Aging in disordered systems

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Abstract

The dynamics of strongly disordered systems becomes extremely slow or glassy at low temperatures, which results in a characteristic aging scenario. This means that the outcome of measurements strongly depends on the history of the system within the glassy phase, even on macroscopic time scale like hours, weeks or years. This area of non-equilibrium dynamics in disordered systems became recently a major focus of research interest, in particular with respect to spin glasses and related systems. Here we give an overview on these activities with a focus on Monte Carlo studies.
I. INTRODUCTION

The physics of strongly disordered systems has been a focal point of research by experimentalists and theoreticians in recent years. Among the most studied materials/models in this category are magnetic systems with impurities and especially spin glasses. However, their glassy features observed in experiments as well as the theoretical problems occurring in spin glass models are also encountered in various different situations: So for instance in the context of structural glasses, manifolds (e.g. polymers) in random media, protein folding, dirty superconductors, charge–density–wave systems with impurities and also other areas like neural networks, population dynamics, immunology and biological evolution.

Much of the theoretical effort has concentrated on the existence and characterization of an equilibrium phase transition in spin glass models. Here much progress has been made, although some questions still await a final answer. An at least equally fascinating subject, for which theory is even harder, is the description of its non-equilibrium dynamics. Experimentally this is the predominant scenario one has to deal with, since equilibration of a spin glass is nearly impossible on laboratory time scales. A major part of glassy dynamics takes place out of equilibrium and a characteristic feature of it is what one calls aging. This has been first observed by experimentalists 10 years ago and denotes the striking dependence of e.g. magnetization measurements in spin glasses on the history (or age) of the system within the frozen phase.

A huge number of experimental investigations of this phenomenon has been performed since then and it turned out that it occurs quite commonly in all different kinds of spin glass materials and can also be observed in other disordered substances like in amorphous polymers, high–$T_c$ superconductors or in charge-density-wave systems. Furthermore it does not depend on the existence of an equilibrium phase transition, for instance also two-dimensional spin glasses exhibit aging. We will argue below that it is a characteristic feature of any disordered or amorphous system with a broad distribution of relaxation times and is therefore observable also in the various contexts mentioned above.

On the theoretical side the aging phenomenon in spin glasses has attracted ever increasing interest in recent years. Due to its extreme mathematical difficulties it was not possible up to now to formulate a microscopic theory for the non-equilibrium dynamics of finite dimensional spin glasses. Only very recently progress has been made in the analytic treatment of aging in mean-field models of Ising spin glasses and simplified or toy models. However, it has not been possible yet to make quantitative predictions that would render a comparison with experiments possible. More successful in this respect are phenomenological theories like the droplet model by Fisher and Huse and the domain theory by Koper and Hilhorst.

Therefore numerical studies play a decisive role in discriminating between various predic-
tions of the existing phenomenological models. As is well known in a Monte-Carlo simulation one can obtain much more detailed information about the dynamical processes and the spatial correlations in the system under consideration. Moreover with increasing computer power one might even be able to come close to the macroscopic time scales that are relevant in real experiments. Much progress has been obtained recently and in this paper we intend to give an overview on our recent numerical studies on aging in spin glasses and other strongly disordered systems.

II. AGING IN SPIN GLASSES

The first observation that one makes by dealing with spin glasses and related systems is that their dynamics is extremely slow at low temperatures and that for instance equilibration cannot be achieved any more on laboratory time scales. This is a disadvantage only as long as one is solely interested in equilibrium quantities, but it becomes a very fascinating subject for investigation as soon as one gives up the pretension to explore this regime that is an unnatural form of existence for glassy materials anyway: they are typically out of equilibrium. In this sense aging is just another word for non-equilibrium dynamics and means that the outcome of any experiment that is done with the system under consideration will depend on the procedures one has applied to it at former times.

Supposed one is interested in the functional form of the time-dependence of some observable $O(t)$, where the point $t = 0$ is chosen deliberately and defines a separation between the beginning of the observation and the system’s former history in the glassy phase of duration $t_w$, the waiting time or the time for which the system has aged. Experimentalists usually apply after this particular time a change in a field $\hat{O}$ that is conjugate to the observable $O$ so that $O(t)$ is essentially the response of the system to this field change. Instead one might also measure (e.g. in Monte-Carlo simulations) the corresponding correlation function $O(t)O(t + t_w)$, which would even contain the same information via the fluctuation dissipation theorem provided equilibrium conditions would hold. Note that one is not interested in this information per se, but only in the characteristic aging scenario where $O(t)$ depends on the whole functional form $\hat{O}(t_w)$ even for macroscopically large waiting times $t_w$ of the order of hours, weeks or even years.

