LETTER TO THE EDITOR

Escape from metastability via aging: non-equilibrium dynamics in a one-dimensional Ising model

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Abstract. The non-equilibrium dynamics of a one-dimensional Ising model with uniform, short-ranged three-spin interactions is investigated. It is shown that this model possesses an exponentially large number of metastable configurations that are stable against single spin flips. This glass-like situation results in a complete freezing of the system at low temperatures for times smaller than an intrinsic time-scale, which diverges exponentially with inverse temperature. Via thermal activation the system eventually escapes from this frozen state, which signals the onset of aging by domain growth.

Glassy dynamics is one of the most fascinating subjects in modern physics [1,2]. It manifests itself in an extremely slow relaxation exceeding laboratory time-scales caused by a rough energy landscape. In spin glasses this complex dynamics is due to frustration and randomness [3] and results in well known aging effects [4,5] meaning a characteristic history dependence of dynamical observations.

However, as is obvious from the situation in e.g. window glass, disorder is not a necessary ingredient for these phenomena to occur. For spin models it has been pointed out a long time ago [8] that frustration without disorder might be able to produce a low-temperature behaviour reminiscent of spin glasses. Indeed, experiments with geometrically frustrated antiferromagnets [6, 7] showed anomalous dynamical behaviour below a certain temperature that was interpreted as a spin-glass transition. The magnetic properties of these materials are supposed to be adequately described by antiferromagnetically-coupled Heisenberg spins on a Kagomé lattice and recent numerical studies of this model also yield indications for dynamical freezing [9] and possibly spin-glass ordering [10] at low temperatures.

On the other side, disorder without frustration can also cause anomalous dynamics and slow relaxation: Diluted or disordered ferromagnets are prominent examples [11, 12] for systems in which non-equilibrium dynamics is characterized by domain growth that is drastically slowed down by pinning of domain walls at vacancy-sites or weak bonds. Obviously at low enough temperatures it becomes very hard to discriminate such a scenario from true spin-glass dynamics. Even non-frustrated, non-disordered models at, or close to, criticality will exhibit anomalously slow non-equilibrium relaxation including aging, originally supposed to be typical for spin glasses [11, 13].

In this short note we present a very simple spin model without any frustration or disorder that possesses many glass-like features at low temperatures. It turns out that, quenching the system from high to low temperatures, the dynamics become trapped within *microscopic* time scales in a metastable configuration without long-range order. The system

remains frozen in this amorphous state for a *macroscopic* time before it will try to reach an energetically more favourable, ordered state via domain growth. This is very reminiscent of the structural glass transition scenario [2], however, this should only be taken as a pictorial analogy.

The model which we consider is a one-dimensional Ising spin system with p-spin interactions defined by the Hamiltonian

$$H = -J \sum_{i=1}^{L} S_i S_{i+1} \cdots S_{i+p-1} \qquad (S_i = \pm 1).$$
 (1)

The constant J fixes the energy scale of the spin interactions, which we set to one from now on, and periodic boundary conditions are imposed. The dynamics is defined to be the usual Glauber-dynamics [14], where each spin is flipped with probability

$$\omega(S_i \to -S_i) = \frac{1}{2} [1 - S_i \tanh(h_i/T)] \tag{2}$$

where the local field h_i is defined to be one half of the energy difference between the configuration with spin $S_i = +1$ and the same configuration with spin $S_i = -1$, and T is the temperature. We use sequential update for the analytic calculations as well as for the numerical simulations. For p = 2 one gets the well known ferromagnetic Ising chain, whose dynamics with random sequential update has been solved by Glauber [14]. Note that for p odd the Hamiltonian (1) does not have the usual spin-flip symmetry $S_i \rightarrow -S_i$. Furthermore the local field is a sum over p terms with values +1 or -1, from which it follows that it can never be identical to zero in the case p odd, whereas for even p the probability for a spin to have zero local field is finite. Thus one has to discriminate between two different situations. For p odd a new situation arises, similar to p = 2 with external field [15]. For p even and $p \ge 4$ features of the latter case will coexist with those already known from the case p = 2 [14]. Therefore from now on we will concentrate on the most simple case with p odd, i.e. p = 3 and leave the study $p \ge 4$ to a more detailed analysis [16].

