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LETTER TO THE EDITOR

Non-equilibrium dynamics and aging in the three-dimensional Ising spin-glass model

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Abstract. The low temperature dynamics of the three-dimensional Ising spin-glass in zero field with a discrete bond distribution is investigated via MC simulations. The thermoremanent magnetization is found to decay algebraically and the temperature dependent exponents agree very well with the experimentally determined values. The non-equilibrium autocorrelation function $C(t, t_w)$ shows a crossover at the waiting (or *aging*) time t_w from algebraic *quasi-equilibrium* decay for times $t \ll t_w$ to another, faster algebraic decay for $t \gg t_w$ with an exponent similar to one for the remanent magnetization.

The measurement of dynamical non-equilibrium quantities in real spin-glasses [1] has a long history. The typical experiment that has been conducted many times [2, 3] is the following: within a magnetic field the spin-glass (for instance Cu(Mn), Au(Fe), $Fe_{0.5}Mn_{0.5}TiO_3$, $(Fe_xNi_{(1-x)})_{75}P_{16}B_6Al_3$, $Cd_xMn_{(1-x)}Te$, etc) is cooled down to temperatures below the freezing temperature T_g and either immediately or after a certain waiting time t_w the field is switched off. Then the so-called (thermo)remanent magnetization $M_{rem}(t)$ is measured as a function of time t. The asymptotic time dependence of this quantity is found to be algebraic well below T_g ($T/T_g \lesssim 0.98$) in the short range Ising spin-glass $Fe_{0.5}Mn_{0.5}TiO_3$ [4, 5] and in an amorphous metallic spin-glass $(Fe_xNi_{(1-x)})_{75}P_{16}B_6Al_3$ [6]. Furthermore the time-dependence of the remanent magnetization depends on the waiting time t_w, a phenomenon called aging [2].

Several attempts have been made to explain this behaviour theoretically [7–11] and a wide variety of functional forms for the time dependence of the remanent magnetization is found. The problem lies in the fact that starting from a microscopic model or model-Hamiltonian one encounters insurmountable difficulties in trying to solve the non-equilibrium dynamics. Therefore additional assumptions have to be made and the final outcome—stretched exponential [7], algebraic [10, 11] or logarithmic [9] decay—depends on them. Even within the mean field approximation it is hard to obtain any analytical [12, 13] or semi-analytical [14] results.

Once a microscopic model for a spin-glass has been formulated, one can in principle try to extract its macroscopic behaviour via Monte Carlo (MC) simulations. In contrast to an analytical treatment, where the calculation of dynamical non-equilibrium quantities within the spin-glass phase (instead of those characterizing equilibrium, see [15]) is even more complicated, MC simulaton can be done with less effort for certain

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non-equilibrium situations, since equilibration times reach astronomical values in the case of spin-glasses [16–18]. The remanent magnetization with zero waiting time has been investigated numerically for the mean field version of a spin-glass model [9, 19] and for the three-dimensional EA (Edwards-Anderson) model only right at the critical temperature [20]. Quite recently attempts have been made to investigate the whole temperature range below T_g numerically [21, 22]. However, a systematic MC study of non-equilibrium correlations and aging phenomena within the frozen phase ($T < T_c$) of the three-dimensional EA spin-glass model has not been made up to now. The results of such an investigation, its theoretical implications and comparison with experiments will be reported in this letter.

The system under consideration is the three-dimensional Ising spin-glass with nearest neighbour interactions and a discrete bond distribution. Its Hamiltonian is

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

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 neighbour interactions J_{ij} take on the values $+1$ or -1 with probability $\frac{1}{2}$. We consider single spin-flip dynamics and used a special, very fast implementation of the Metropolis algorithm on a Cray YMP (see [23] for details). The simulations were done in the frozen phase, that means at temperatures below $T_c = 1.175 \pm 0.025$ (see [16–18]). All measured quantities are averaged over at least 128 samples (smaller system sizes were averaged over up to 1280 samples). The system size was increased until no further size dependence of the results were observed within the simulation time ($t \leqslant 10^6$), which is measured in MC sweeps through the whole lattice. It turns out that $L = 32$ is large enough for this time range (see [18]).

