Glassy timescale divergence and anomalous coarsening in a kinetically constrained spin chain

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We analyse the out of equilibrium behavior of an Ising spin chain with an asymmetric kinetic constraint after a quench to a low temperature \( T \). In the limit \( T \to 0 \), we provide an exact solution of the resulting coarsening process. The equilibration time exhibits a ‘glassy’ divergence \( t_{eq} = \exp(\text{const}/T^2) \) (popular as an alternative to the Vogel-Fulcher law), while the average domain length grows with a temperature dependent exponent, \( d \sim t^{T \ln 2} \). We show that the equilibration time \( t_{eq} \) also sets the timescale for the linear response of the system at low temperatures.

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Even after decades of research, understanding the dynamics of glasses remains a challenging problem (see e.g. \textsuperscript{[1,2]}). One of the main features of glassy systems is that their relaxation time \( \tau \) increases quickly as the temperature \( T \) is lowered. A popular representation of this increase (for so-called ‘fragile’ glasses \textsuperscript{[2]}\textsuperscript{2}) is the Vogel-Fulcher (VF) law, \( \tau \sim \exp[-\text{const}/(T - T_0)] \). This predicts that \( \tau \) diverges at temperature \( T_0 \), and the latter has therefore been associated with the temperature at which a true thermodynamic glass transition (achievable only in the limit of infinitely slow cooling) would take place. However, other functional forms for \( \tau(T) \) that have been proposed do not exhibit singularities at any finite \( T \), indicating the absence of a thermodynamic glass transition. Among these, the exponential inverse temperature squared (EITS) form \( \tau \sim \exp(\text{const}/T^2) \) is popular. Experimentally, it is difficult to distinguish between VF and EITS behavior due to obvious limitations on the longest accessible timescales; both can represent the experimentally observed \( \tau(T) \) in many materials \textsuperscript{[3,4]}. Thus analytical results are desirable to shed light on this controversy. In this work we solve a simple dynamical model exhibiting glassy dynamics and find EITS behavior.

To model relaxation in glassy systems theoretically, one can postulate some kind of quenched disorder, either in terms of some underlying microscopic Hamiltonian (as is done in spin glasses) or more phenomenologically by making assumptions about the phase space of the system (e.g. in terms of hierarchical or ultrametric structures \textsuperscript{[5,6]} or energy barrier distributions \textsuperscript{[7,8]}). The alternative is to consider simple models whose dynamics directly induce glassiness. Examples include systems with kinetic constraints \textsuperscript{[9,10]} or entropic barriers \textsuperscript{[11]}, and driven diffusive models \textsuperscript{[12,13]}. Such an approach is more obviously relevant to the dynamics of structural glasses (where quenched disorder is absent) since one does not need additional arguments that relate quenched and dynamically ‘self-induced’ disorder \textsuperscript{[14,15]}.

The model that we consider is a chain of spins in a uniform field, whose dynamics is nontrivial due to an asymmetric kinetic constraint: A spin can flip only if its left neighbor is up. This model was introduced by Jäckle and Eisinger \textsuperscript{[16]} and has recently been rediscovered \textsuperscript{[17,18]}. We study in particular the behavior after a quench to a low temperature \( T \to 0 \). We solve the resulting coarsening dynamics exactly in this limit and find two main results: Firstly, the equilibration time of the system diverges as \( t_{eq} \sim \exp(1/2 T^2 \ln 2) \), thus providing an example of a system without quenched disorder with a timescale that provably follows an EITS law. Secondly, before equilibrium is reached, the average domain length grows as \( d \sim t^{T \ln 2} \), with an exponent that varies continuously with temperature. This novel anomalous coarsening is a consequence of the dynamical constraint, which produces scale-dependent energy barriers which grow as the logarithm of the domain size. Finally, we show that \( t_{eq} \) is not just the timescale for equilibration after a quench, but in fact is also the timescale for relaxation of spin-spin correlations in equilibrium (at low \( T \)); this relaxation time therefore also has an EITS divergence at low \( T \).

The model comprises a chain of \( L \) spins \( s_i \in \{0,1\} \) where \( 1 \leq i \leq L \); periodic boundary conditions imply that the left neighbor of \( s_1 \) is \( s_L \). The dynamics for a given temperature \( T \) are defined as follows: At any time, only spins whose left neighbor is up (i.e., has the value 1) can flip. For such ‘mobile’ spins, the rate for down-flips \( 1 \to 0 \) is 1, while the rate for up-flips \( 0 \to 1 \) is \( \epsilon = \exp(-1/T) \). Detailed balance is obeyed, and the stationary distribution is the Boltzmann distribution for the trivial Hamiltonian \( H = \sum_{i=1}^{L} s_i \). For low temperatures the equilibrium concentration \( c = \epsilon/(1 + \epsilon) \) of up-spins is small. Since these spins facilitate the dynamics, the system evolves slowly for small \( T \). Moreover to eliminate an up-spin one first has to generate an adjacent up-spin. Thus there are energy barriers in the system’s evolution.

