Thermocycling experiments with the three-dimensional Ising spin glass model

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Abstract

A characteristic feature of the non–equilibrium dynamics of real spin glasses at low temperatures are strong aging effects. These phenomena can be manipulated by changing the external parameters in various ways: a thermo-cycling experiment consists for instance of a short heat pulse during the waiting time, by which the relaxation might be strongly affected. Results of numerical experiments of this kind, performed via Monte Carlo simulations of the three dimensional Ising spin glass model, are presented. The theoretical implications are discussed and the scenario found is compared with the experimental situation.

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1 Introduction

The non-equilibrium dynamics of spin glasses has been a major focus of research activity since the seminal work of Lundgren et al. [1] of 1983. Two years later the so called aging phenomena of spin glasses became manifest, when experimentalists realized [2] that magnetic properties of spin glasses depend strongly on the time they spent below the freezing temperature T_g. These effects are a consequence of the extremely slow dynamics of spin glasses at low temperatures, regardless of the existence of an equilibrium phase transition (for an overview of their equilibrium properties see [3]).

Following the arguments of the droplet theory [4] one imagines the dynamical process at low temperatures to be governed by a growth of domains, which will reach some typical size after a certain waiting time. This length/time scale becomes manifest in a crossover observable e.g. in the thermo-remanent magnetization decay (see also [5]). On the other hand, inspired by Parisi's solution of the mean–field model of spin glasses [6], it has been proposed that the many metastable states existing in the rough free energy landscape of spin glasses might be organized in a hierarchical way[7]. Dynamics then explores states with decreasing free energy, and the escape from these valleys becomes harder, which means that it takes longer time. In this way the depth of the valley reached during the waiting time becomes manifest again as a crossover in observable quantities (see also [8]).

Thermo-cycling experiments consist of two temperature changes within the spin glass phase [9]: either a short heat pulse is applied to the spin glass during the waiting time after which the relaxation of e.g. the thermo-remanent magnetization is measured, or a short negative temperature cycle is performed. It has been pointed out [10] that this kind of experiments can discriminate between the droplet picture and the hierarchical picture.

Within the hierarchical picture a heat pulse experiment and a negative temperature cycling experiment should have an asymmetric outcome: The hierarchical organization of the metastable states depends on temperature in such a way that the free–energy–valleys split into several, steeper valleys with decreasing temperature. Here an escape becomes even more difficult, resulting in a freezing of the aging process during a negative temperature cycle. Upon heating several valleys melt together, thus facilitating the escape. After completion of the cycle the system is again in a narrow valley with a higher free energy, similar to the beginning of the experiment and thus restarting the aging process. Experiments using the insulating spin glass $CdCr_{1.7}In_{0.3}S_4$ [9, 10] can be nicely interpreted within this picture.

On the other hand within the droplet theory a heat pulse experiment and a negative temperature cycling experiment should have qualitatively a symmetric outcome: in both cases the domains that have grown so far should be reduced in size (or even destroyed) by the temperature cycle, and thus reinitialize the aging process. This is a consequence of the fact that spatial correlations among equilibrium spin glass states at different temperatures below T_g are short ranged with a typical length scale decresing rapidly with increasing temperature difference [4, 5, 13]. Experiments in Cu(Mn) spin glasses [11] and Cu(Mn) spin glass films [12] have reported a scenario that speak in favor of this interpretation.

Besides these two phenomenological approaches cited above some success has been made very recently in the analytical and numerical investigation of microscopic mean-field models of aging in spin glasses [14, 15, 16] or related, simplified models [17, 18]. However, up to now the study of microscopic models of aging phenomena in two– or three–dimensional model of spin glasses had to be performed exclusively via numerical simulations [19, 20]. Here not only a qualitative agreement among simulation results and simple aging–experiment (without temperature cycle) could be established, but also numerical values for various exponents determining the functional form of the decay of the thermo-remanent magnetization have been shown in [20] to be the same in certain spin glasses $(Fe_xNi_{(1-x)})_{75}P_{16}B_6Al_3$ and $Fe_{0.5}Mn_{0.5}TiO_3$) and the three–dimensional Edwards–Anderson model with a heat–bath dynamics.

One might ask, whether temperature cycling in Monte–Carlo simulations will also show such a remarkable concurrence with the experimental scenario. In this paper we present the results of such simulations. In the next section we introduce the model, give some numerical details and define the quantities that have been calculated. In section 3 we present the results, which are discussed in section 4.