The system was prepared in a fully magnetized initial configuration and then the simulation was run for a time t_w (waiting time) and then the spin configuration $\sigma(t_w)$ was stored. From now on after each MC step (data were then averaged over appropriate time intervals, see [18]) the following correlation function was measured:

$$C(t, t_w) = \frac{1}{N}\sum_i \overline{\langle \sigma_i(t+t_w)\sigma_i(t_w)\rangle} \tag{2}$$

where $\langle \ldots \rangle$ 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. The quantity $C(t, 0)$ corresponds to the remaining magnetization of the system after a time t.

$$M_{\mathrm{rem}}(t) = C(t, 0). \tag{3}$$

This quantity is directly related to the experimentally determined thermoremanent magnetization with zero waiting time (i.e. without aging) and nearly saturated initial magnetization. The result for the remanent magnetization $M_{\mathrm{rem}}(t)$ is shown in figure 1 within a log-log plot. Its decay clearly obeys a power law for large times and temperatures in the range $1.1 \geqslant T \geqslant 0.5$. The exponent $\lambda(T)$ for the fit

$$M_{\mathrm{rem}}(t) \propto t^{-\lambda(T)} \qquad (t \geqslant 10^2) \tag{4}$$

is plotted in figure 2, upper curve. It starts at $\lambda = 0.36 \pm 0.01$ for $T = 1.1$ (and can be extrapolated via the fit indicated in figure 2 to 0.39 ± 0.01 for $T = T_c$, which was already found in [20]) and decreases monotonically with temperature. For the short range Ising spin-glass $Fe_{0.5}Mn_{0.5}TiO_3$ and for certain amorphous metallic spin-glasses not

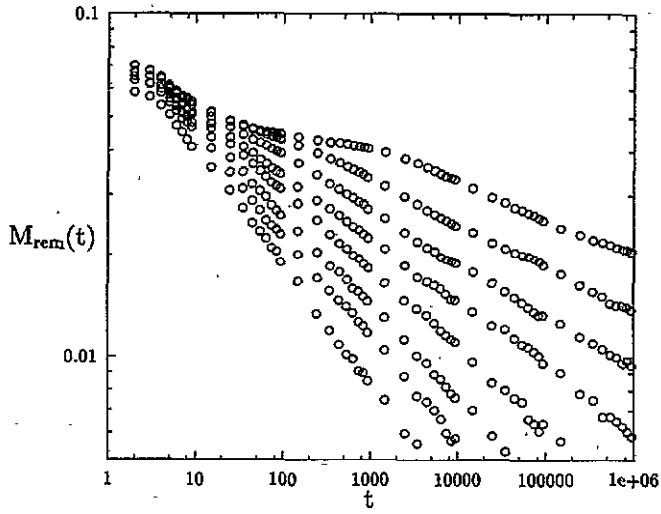

Figure 1. The remanent magnetization $M_{rem}(t)$ versus the time t in a log-log plot for varying temperatures. From top to bottom we have $T = 0.4$, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 and 1.1. the system size is $L = 32$ and the data are averaged over 128 samples. The error bars are of the size of the symbols for $M_{rem} \leq 0.01$ and much smaller for larger M_{rem}.