To be concrete let us consider the Edwards-Anderson (EA) model of an Ising spin glass in three dimensions, which (most probably) has a phase transition into a spin glass phase at some finite temperature:

$$H = - \sum_{(ij)} J_{ij} S_i S_j .$$

(1)
The Ising spins $S_i = \pm 1$ are put on a simple cubic lattice of linear dimension $L$ with periodic boundary conditions. The interaction strengths $J_{ij}$ are quenched random variables obeying a Gaussian distribution with zero mean and variance one, the spin glass transition temperature is $T_g \approx 0.91$. Usually we are interested in a stochastic, microscopic, single-spin-flip dynamics that is non-conservative in energy and magnetization, modeling the coupling of the magnetic moments in real spin glasses to a heat-bath representing the lattice phonons. Hence we choose the so-called heat-bath algorithm, which flips single spins with a probability $w(S_i \to -S_i) = \min\{1, \exp(\Delta E_i/T)\}$, $\Delta E_i$ being the energy difference $H(S_i) - H(-S_i)$ between the old and the new configuration. However, the results will not depend significantly on this choice, as we have checked explicitly.

The quantity that convincingly demonstrates the aging phenomena and which is best accessible for a quantitative analysis in numerical simulations is the spin autocorrelation function

$$C(t, t_w) = \frac{1}{N} \sum_i \left\langle (S_i(t + t_w)S_i(t_w)) \right\rangle_{av},$$

where for instance $S(t_w)$ is the configuration of the system after the waiting time $t_w$ and time is measured in number of Monte-Carlo sweeps through the whole lattice. The angular brackets indicate the average over different initial conditions and $\left\langle \cdots \right\rangle_{av}$ mean the disorder average. Note that as mentioned before in experiments usually the corresponding response function, i.e. the thermo-remanent magnetization decay after a field change at time $t_w$ is measured. In fig. [1] the result for one particular temperature (in the spin glass phase) is shown in a log-log plot. Several characteristic features can be read off immediately, like the crossover from a slow quasi-equilibrium decay for $t \ll t_w$ to a faster non-equilibrium decay for $t \gg t_w$ and the functional form of these decays being algebraic rather than logarithmic, which can be subsumed in the scaling formula $^{21, 22}$

$$C(t, t_w) = t^{-\frac{x(T)}{2}} \Phi_T(t/t_w),$$

with $\Phi_T(y) = c_T$ for $y = 0$ and $\Phi_T(y) \propto y^{x(T)-\lambda(T)}$ for $y \to \infty$. The most important observation is the $t/t_w$ scaling behavior, in contrast to e.g. the prediction $C(t, t_w) \sim (\ln t)^{-\theta/\psi} \tilde{\Phi}\{\ln(t/\tau)/\ln(t_w/\tau)\}$ by the droplet theory. Nevertheless we think that the domain growth or coarsening picture of the latter theory is appropriate: for the length and time scales under consideration only a basic scaling assumption has to be modified in order to be consistent with the result (3), see $^{2}$ for details.

The domain growth taking place during the waiting time $t_w$ can be studied in a straightforward manner within Monte-Carlo simulations by calculating the spatial correlation function $G(r, t_w) = \left\langle (S_i(t_w)S_{i+r}(t_w))^2 \right\rangle_{av}$. From this one can extract the correlation length $\xi(t_w)$.
either with the help of the expected scaling form $G(r, t_w) \sim \tilde{g}(r/\xi(t_w))$ or via the integral 
$\xi(t_w) = 2 \int dr \, G(r, t_w)$. In fig. 2 the waiting time dependence of this correlation length for a particular temperature is shown in a log-log plot. It turns out that a fit of the waiting time dependence of this correlation length to an algebraic growth law $\xi(t_w) \sim t_w^{\alpha(T)}$ works very well, which is consistent with the asymptotic algebraic decay of the autocorrelation function $C(t, t_w)$ and its $t/t_w$-scaling behavior.

In addition to waiting time experiments described above also other procedures (in terms of the function $\hat{O}(t_w)$ mentioned in the first paragraph of this section) have been applied experimentally. For instance so-called temperature cycling experiments, which consist of two temperature changes during the time in which the material is aged in the spin glass phase: 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, which is the same as a heat pulse but with a negative temperature shift during the pulse. It has been pointed out that this kind of experiments can discriminate between the droplet picture and the hierarchical picture. The interpretation of the experimental situation is still controversial and as long as numerical simulations follow exactly the lines of the experiments the outcome is pretty similar, meaning inconclusive. However, in numerical studies one has a much broader spectrum of quantities that can be analyzed and in the overlap-correlation function $\langle S_i S_{i+r} \rangle_T \langle S_i S_{i+r} \rangle_{T \pm \Delta T}$ was calculated explicitly. Here no indication of the existence of an overlap-length, which is one of the underlying concepts of the droplet theory, could be found.