2 Numerical Procedure

The system under consideration is the same as in [20], the three–dimensional Ising spin glass model with nearest neighbor interactions and a discrete ($\pm J$)

bond distribution. Its Hamiltonian is

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \ , \tag{1}$$

where the spins $\sigma_i = \pm 1$ occupy the sites of a $L \times L \times L$ simple cubic lattice with periodic boundary conditions and the random nearest neighbor interactions J_{ij} take on the values $+1$ or -1 with probability $1/2$. The quantity h is an external magnetic field. The dynamics is the so called Metropolis algorithm, defined by the probability for single spin flips

$$w(\sigma_i \to -\sigma_i) = \min\{1, \exp(-\Delta E/T)\} \ , \tag{2}$$

where ΔE is the energy difference between the old state and the new state in which the spin at site i is flipped. The most efficient implementation of this algorithm on a Cray-YMP has been used (see [21] for details).

To mimic the temperature cycling experiments [9, 10, 11, 12] the following procedure has been applied: First the system is initialized in a random state at a temperature $T < T_g \approx 1.2$ (T_g is the freezing or spin glass transition temperature of the model (1), see [22], however, note also [23]), which corresponds to a fast quench from the paramagnetic phase into the spin glass phase. Then the system is kept at the temperature T for a first waiting time t_{w1}, during which the initial aging takes place. Note that time is measured in Monte–Carlo seeps through the lattice. Then the temperature is changed to T_p, which is larger than T in a heat pulse experiment and smaller than T in a negative temperature cycle experiment. The system is kept at the temperature T_p for a time t_p. Finally the cycle is completed by changing the temperature back again to the initial temperature T, where the system is aged again for a time t_{w2}. After this time (note that up to this point $t_{\rm age} = t_{w1} + t_p + t_{w2}$ Monte–Carlo sweeps have been done).

We performed two different kind of experiments: In the first the whole simulation is done in zero field, and we stored the spin configuration at time $t_{\rm age}$ and measured its overlap with the spin configurations of the system t Monte–Carlo steps later:

$$C(t, t_{\rm age}) = \frac{1}{N}\sum_i \overline{\langle \sigma_i(t + t_{\rm age})\sigma_i(t_{\rm age})\rangle} \ . \tag{3}$$

Here $\langle \cdots \rangle$ means a thermal average (i.e. an average over different realizations of the thermal noise, but the same initial configuration) and the bar means an average over different realizations of the bond–disorder.

In the second experiment we keep the system within an external field h during the whole temperature cycling procedure and switch it off after the the procedure has been completed (i.e. after t_{age}). From that moment on the thermo-remanent magnetization

$$M_{\mathrm{TRM}}(t, t_{\mathrm{age}}) = \frac{1}{N} \sum_i \overline{\langle \sigma_i(t + t_{\mathrm{age}}) \rangle} \ , \tag{4}$$

is measured. This field–cooling experiment is exactly what is done with real spin glasses [9, 10, 11, 12].

The linear system size of the samples is L=32 (i.e. $\sim 3 \cdot 10^4$ spins), and we averaged over 256 different realizations of the disorder. There are *no* finite size effects observable within the time scale of 10^6 Monte–Carlo steps, which means that the typical correlation length (or linear domain size within the language of the droplet picture) is still smaller than half of the linear system size after $t = 10^6$. We believe that our results do not depend significantly on the choice of the dynamics (2). Let us adopt the point of view that spin glasses are critical for all temperatures below the spin glass transition temperature T_g (note that the correlation length in the frozen phase is infinite for all temperatures). In this case we would expect that any microscopic dynamics without order-parameter conservation (model A in the classification of Hohenberg and Halperin [25]) will give the same universal results for all temperatures below T_g as long as the spins are of Ising type and the interactions are short ranged (so, for instance, also in the case of the short–ranged Ising spin glass $\mathrm{Fe}_{0.5}\mathrm{Mn}_{0.5}\mathrm{TiO}_3$ [24]. As soon as one considers e.g. Heisenberg spins or RKKY–interactions the quantitative behavior might change, although we have nor reason to believe that the qualitative picture of the results presented here changes significantly.