We will be interested mainly in the behavior after a quench from equilibrium at some high initial temperature \( T_i \gtrsim 1 \) to a low temperature \( T \ll 1 \). The basic objects that we use for the description of the system are domains. As shown by the vertical lines in
At the final temperature \( T \) call the maximum number of up-spins (not counting encountered along a path its height, and define \( h \) spin where all spins \( n \) state space from \( \ldots 1|0001|1|01|001|1|01|0 \ldots \) a domain consists of an up-spin and all the down-spins that separate it from the nearest up-spin to the left. The length \( d \) of a domain also gives the distance between the up-spin at its right edge and the nearest up-spin to the left. Note that adjacent up-spins are counted as separate domains of length \( d = 1 \). In equilibrium, the distribution of domain lengths and its average are

\[
P_{\text{eq}}(d) = e/(1 + e)^d, \quad d_{\text{eq}} = 1 + 1/e. \tag{1}
\]

Now consider what happens after a deep quench to \( T \ll 1, e \ll 1 \). The equilibrium concentration of up-spins at the final temperature \( T \) is \( e = 1/d = e + O(e^2) \); hence the equilibrium probability of finding an up-spin within a chain segment of finite length \( d \) is \( O(de) \) and tends to zero for \( e \to 0 \). In this limit \( e \to 0 \) at fixed \( d \), the flipping down of up-spins therefore becomes irreversible to leading order. In terms of domains, this means that the coarsening dynamics of the system is one of coalescence of domains: an up-spin that flips down merges two domains (the one that it bounds on its left and the next one to the right) into one large domain. During such a coarsening process, no correlations between the lengths of neighboring domains can build up if there are none in the initial state. For the present model the equilibrated initial state consists of domains independently distributed according to \((\ref{1})\). Therefore a ‘bag model’ \((\ref{1})\) or ‘independent interval approximation’ for the dynamics, which is defined by neglecting correlations between domains, becomes exact in the low-temperature limit (always taken at fixed \( d \)). A formal proof of this statement will be given in a longer paper [53].

We now estimate the typical rate \( \Gamma(d) \) at which domains of length \( d \) disappear by coalescing with their right neighbors. Because domain coalescence corresponds to the flipping down of up-spins, \( \Gamma(d) \) can also be defined as follows. Consider an open spin chain of length \( d \), with an extra ‘clamped’ up-spin (\( s_0 = 1 \)) added on the left end. Starting from a configuration where all spins except \( s_0 \) and \( s_0 \) are down, \( \Gamma^{-1}(d) \) is the typical time needed to reach the state where all spins (except \( s_0 \)) are down, \( \epsilon \), where spin \( s_0 \) has ‘relaxed’. One might at first suspect that this relaxation process needs to proceed via the state where all spins \( s_1, \ldots, s_{d-1} \) have been flipped up. In fact, spin \( s_2 \) can be relaxed in a much more efficient manner. To see this, think of the relaxation process as a path in state space from \((s_0, s_1, \ldots, s_d) = 10 \ldots 01 \to 10 \ldots 00 \) into one large domain. During such a process, we call these the ‘active’ domains. This process takes place on a timescale of \( \mathcal{O}(\Gamma^{-1}(d)) = \mathcal{O}(e^{d-1}) \). In principle there are also ‘entropic’ contributions to \( \Gamma(d) \), related to the number of different paths by which \( s_0 \) can be relaxed. But as long as we keep \( d \) finite when taking the limit \( e \to 0 \), the number of paths also remains finite and hence does not change the scaling of \( \Gamma(d) \) with \( e \).

Before continuing with the exact analysis, we can already see at this stage from \((\ref{2})\) the key feature of the dynamics: the relaxation rate for domains of size \( d \) is \( \Gamma(d) \sim e^{-d} \ln 2 \). One can think of the energy barrier for the growth of domains increasing logarithmically with domain size. This implies that the typical domain size will grow as \( d \sim t \ln 2 \). Also, since \( d_{\text{eq}} \sim e^{-1} \ln 2 \) the equilibrium time will grow according to an EITS law \( t_{\text{eq}} \sim e^{-1} \ln 2 \).