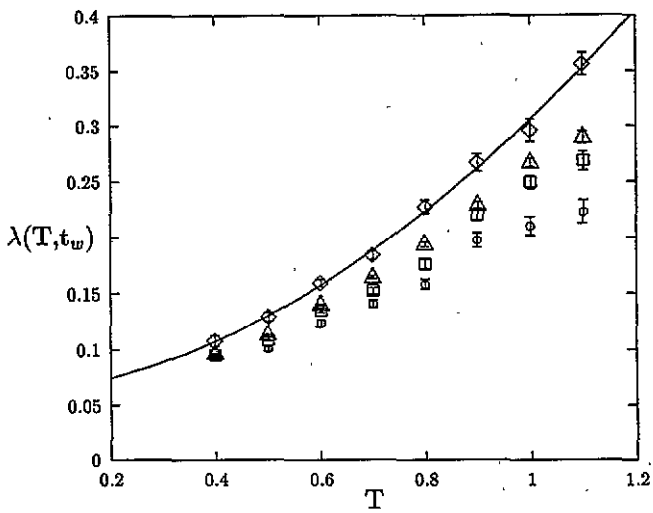

Figure 2. Upper curve: The exponent $\lambda(T)$ for the remanent magnetization (3) versus temperature. The points represented by diamonds (◇, plus errorbars) are those extracted from figure 1 and the full curve is a least square fit to a quadratic polynomial as a guideline to the eye. Lower points: The non-equilibrium exponent $\lambda(T, t_w)$ (see equation (5)) extracted from the long-time behavour ($t \gg t_w$) of the non-equilibrium correlation function $C(t, t_w)$ (see figure 3) for fixed values of t_w versus the temperature T. From top to bottom we have: (△) $t_w = 10$, (□) $t_w = 100$ and (○) $t_w = 1000$. The errorbars are indicated.

only the same algebraic decay of the remanent magnetization has been observed, but also the shape of the functional temperature dependence of the exponent $\lambda(T)$ and even its numerical values are in excellent agreement: from figure 4(b) in [6] one may for instance read off $\lambda(T_g) \approx 0.38$ and $\lambda(0.5T_g) \approx 0.12$, concurring within the errorbars to the corresponding data plotted in figure 2.

It was argued [9] that the decay of $M_{rem}(t)$ should be logarithmic (i.e. $M_{rem}(t) \propto (\ln t)^{-\lambda/\psi}$) below T_c, but a fit of the data in figure 1 for $T \geq 0.5$ does not yield acceptable results over the range of the observation time. We want to focus some attention to the $T = 0.4$ curve: It bends upward in the log–log plot for $t > 10^4$, which could indicate the onset of a slower than algebraic decay for temperatures smaller than 0.5, logarithmic for instance.

Another indication that something new happens at lower temperatures can be obtained by looking at the short-time behaviour of $M_{rem}(t)$: At $T \approx 0.5$ a plateau begins to develop for $t < 10^2$, which can clearly be seen for $T = 0.4$ and becomes even more pronounced and wider for even smaller temperatures. It can be exactly reproduced in shape and location for smaller and larger sizes and number of samples, which means that it is a physical effect and not only a fluctuation. A possible interpretation might be that the system gets trapped in metastable states, whose lifetime grows with decreasing temperatures.

Next we turn our attention to the correlation function $C(t, t_w)$ with $t_w = 10^a$ ($a = 1, \ldots, 5$). In contrast to $M_{rem}(t)$ the correlation function $C(t, t_w)$ for $t_w \neq 0$ is not directly related to the thermoremanent magnetization $M(t, t_w)$ at time $t + t_w$ in a temperature-quench experiment, where the field H is switched off at time t_w after the quench (see e.g. [24]). In equilibrium $(t_w \to \infty) C(t, \infty)$ is related to the relaxation function $R(t, \infty) = M(t, \infty)/H$ via the fluctuation dissipation theorem (FDT) $R(t, \infty) = C(t, \infty)/k_B T$. However, in a non-equilibrium situation, like the one considered here, slight differences between them exist [21, 25] (e.g. in the location of the maximum relaxation rate). The magnetization that is induced by a small external field ($H \ll 1$) for model (1) is rather small, therefore the functional form of $M(t, t_w)$ is harder to determine accurately via MC-simulations. This is the reason why in this letter the focus is on $C(t, t_w)$.

A typical set of data for a particular temperature ($T = 0.8$) is shown in figure 3 in a log–log plot. One observes a crossover from a slow algebraic decay for $t \ll t_w$ to a faster algebraic decay for $t \gg t_w$. The crossover time is simply defined as the intersection of the two straight line fits for short- and long-time behaviour in the log–log plot. For the long-time behaviour the fit to