First we study the zero-temperature properties of this model. The groundstate of this system has a 4-fold degeneracy (in general 2^{p-1}) given by \dagger

$$(1) \cdots + + + + + + + + + + + \cdots$$

$$(2) \cdots + - - + - - + - - \cdots$$

$$(3) \cdots - + - - + - - + - \cdots$$

$$(4) \cdots - - + - - + - - + \cdots$$

$$(3)$$

Introducing a local energy-variable $\tau_i = S_{i-1}S_iS_{i+1}$ all groundstate configurations are described by $\tau_i = +1$ for all sites i. Consider a configuration in τ and S variables

[†] For simplicity we stipulate that L is a multiple of p.

which consists of two domains, both being in a minimum energy configuration, separated by a domain wall located at site i (note that in general one has 2^{p-1} different kinds of domains, corresponding to the groundstate degeneracy). A closer look at the transition probabilities (2) tells us that it costs an energy amount of $2S_jh_j = 2(\tau_{j-1} + \tau_j + \tau_{j+1})$ to flip one spin, i.e. in configuration (4) 6J for spins within the domains and 2J to flip the spins at the three sites i-1, and i+1 surrounding the domain wall. Thus this configuration is stable against single spin flips and at finite, but small, temperatures it needs a time

$$\tau_{\text{freeze}} \approx \exp(2J/T)$$
 (5)

to move the domain wall one lattice spacing to the left or right. This is the time scale (which is quite large for $T \ll J$) on which the particular configuration remains frozen for small temperatures. Moreover, it can be shown that all configurations of the type (4) consisting (expressed in τ -variables) of strings of arbitrary length $l \ge 2$ with $\tau = +1$ separated by isolated sites with $\tau = -1$ are indeed metastable: From what has been said above it is clear that the criterion for metastability is $\tau_{i-1} + \tau_i + \tau_{i+1} > 0$ for all sites i. Thus in any triplet $(\tau_{i-1}, \tau_i, \tau_{i+1})$ at most one minus sign may occur. Hence any metastable configuration can be represented by an arbitrary sequence of two elementary units + + + and + +. The total number n_L of all possible sequences in a system with L sites can be calculated via the Fibonacci-like iteration $n_L = n_{L-1} + n_{L-3}$. The result for $L \to \infty$ is

$$n_L \sim x^L$$
 with $x = \sqrt[3]{\frac{29 + \sqrt{837}}{54}} + \sqrt[3]{\frac{29 - \sqrt{837}}{54}} \approx 1.46557.$ (6)

Starting with a random initial state the sequential update procedure at zero temperature will drive the system into one of these exponentially large number of metastable states within only two sweeps through the whole chain. A random sequential update and small non-vanishing temperature will not change this scenario significantly. Thus after $2\tau_0$, where τ_0 is the microscopic time scale, the system will be frozen for a time $\tau_{\text{freeze}} = \exp(2J/T)$.

What has been said so far can be quantified by looking at the spin autocorrelation function $C_T(t,t_\omega)=1/L\sum_{i=1}^L\langle S_i(t+t_\omega)S_i(t_\omega)\rangle_T$ and the time-dependent energy $E_T(t)=1/L\sum_{i=1}^L\langle t_i(t)\rangle_T$ where $\langle \cdots \rangle_T$ means the expectation value with respect to the (time-dependent) probability distribution of spin configurations determined by the master equation for the stochastic process considered here (in the limit $L\to\infty$). These quantities can easily be calculated for the ferromagnetic Ising chain (i.e. p=2) [14]. In the present case such a treatment is not possible for the same reasons as in the ferromagnetic Ising chain in an external field or the Cayley tree with branching number two [15]. However, the remanent magnetization $C_T(t,t_\omega)$ and the energy $E_T(t)$ can be calculated analytically for zero temperature with the tools introduced in [15]. In this letter we only note that an important ingredient for this problem to be exactly solvable is the fact that the local field acting on the spins never vanishes (details will be published elsewhere [16]):

$$C_{T=0}(t,0) = 0.475$$
 for $t \ge 2$
 $C_{T=0}(1,0) = 0.5$ $E_{T=0}(1) = -0.5$
 $C_{T=0}(1,1) = 0.9$ $E_{t=0}(t) = -0.6$ for $t \ge 2$
 $C_{T=0}(t,t_{\omega}) = 1$ for $t_{\omega} \ge 2$. (7)

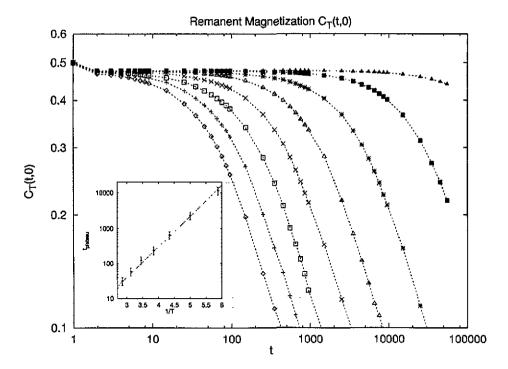


Figure 1. The remanent magnetization for various temperatures calculated via Monte Carlo simulation of a system with 10^6 spins. From right to left: T=0.14, 0.17, 0.20, 0.23, 0.26, 0.29, 0.32 and 0.35. The insert shows the temperature dependence of $t_{\rm plateau}$ defined in the text, the straight line is the predicted dependency $\tau_{\rm freeze} \sim \exp(2J/T)$ (J=1).