3 The correlation function $\mathbf{C}(\mathbf{t}, \mathbf{t}_{\mathrm{age}})$

The autocorrelation function $C(t, t_{\mathrm{age}})$ defined in equation (3) measures the overlap of spin configurations at time $t + t_{\mathrm{age}}$ with that achieved after aging the system for a time t_{w1} at temperature T, exerting a heat pulse of duration t_p with temperature T_p and finally aging the system again for a time t_{w2} at temperature T. In figure 1 we choose $T = 0.7$, $t_{w1} = 10^4$, $t_p = 10^2$, $t_{w2} = 10^1(a), 10^2(b)$ and various heat pulse temperatures T_p. In figure 1 one observes that the short heat pulse diminishes the correlations and $C(t, t_{\rm age})$ varies smoothly between the two curves obtained by $T_p = T$ (no heat pulse) and $T_p = \infty$. The latter curve is identical to that obtained by simple aging with waiting time t_{w2} since $T_p = \infty$ destroys all correlations grown during the first waiting time t_{w1}. Thus the heat pulse tends to reinitialize aging, however, not completely as long as T_p is not high enough. Partial re-initialization has been observed in some experiments [11, 12]. On the other hand, figure 1 is at variance with other experiments [9, 10], where aging is fully reinitialized by applying a heat pulse of temperature only slightly above T and still significantly below the freezing temperature T_g.

In figure 2 the same parameters as above are used up to the duration of the pulse, which is now $t_p = 10^3$. Note that now the heat pulse is only one decade shorter than the first waiting time t_{w1} and one observes differences to figure 1: For $T_p = 1.0$ and 1.3 the correlations are larger at long times t than those without heat pulse. One possible interpretation is that on one side the longer heat pulse destroys some of the correlations originating from the first aging (note that for small t all curves with $T_p > T$ lie below $T_p = T$), but drives the system into energetically more favorable states (deeper valleys) like in simulated annealing [26]. Thus it is harder for the system to escape from the vicinity of the state reached after $t_{\rm age}$, which enhances the correlations at long times.

This picture is supported by figure 3, where $T = 0.7$, $T_p = 1.0$ and the sum of first waiting time and duration of the heat pulse is kept constant: $t_{w1}+t_p = 1000$. The longer the heat pulse the larger the correlations $C(t, t_{\rm age})$ at large times t. For comparison we have inserted a plot of the function $C(t, t_w = 10^5)$ obtained by simple aging with a much longer waiting time $t_w = 10^5 \gg t_{\rm age}$.

This effect is completely absent if one performs a negative temperature cycling experiment with the same data for t_{w1}, t_p and t_{w2}. The result for $T = 0.9$ and $T_p = 0.7$ (note that now $T_p < T$ is depicted in figure 4: For increasing duration of the "cold" pulse the correlation function $C(t, t_{\rm age})$ is clearly diminished. It seems that aging is partially frozen during the negative temperature cycle, the system cannot reach valleys as deep as those it would explore during simple aging at temperature T (corresponding to the $t_p = 0$ curve). However, freezing is only partial, since compared with the simple aging curve $C(t, t_w = t_{w2})$ the correlations are still higher. Let us conclude this section with this observation of a clear asymmetry between heat pulse experiments shown in figures 1–3 and negative temperature cycling experiments shown in figure 4.

4 The magnetization $\mathbf{M}(\mathbf{t}, \mathbf{t}_{\rm age})$

The correlation function that has been investigated in the last section is hard to measure in experiments with real spin glasses. Nevertheless it has a physical meaning and it yields the same information as the usual susceptibility–measurements in equilibrium (because of the fluctuation–dissipation theorem, see [19, 20]) and additional information in non-equilibrium. In this section we perform the following procedure already mentioned in section 2, which mimics exactly the experimental situation described in [9, 11, 12]: the temperature cycle is done within a weak external field, by which a magnetization is induced. After the completion of the cycle the field is switched off and the decay of the (thermo)-remanent magnetization (4) is measured.

We show in the following results for rather strong magnetic fields ($h = 0.5$), for the simple reason that the data are less scattered, since the signal (magnetization) is stronger. We performed also simulations for $h = 0.2$ and $h = 0.1$, which give qualitatively the same results. The differences originating in the fact that $h \sim 0.5$ is certainly outside the linear response regime are not observable on these time scales.