$$C(t, t_w) \propto t^{-\lambda(T, t_w)} \qquad t \gg t_w \tag{5}$$

yields a set of exponents that is depicted in figure 2. For increasing t_w the exponent $\lambda(T, t_w)$ decreases only slightly and the waiting time dependence becomes weaker for lower temperatures. By looking at figure 3 one observes that it is difficult to extract $\lambda(T, t_w)$ for $t_w = 10^4$ and 10^5 since there are only 2 or 1 decades left to fit the exponent—therefore they are not shown in figure 2. The exponent describing the short-time ($t \ll t_w$) behaviour of $C(t, t_w)$,

$$C(t, t_w) \propto t^{-x(T)} \qquad t \ll t_w \tag{6}$$

which is depicted in figure 4, is independent of the waiting time t_w. Since the system was able to equilibrate over a time t_w, all processes occurring on timescales smaller than t_w have the characteristics of equilibrium dynamics and therefore the exponent

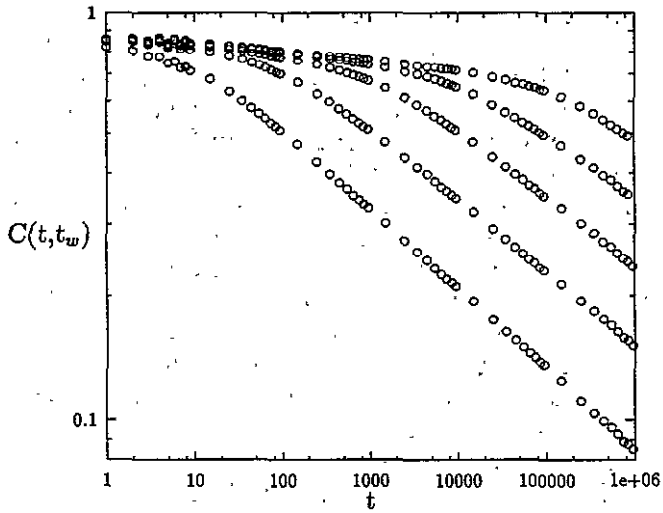

Figure 3. The averaged non-equilibrium spin autocorrelation function $C(t, t_w)$ of equation (2) for fixed values of t_w versus time t on a double logarithmic timescale. The temperature is fixed to be $T=0.8$ and from top to bottom we have $t_w=10^5$, 10^4, 10^3, 10^2 and 10. The system size is $L=32$ and the data are averaged over 128 samples. The size of the errorbars is only a fraction of the size of the symbols.

$x(T)$ is identical to that describing the decay of the equilibrium autocorrelation function $q(t)=\lim_{t_w\to\infty} C(t, t_w)$. The latter was investigated in [18] and the exponents that are reported there for $T \geqslant 0.7T_c$ agree with the values shown in figure 4. They also agree with those determined experimentally [5] in the short range Ising spin-glass

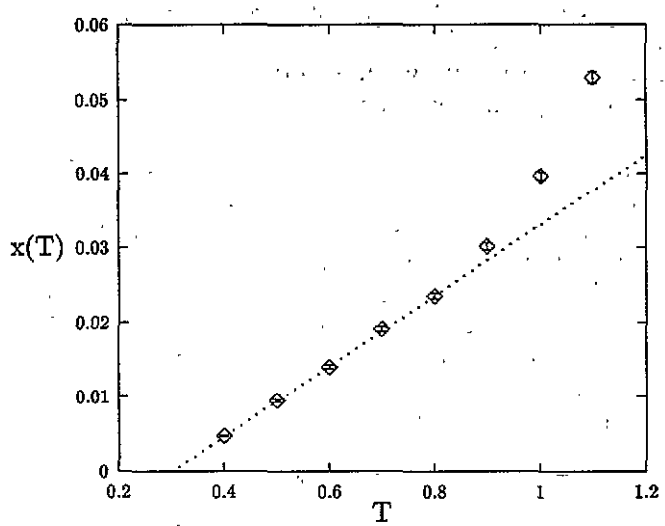

Figure 4. The equilibrium exponent $x(T)$ for the equilibrium autocorrelation function $q(t)$ *extracted from the short-time behaviour* ($t \ll t_w$) *of the non-equilibrium correlation function* $C(t, t_w)$ (see equation (6)) versus the temperature T. The errorbars are smaller than the symbols, as indicated. For $T \leqslant 0.8$ the data are fitted to a straight line, which shows that at approximately $T=0.3$ the exponent $x(T)$ vanishes.

