $\gamma = 0.85$ the prediction for $t_{\text{eff}}$ becomes the one plotted with a full line in Fig. \( \text{D} \) which is a much better interpolation of the numerical data.

In figure \( \text{A} \) we present the analogous data for I4D and H3D, and we compare them with a cumulative hypothesis based on $\gamma = 1$ (this is only to allow to compare to a scenario where $\xi$ grows as a power of the time: at least for the Heisenberg case we have no precise hints about a given rate of growth, so that the fact that the solid curve does not fall on the numerical
data cannot be seen as a “discrepancy”). Data for H3D show a very weak dependence of $t_{\text{eff}}$ (and of $\xi(t)$) on $T$, which deserves (and is undergoing) deeper investigations \cite{10}.

The authors of \cite{5} find cumulative aging only for small $\Delta T$, while for $\Delta T \geq 0.3$ their data are incompatible with the cumulative aging scenario. This incompatibility shows up as an asymmetry in the laws for transforming times from $T_1$ to $T_2$ and that from $T_2$ to $T_1$. In the cumulative aging scenario these two functions should be the inverse of each other, while in \cite{5} they are shown not to be so. This discrepancy could be due to the fact that $T$-shift experiments of \cite{5} also take into account the very first part of the relaxation after the initial quench, which is typically plagued by finite time effects. We believe that in order to avoid this kind of problems any measurement should be taken late enough after the initial quench, in such a way that the system has already entered the asymptotic aging regime (and in any case all the region of very large $\Delta T$ is bound to be affected by non-universal effects, very resilient to a clean theoretical analysis).

In order to investigate this potential problem we have repeated the “twin-experiments” of \cite{5,11}. They are based on four stages: the first stage ($t_1$ steps at $T_1$) is the same in both twin experiments, and it is only used to bring the system in the asymptotic aging regime (in this stage there are no measurements). In the following two stages the two experiments are complementary: one consists of $t_2$ steps at $T_2$ and then $t_3$ steps at $T_3 = T_1$, while the other goes first with $t_3'$ steps at $T_3 = T_1$ and then $t_2'$ steps at $T_2$. In the fourth and last stage both experiments are run at the same temperature $T_4 = T_1$.

Assuming the validity of the cumulative aging hypothesis, it is not difficult to choose times $t_1$, $t_2$, $t_2'$, $t_3$ and $t_3'$ at fixed temperatures $T_1$ and $T_2$ such that the correlation length takes the same value at the end of the complementary stages (the second and the third ones). If the cumulative aging hypothesis is correct, one should observe that in the fourth stage measurements from the twin experiments coincide. We show in figure \ref{fig:5} the results of measurements of $G(1)$ from twin experiments of I3D with $T_1 = 0.7$, $T_2 = 0.4$: stage durations are marked by dotted vertical lines. In the fourth stage measurements of $G(x)$ turn out to coincide (in our statistical accuracy) even for large values of $x$: the structures built by the two systems undergoing different histories are, as far as we can check, equivalent.

We believe that we have been able to give quantitative evidence that aging in finite dimensional spin glasses is cumulative in nature. It is clear that, as always in numerical simulations, our statements are valid in the limit of, among others, the time scales we

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Stage durations were predicted using a power law cumulative hypothesis and imposing the equivalence of the coherence length at the end of the third stage.

are able to investigate (that are far shorter than the experimental ones). Still, our search for some potential asymptotic restoration of true, experimental-like RME has failed. Our findings concern both Ising and Heisenberg systems, both in 3D and in 4D: in our time windows the behavior is not substantially affected under a sizable change of time window, even if we should not forget that we are still very far from the experimental time scales.

It is clear that further studies are required. There is a clear mismatch with experimental data, where a non-trivial aging is observed.

This work was partially supported by the European Community’s Human Potential Programme under contracts HPRN-CT-2002-00307, Dyglagemem, and HPRN-CT-2002-00319, Stipco.
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