In figure 5 we depicted the results of heat pulses with various temperatures. The initial aging temperature was $T = 0.7$ and $t_{w1} = 10^4$, the duration of the pulse was $t_p = 10^2$ and the final waiting time is $t_{w1} = 10^1$. For comparison the remanent magnetization obtained from simple aging at temperature $T = 0.7$ and waiting time $t_w = 10$ is shown. One observes that the heat pulse diminishes the magnetization for times smaller than $0.1 \cdot t_{w1}$, like it does with the correlations in figure 1. The aging process is again only partially reinitialized, the temperature of the heat pulse has to be very high nullify the magnetization obtained during the first waiting time t_w. This is of course a consequence of the high magnetic field, for smaller magnetic fields the temperatures needed to completely re-initialize the aging process are significantly smaller.

Furthermore one observes that for $t > 0.2 \cdot t_{w1}$ the heat-pulse is able to enhance the magnetization, an effect that becomes more pronounced the longer the heat pulse is. This effect can be interpreted in the same way as in the preceding section about the correlation function $C(t, t_{\rm age})$. Here the heat pulse destroys some of the magnetized domains of the system, however not completely. Simultaneously it drives the system into energetically more favorable states, which have a non-vanishing magnetization. After the completion of the temperature cycle the initial magnetization is smaller, but it takes longer to escape from this magnetized state and to approach zero magnetization.

Again, if this picture is correct in essence, one might expect a different outcome in a negative temperature cycle experiment. In figure 6 we show such an experiment with $T = 0.9$ and cycle temperature $T_p = 0.6$ (note that $T_p < T$ now). The initial waiting time is $t_{w1} = 10^3$, the final waiting time is $t_{w2} = 10^2$. For increasing heat pulse length t_p the remanent magnetization is either unchanged or slightly increased for all times t. Thus the negative temperature cycle destroys nothing of the magnetization obtained during the initial aging process. The magnetized domains continue to grow during the cycle (however, at a much smaller rate), for comparison the magnetization curve obtained for simple aging at $T = 0.9$ with a waiting time $t_w = 10^5$ is shown, which shows a still larger magnetization than that of negative temperature cycling with $t_p = 10^5$.

We conclude that TRM–measurements in temperature cycling experiments manifests again an asymmetry between heat pulse and negative temperature cycle experiments and therefore yield the same picture as that obtained from the calculation of the autocorrelation function $C(t, t_{\rm age})$ described in the last section.

5 Discussion

In this section we will summarize and discuss the results of the numerical experiments presented in this paper. By calculating the autocorrelation function $C(t, t_{\rm age})$ and the thermo-remanent magnetization $M_{\rm TRM}(t, t_{\rm age})$ we tried to explore the effect of temperature cycling on the aging process within the three–dimensional Ising spin glass model. We demonstrated that by a heat pulse, which is short compared to the initial waiting time, the aging process is partially re-initialized. On the other side, a negative temperature cycle experiment partially freezes the system into the (domain)–state reached during the initial aging process. Some experiments on real spin glasses show a much clearer outcome [9, 10], which, nevertheless, might be interpreted to concur with our observation. And finally — as pointed out in [10] — this asymmetry would pledge in favor of the hierarchical picture mentioned in the introduction and against the droplet picture.

However, our results are on a very qualitative level and the dynamical processes involved are still microscopic on a logarithmic time scale. Thus it might be hard to verify one phenomenological, macroscopic theory and falsify another on the ground of our numerical data, although they have been obtained by state–of–the–art simulations with the most efficient existing algorithm implemented on one of the fastest computers of today. The parameter space for this kind of experiments is essentially six–dimensional (T, T_p, t_{w1}, t_p, t_{w2} and h), therefore a systematic investigation, as was done for simple aging experiments in the same model [20], seems to be forbidden. Therefore we had to confine ourselves to demonstrate what kind of scenario for temperature cycling experiments is obtained for the model, time scales and quantities under considerations and can only offer a possibly speculative interpretation.

Furthermore we would like to point out that very strong crossover phenomena are observable within our results as soon as the duration of the heat pulse of the final waiting time become comparable to the initial aging time. We interpreted them within a picture of a relaxation in a rough free energy landscape, which again seems to be most appropriate for the results we obtained. This picture is rather flexible and is able to explain a lot of features in a frustrated system — real or theoretical, and regardless of the existence of a phase transition. One of the phenomena that are fully neglected in a theory that is based on the assumption of a relaxation within a complicated free energy landscape is that of the growth of spatial correlations during the aging process. They are on the other side the basic ingredience of the droplet model [4]. Although both theories seem to make contradicting predictions (e.g. the symmetry or asymmetry of heat pulse and negative temperature-cycling experiments) our impression is that they have more in common than usually admitted.