$Fe_{0.5}Mn_{0.5}TiO_3$ via the above the mentioned relaxation function $R(t, t_w) = M(t, t_w)/H$ for $t \ll t_w$ (note that in this quasi-equilibrium regime $C(t, t_w)$ and $R(t, t_w)$ are related via the FDT [21, 25], yielding the same exponents for both): close to $T_g (T/T_g = 1.029)$ they obtain $x = 0.07$. Furthermore there seems to be a temperature at about 0.3, where $x(T)$ becomes zero, which could be another indication for the above mentioned onset of a logarithmic decay of the correlation functions†.

Although the decay of the non-equilibrium correlations in the temperature range $0.5 \leqslant T \leqslant 1.1$ is algebraic rather than logarithmic as predicted by the droplet picture proposed in [9], this picture might not be inappropriate. Let us assume the following scaling law for the dependence of the free energy barriers B on a length scale L of the regions to be relaxed: $B = \Lambda \ln L$ instead of $B \propto L^{\psi}$ as in [9]. Then one ends up with an algebraic decay of, e.g., the remanent magnetization by observing (see [9]) that the typical length scale of domains R_t now grows with time according to $\Lambda \ln R_t \sim T \ln t$, which means $R_t \propto t^{T/\Lambda(T)}$, leading to equations (3)–(6).

In the context of the phenomenological model for the dynamics and aging in disordered systems developed in [11], the algebraic decay of correlations found so far implies that the probability distribution of free energy barriers is exponential in the temperature range of $0.5 \leqslant T \leqslant 1.1$ for the system under consideration. Furthermore we would like to mention that a fit to the functional form for the short time behaviour $(t \ll t_w) C(t, t_w) \sim 1 - a(t/t_w)^{y}$ proposed in [11] works also quite well for our data, although not as convincingly as equation (6).

Guided by equations (4) and (5) we tried to put our results into the following scaling form:

$$C(t, t_w) = c_T t^{-x(T)} \Phi_T(t/t_w) \tag{7}$$

where $\Phi_T(y) = 1$ for $y = 0$ and $\Phi_T(y) \propto y^{x(T)-\tilde{\lambda}(T)}$ for $y \to \infty$. The form (7) has recently been used [27] successfully to extract the critical dynamical exponent z from the non-equilibrium correlation function (2) via finite size scaling, where the waiting time t_w has been replaced by the relaxation time $\tau \propto L^z$ in the critical region. For temperatures below $T = 0.8$ equation (7) yields an acceptable fit (which can already be deduced from the negligible waiting time dependence of the exponents $\lambda(T, t_w)$ for $T \leqslant 0.7$, see figure 2).

Concluding, we have reported new results of numerical non-equilibrium simulations that show an excellent concurrence with experiments on the short range Ising spin-glass $Fe_{0.5}Mn_{0.5}TiO_3$ and on amorphous metallic spin-glasses: not only a single exponent but a whole continuum of (temperature dependent) exponents for the remanent magnetization are found to agree within the numerical errors. Although the values for the exponents extracted from experiments might vary somewhat depending on the microscopic details (range of interactions, spin-type) the main features of the relaxation and the dynamics of many different three-dimensional spin-glasses are very similar and the functional forms of the remanent magnetization decay should be the same for different systems [28].

Furthermore we have shown that aging phenomena in the spin-glass model under consideration can be observed via the measurement of a particular correlation function and that its non-equilibrium dynamics is indeed governed by its equilibrium characteristics for timescales smaller than the imposed waiting (or aging) time. This gives an

† According to [26], also the equilibrium autocorrelation function $q(t)$ should decay logarithmically $q(t) \propto (\ln t)^{-\theta/\psi}$.

interesting new perspective (see also [27, 29]) to extract equilibrium quantities, which are hard to obtain via MC simulations within the spin-glass phase. Finally, by observing plateaus in the short time behaviour and slowing down of the algebraic decay of the remanent magnetization, we revealed a dynamical scenario at very low temperatures that is not yet fully understood.

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