Finally it should be noted that the microscopic theory for the off-equilibrium dynamics of mean field models of spin glasses has been pushed forward recently. The mathematical difficulties for an analytically exact solution of the dynamical off-equilibrium mean field equations for e.g. the SK-model come from the lack of the fluctuation-dissipation theorem (FDT) that relates autocorrelation and response function. The new approaches circumvent this by considering a so-called fluctuation-dissipation ratio defined via

$$x(t, t') = \frac{r(t, t')}{\beta \partial C(t, t')/\partial t'} \quad (4)$$

and postulating a particular set of properties for this function $x(t, t')$ in various asymptotic limits, essentially setting up an "ultrametric" for timescales. In this way Parisi’s static, equilibrium (!) order parameter function $q(x)$ finds its counter-part in off-equilibrium dynamics. This scenario has been checked in numerically in three dimensions. Indeed a nontrivial function $x(q)$ was found (the validity of the FDT-theorem would imply simply $x(q) = 1$) and it seems that these concept might also be applicable in finite dimensions.
III. INTERRUPTED AGING

Two-dimensional spin glass models do not have a spin glass transition at a finite temperature. This means that the equilibrium correlation length $\xi_{eq} = \lim_{t_w \to \infty} \xi(t_w)$ (where $\xi(t_w)$ is defined in the last section) stays finite if $T > 0$. Moreover there is a finite, but very large, equilibration time $\tau_{eq}$ characterized by $\xi(t_w) \sim \xi_{eq}$ for $t_w \geq \tau_{eq}$. In terms of a coarsening picture this means that after a temperature quench domains will steadily grow for a some time and aging in the sense described above will persist. However, as soon as the waiting time reaches the order of $\tau_{eq}$ the system is equilibrated and aging is interrupted.

Monte-Carlo simulations of the two-dimensional EA-model of an Ising spin glass (identical to (1) but on a square lattice) indeed confirm this picture of interrupted aging\(^{26}\). In fig. 3 the autocorrelation function (2) is shown for different temperatures. Here it is nicely demonstrated that for higher temperatures the system reaches equilibrium and the different curves for $C(t, t_w)$ collapse onto a single curve $C_{eq}(t)$ for waiting times large than the equilibration time $\tau_{eq}$. For lower temperatures the figure becomes indistinguishable from the three dimensional case, fig. 4, which is a consequence of the fact that the equilibration cannot take place any more on time scales that are accessible. This is also the situation that is reported in experiments on two-dimensional spin glasses\(^{16}\). Moreover, it can be shown\(^{26}\) that for these temperatures the correlation length grows algebraically with a temperature dependent exponent, similar to the three-dimensional case. At higher temperatures the domain growth saturates at some finite correlation length as expected.

Up to now only frustrated systems were considered, however, glassy dynamics and aging also occurs in non-frustrated systems. We studied the non-equilibrium dynamics and domain growth in the random Ising chain\(^{27}\)

$$H = -\sum_{i=1}^{L} J_i S_i S_{i+1} ,$$

with random ferromagnetic bonds $J_i$ (note that the distribution does not need to be confined to positive couplings since their sign can be removed by a simple gauge transformation). Although this system does not have any frustration a typical (interrupted) aging scenario at low temperatures can be observed. A broad distribution of (free) energy barriers results in a very slow domain growth results. The latter can easily be studied in this context, since domains are simply ferromagnetically ordered segments of the chain.
IV. NON-CONVENTIONAL AGING

From what has been said in the last section it might occur that only a very few ingredients might be necessary in order to observe aging at least over some time scale. Indeed, aging becomes manifest already in the ferromagnetic Ising chain \( H = -J \sum_i S_i S_{i+1} \) at zero temperature\(^2\), where the dynamics is simply described by kink diffusion and annihilation. In particular the autocorrelation function \( C(t, t_w) \) scales with \( t/t_w \) as observed in many other models with and without disorder or frustration, too. However, this is not the only possible scenario one can think of and some systems show deviations from this \( t/t_w \) scaling, which we call *non-conventional aging*. For instance it is also possible that after the temperature quench the system gets trapped in narrow (free) energy minima of a particular depth in such a way that continuous domain growth (or steady equilibration) is not possible any more. In this way, very reminiscent of the structural glass transition, the system is frozen into an amorphous metastable state for an astronomically long time.