According to the above arguments the relations (7) also hold for $T \neq 0$ as long as $t \ll \tau_{\text{freeze}}$. To check this we performed Monte Carlo simulations of this model and results for the remanent magnetization $C_T(t,0)$ at various temperatures are shown in figure 1. One observes the plateau at the value 0.475 extending to larger and larger times for decreasing temperatures. For low temperatures the final decay of $C_T(t,0)$ seems to be algebraic (before it will crossover to an ultimately exponential decay at times comparable to the equilibration time, cf [11]). Fitting a straight line to this decay in a log-log plot yields an intersection with the (imaginary) line $C_T = 0.475$, by which we define the time scale t_{plateau} for the lifetime of the metastable state. The temperature dependence of this quantity is depicted in the insert of figure 1 and yields, as expected $t_{\text{plateau}} \propto \tau_{\text{freeze}}$.

We also looked for the waiting time (t_{ω}) dependence of $C(t,t_{\omega})$ and found that the zero-temperature-predictions (7) are indeed also fulfilled for finite temperatures as long as $t < \tau_{\rm freeze}$. Note that obviously for $t < \tau_{\rm freeze}$ scaling laws like $C(t,t_{\omega}) \sim \tilde{c}(t/t_{\omega})$, which apply in many aging scenarios [11,17] cannot hold. However, for $t > \tau_{\rm freeze}$ this conventional scaling is restored. Furthermore we calculated the remanent energy $E_T(t)$ in Monte Carlo simulations. The result is depicted in figure 2. As for the remanent magnetization one sees the characteristic initial plateau. Furthermore by plotting the value of $E_T(t)$ versus temperature T for fixed time t one gets a characteristic non-monotonic behaviour. However, for $t \to \infty$ the location of the minimum approaches T=0 and one obtains a monotonic increase with temperature as expected for an equilibrium-thermodynamical internal energy.

Inspecting again configuration (4) and the following analysis one might expect that once

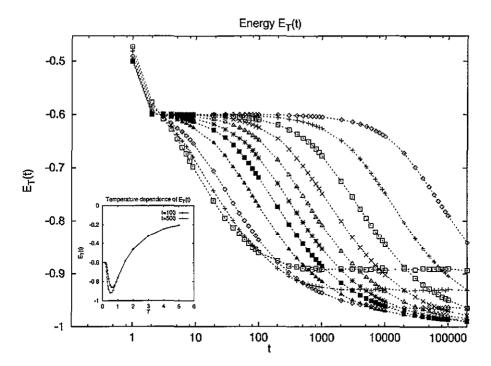


Figure 2. The energy $E_T(t)$ for various temperatures. From right to left: 0.17, 0.20, 0.23, 0.26, 0.29, 0.32, 0.35, 0.4, 0.5, 0.6 and 0.7. The insert shows the temperature dependence of $E_T(100)$ and $E_T(500)$.

the observation time reaches the time scale τ_{freeze} the domain wall will perform a random walk. In an arbitrary metastable configuration domain walls will randomly diffuse on a characteristic time scale τ_{freeze} and annihilate when two of them meet. This scenario will results in a \sqrt{t} growth of the domain size. To check this, we measured the average domain size in Monte Carlo simulations. We define size l of a domain to be equal to the number of spin pairs between two succeeding τ -variables that have the value -1. Then, at a time t, we count the number $n_l(t)$ of domains of size l. This defines the probability $P_T(l,t) = \ln_l(t)/L$ for a spin pair to be contained in a segment of length l.

In figure 3 we show the result of the average domain size at time t after the quench $d(t) = \sum_l l P_T(l,t)$ in a log-log plot. Again one recognizes the frozen regime from d(t) being constant for $t \ll \tau_{\text{freeze}}$. For larger times an intermediate growth regime follows and we inserted a graph of $d(t) \propto \sqrt{t}$ comparison. One concludes that the above mentioned picture of domain wall diffusion and annihilation is indeed to be applicable here. As soon as t reaches the order of the equilibration time τ_{eq} , the domains stop growing and d(t) saturates at a value proportional to the equilibrium correlation length $\xi_{\text{eq}}(T)$, which can be calculated analytically [16]

$$\xi_{\text{eq}}(T) = \frac{3}{2} |\log \tanh(J/T)|^{-1} \propto \exp(J/T) \qquad \text{for } T \ll J.$$
 (8)

Apart from the prefactor 3/2 (in general p/2) the result (8) is identical to the case p=2 [14]. This is a general feature of the model (1): although the dynamics shows drastic differences between p even and odd it turns out that the equilibrium behaviour of static quantities is very similar.