We think that it might be very useful to try to find a synthesis of both models, not only in order to be able to describe the growth of spatial correlations and their destruction by a heat pulse and their freezing during a negative temperature cycle. Domain growth has not been investigated by direct measurements up to now (for experiments that investigate this matter indirectly see [12, 27, 28]). However, in numerical simulations one has an immediate access to the quantities of interest and work on this subject is in progress[29]. It is our impression, obtained from the results presented in this paper and in other publications [19, 20], that the simulation of finite dimensional Ising spin glass models can make relevant predictions for real spin glasses, too, and will prove to be a very useful tool in testing and improving phenomenological theories for them.

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Figure Captions

Fig. 1 The spin autocorrelation function $C(t, t_{\rm age})$ defined in (3) in dependence of t (number of MC–steps) for various heat pulse temperatures T_p. The other temperature cycling parameters are $T = 0.7$, $t_{w1} = 10^4$, $t_p = 10^2$ and $t_{w2} = 10^1$ in the upper figure and $t_{w2} = 10^2$ in the lower figure. From top to bottom it is $T_p = T$ ($\circ$), $T_p = 1.0$, 1.3, 1.6, 1.9, 2.2, 2.5 (full lines) and $T_p = \infty$ ($\Box$). The error bars are significantly smaller than the symbols for the curves plotted with points.

Fig. 2 Same as in figure 1, but with a longer duration of the heat pulse $t_p = 10^3$ and pulse temperatures (from top to bottom at $t \sim 10^3$) $T_p = T$ ($\circ$), $T_p = 1.0$, 1.3, 1.6, 2.0 (full lines) and $T_p = \infty$ ($\Box$).

Fig. 3 $C(t, t_{\rm age})$ in dependence of t with $T = 0.7$, $T_p = 1.0$ and $t_{w2} = 100$. The sum $t_{w1} + t_p = 1000$ is constant, from bottom to top it is $t_p = 0$ ($\diamond$), $t_p = 10$, 100, 300, 500 and 900 (full lines). The top curve ($\Box$) is just for comparison — it is the function $C(t, t_w = 10^5)$ obtained from simple aging with waiting time $t_w = 10^5 \gg t_{\rm age}$.

Fig. 4 $C(t, t_{\rm age})$ from a negative temperature cycling experiment with $T = 0.9$, $T_p = 0.7$ ($< T$!) and $t_{w2} = 100$. As in figure 3 the sum $t_{w1} + t_p = 1000$ is constant, from top to bottom it is $t_p = 0$ ($\diamond$), $t_p = 10$, 100, 500 and 900 (full lines). The bottom curve ($\Box$) is just for comparison — it is the function $C(t, t_w = 10^2)$ obtained from simple aging with waiting time $t_w = 10^2 = t_{w2}$.

Fig. 5 The thermo-remanent magnetization $M_{\rm TRM}(t, t_{\rm age})$ defined in (4) in dependence of t (number of MC–steps) for various heat pulse temperatures T_p. The other temperature cycling parameters are $T = 0.7$, $t_{w1} = 10^4$, $t_p = 10^2$ and $t_{w2} = 10^1$. From top to bottom (at $t = 100$) it is $T_p = T$ ($\diamond$), $T_p = 1.0$, 1.3, 1.6, 1.9, 2.2, 2.5 (full lines) and $T_p = \infty$ ($\Box$). The error bars are significantly smaller than the symbols for the curves plotted with points.

Fig. 6 $M_{\mathrm{TRM}}(t, t_{\mathrm{age}})$ from a negative temperature cycling experiment with $T = 0.9$, $T_p = 0.6$ ($< T$!), $t_{w1} = 10^3$ and $t_{w2} = 10^2$. From bottom to top (at $t = 1000$) it is $t_p = 0$ ($\Box$), $t_p = 10^2$, 10^3, 10^4 and 10^5. The top curve ($\diamond$) is just for comparison — it is the function $M_{\mathrm{TRM}}(t, t_w = 10^5)$ obtained from simple aging with waiting time $t_w = 10^5$.