To illustrate this sort of behavior we studied a very simple spin model without any frustration or disorder that possesses many glass like features at low temperatures. It is defined by the following \( p \)-spin interaction Hamiltonian for Ising spins on a chain\(^2\):

\[
H = -J \sum_{i=1}^{L} S_i S_{i+1} \cdots S_{i+p-1} .
\]

For simplicity we consider the case \( p = 3 \). The groundstate of this system has a 4-fold degeneracy (in general \( 2^p-1 \)). Introducing a local energy-variable \( \tau_i = S_{i-1} S_i S_{i+1} \) all groundstate configurations are described by \( \tau_i = +1 \) for all sites \( i \). Consider a configuration in \( \tau \) and \( S \) variables

\[
(\tau) \cdot + + + + + + + + + + + + + + + + + + + + + + + + + + + + + \cdots
\]

\[
(S) \cdot + + + + + + + + + + + + + + + + + + + + + + + + + + + + + \cdots
\]

which consists of two domains, both being in a minimum energy configuration, separated by a domain wall located at site \( i \). It costs an energy of \( 2J \) to move the domain wall at position \( i \) to the right or left, thus the system is frozen into such a metastable configuration for a time \( t_{\text{freeze}} \approx \exp(2J/T) \). Moreover, it can be shown that all configurations of the type \( (\tau) \) consisting (expressed in \( \tau \)-variables) of strings of arbitrary length \( l \geq 2 \) with \( \tau = +1 \) separated by isolated sites with \( \tau = -1 \) are indeed metastable. In a chain of length \( L \) an exponentially large number \( n_{\text{stable}} \sim L^{1.4655} \) of these configurations exist. Starting with a random initial state the sequential update procedure at zero temperature will drive the system into one of this exponentially large number of metastable states within only two
sweeps through the whole chain. Thus after $2t_0$, where $t_0$ is the microscopic time scale, the system will be frozen for a time $t_{\text{freeze}} = t_0 \exp(2J/T)$. This can be seen for instance by looking at the waiting time depends of the average domain size, which enters a plateau at a small value (which can be calculated exactly to be 5.775 lattice spacings) after two time steps that extends to infinity for $T \to 0$ as is shown in fig. 4.

As mentioned before this is an extremely simplified model with one single characteristic energy barrier that prevents the system from relaxing into its equilibrium configuration for an exponentially large time. By allowing the interaction strengths to vary spatially and arranging them for instance in a hierarchical way one generates spatially varying energy barriers and a broad distribution of exponentially large trapping times. On the other hand it is possible to generalize this model to higher dimensions. In this case even a true equilibrium phase transition is possible and a closer contact to the physics of the structural glass transition might become feasible.

V. SUMMARY

As we have seen the non-equilibrium dynamics of strongly disordered systems is a very fascinating subject. Experimentally as well as numerically one is confined to rather restricted time and length scales for which a complete theory is still missing (although some progress has been announced). Aging does not only occur in frustrated systems, as has been demonstrated in the random bond Ising chain, and can even be observed in systems without any disorder. Most systems show an aging behavior in which spin autocorrelations scale with $t/t_w$ and the domain growth depends algebraically on the waiting time $t_w$. However also other scenarios are possible and models are currently under investigation that are very reminiscent of the structural glass transition.

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FIG. 1. Autocorrelation function $C(t, t_w)$ for the EA-spin glass model in three dimensions as a function of time $t$ for $t_w = 5^n$ ($n = 1, \ldots, 8$) at $T = 0.6$. The system size is $L = 24$ and the disorder average was performed over 256 samples.
FIG. 2. Waiting time dependence of the correlation length $\xi(t_w)$ in three dimensions for different temperatures. The straight lines are least square fits to an algebraic growth law $\xi(t_w) \sim t_w^{\alpha(T)}$ with the exponent $\alpha(T)$ varying approximately linear between $\alpha(T = 0.2) = 0.026$ and $\alpha(T = 0.7) = 0.081$. 
FIG. 3. Autocorrelation function $C(t, t_w)$ for the EA-spin glass model in two dimensions as a function of time $t$ for $t_w = 5^n$ ($n = 1, \ldots, 8$) at $T = 1.0$ and 0.8, ($n = 2, \ldots, 8$) at 0.6 and 0.2. The system size is $L = 100$ and the disorder average was performed over 256 samples. The errorbars are smaller than the symbols.
FIG. 4. Average domain size in dependence of the waiting time $t$ of the Ising chain with 3-spin interactions \(^{(k)}\) for various temperatures calculated via Monte-Carlo simulation of a system with \(10^6\) spins. The intermediate growth (between melting of the frozen domains and final saturation by equilibration) can be fitted nicely to $d(t) \sim t^{1/2}$ (solid line).