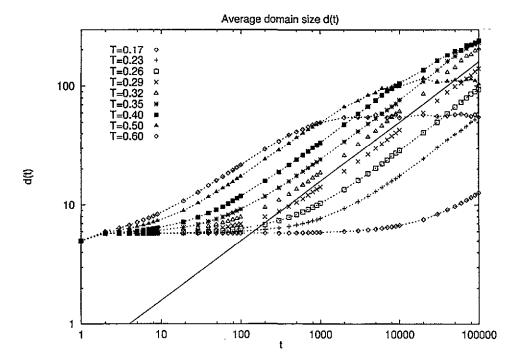


Figure 3. Average domain size in dependence of the waiting time t in a log-log plot. The intermediate growth (between melting of the frozen domains and final saturation by equilibration) can be fitted nicely to $d(t) \sim t^{1/2}$ (solid line).

At zero temperature one can again calculate the average domain size exactly, and also beyond that the whole probability distribution $P_{T=0}(l,t)$ for a site being contained within a domain of size l at time t. Here we only give the result, details of the calculation will be published elsewhere [16]:

$$P_{T=0}(l, t=1) = l(l-1)(\frac{1}{2})^{l+2}$$
 for $l \ge 2$ (9)

and

$$P_{T=0}(l=2, t \ge 2) = 0$$

$$P_{T=0}(l=3, t \ge 2) = \frac{9}{64}$$

$$P_{T=0}(l \ge 4, t \ge 2) = l(3l - \frac{26}{5})(\frac{1}{2})^{l+3}.$$
(10)

Remember that after two timesteps the system is frozen at zero temperature. The average domain size $d_{T=0}(t)$ at zero temperature is then given by:

$$d_{T=0}(t=1) = 5$$
 $d_{T=0}(t \ge 2) = \frac{231}{40} = 5.775.$ (11)

These analytical results are compared with data obtained from Monte Carlo simulations in figure 4(a). The agreement is excellent even at finite temperatures for $t \ll \tau_{\text{freeze}}$. In figure 4(b) we also show results for $P_T(l,t)$ at higher temperatures for t=1,2, an

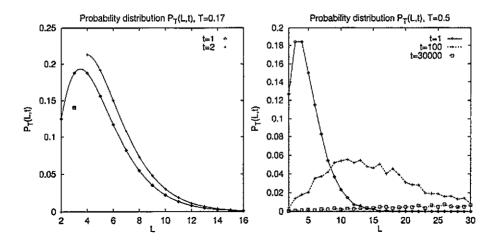


Figure 4. Probability distribution $P_T(l,t)$ for domain sizes l at time t obtained from Monte Carlo simulations. Left: T=0.17 and t=1,2, the full curves are the analytical result. Right: T=0.5 and t=1, t=100 and $t=30\,000 \sim \tau_{\rm en}$.

intermediate time (in the growth regime) and a time larger than the equilibration time—thus reflecting the equilibrium distribution.

To conclude we have presented and analysed a simple one-dimensional model whose non-equilibrium dynamics seems to share many features with a glass transition. One of them is, for instance, the complete freezing of the system in an 'amorphous' state for a macroscopic time when cooled rapidly to low temperatures. Another is that this complex dynamics is achieved without putting in any disorder by hand. Of course, due to its one-dimensionality, it does not have a phase transition and also no particular temperature can be identified with a glass transition (leaving aside the question whether the latter is a true equilibrium phase transition or of purely dynamical origin). However, demonstrating that even very simple models yield a very rich dynamical behaviour, gives us some confidence that in higher dimensional models one might find indeed a candidate that shares more or even all features with a glass transition (as presently discussed in the context of geometrically frustrated models [10]).

As we have shown many new features of our model arise from the presence of multi-spin interactions. Thus it seems worthwhile to have a closer look to such models in two or three dimensions, as already discussed in [18]. To support this view let us mention that it has been pointed out several years ago [19] that mean-field models with p-spin interactions (see also [20]) show a dynamical behaviour that is identical to that found in mode-coupling theories of the structural glass transition. Moreover, very recent work on self-induced disorder in models with long-range interactions [21] heavily rely on multi-spin interactions, too.

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