From the scaling of \( \Gamma(d) \), we see that the coarsening dynamics in the limit \( e \to 0 \) naturally divides into stages distinguished by \( n = h(d) + 1 = 0, 1, \ldots \). During stage \( n \), the domains with lengths \( 2^n < d \leq 2^n \) disappear in the considered active domains. This process takes place on a timescale of \( \mathcal{O}(n^{-1}(d)) = \mathcal{O}(e^{-n}) \); because the timescales for different stages differ by factors of \( 1/e \), we can treat them separately in the limit \( e \to 0 \). During stage \( n \), the distribution of inactive domains \( d > 2^n \) changes only because such domains can be created when smaller domains coalesce. Combining this with the (exact) bag model discussed above, we have for \( d > 2^n \)

\[
\partial_\tau P(d, \tau) = \sum_{2^n-1 < d' \leq 2^n} P(d - d', \tau) [-\partial_\tau P(d', \tau)]. \tag{3}
\]

The term in square brackets is the rate at which active domains disappear; the fact that inactive domains do
not disappear enforces the restriction $d' \leq 2^n$. The time variable has been rescaled according to $\tau = tf^n$; during stage $n$ of the dynamics and in the limit $\epsilon \to 0$, it can take on any positive value $\tau > 0$. The initial condition for $\mathcal{P}_n$ is the domain length distribution at the end of stage $n - 1$ of the dynamics, which we call $P_n(d) = P(d, \tau \to 0)$. We want to calculate $P_{n+1}(d) = P(d, \tau \to \infty)$. To do this, introduce the generating function $G(z, \tau) = \sum_d P(d, \tau)z^d$ (14), and its analogue for the active domains, $H(z, \tau) = \sum_{2^{n-1} < d \leq 2^n} P(d, \tau)z^d$. From (14), one then finds

$$\partial_\tau [G(z, \tau) - H(z, \tau)] = -G(z, \tau) \partial_\tau H(z, \tau).$$

This can be integrated to give $[1-G(z, \infty)]/[1-G(z, 0)] = \exp[H(z, 0) - H(z, \infty)]$. But at the end of stage $n$, all domains that were active during that stage have disappeared, and so $H(z, \infty) = 0$. We define the initial condition for $G$ as $G_n(z) \equiv G(z, 0) = \sum_d P_n(d)z^d$ and similarly for the active domains, $H_n(z) \equiv H(z, 0)$. We then have finally

$$G_{n+1}(z) - 1 = [G_n(z) - 1] \exp[H_n(z)]. \quad (4)$$

This exact result relates the domain length distributions $P_n(d)$ and $P_{n+1}(d)$ at the end of stages $n - 1$ and $n$ of the dynamics, as expressed through their generating functions. Iterating it from a given initial distribution $P_0(d)$ gives $P_n(d)$ for all $n = 1, 2, \ldots$. We do this numerically by expressing (14) directly in terms of the probability distributions; the exponential is thus expanded into a series of convolutions of increasing order. Fig. 1 shows the results for the case where $P_0(d)$ is the equilibrium distribution (15) corresponding to an initial temperature of $T_i = \infty$. Not unexpectedly, a scaling limit is approached for large $n$: The rescaled distributions $\tilde{P}_n(x) = 2^{n-1}P_n(d)$, where the scaled domain size is $d = d/2^{n-1}$, converge to a limiting distribution $\tilde{P}(x)$ which is independent of the initial condition. Invariance under (15) gives an equation for the corresponding Laplace transforms $g(s)$ and $h(s)$ of $\tilde{P}(x)$

$$g(2s) - 1 = [g(s) - 1] \exp[h(s)]. \quad (5)$$

We find a self-consistent solution (16)

$$\tilde{P}(x) = \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m!} \int_1^\infty \prod_{r=1}^m \frac{dx_r}{x_r} \delta \left( \sum_{s=1}^m x_s - x \right) \quad (5)$$

$$= \Theta(x-1) \frac{1}{x} - \Theta(x-2) \frac{\ln(x-1)}{x} + \ldots$$

where $\Theta(x)$ is the Heaviside step function. This series has singularities in the $k$-th derivative at the integer values $x = k + 1, k + 2, \ldots$. The calculated $\tilde{P}(x)$ agrees well with the previous results obtained by direct iteration of (15) (Fig. 2). The average domain length in the scaling limit is given by $\bar{d}_n = 2^{n-1}\bar{x}$; from the results for $\tilde{P}(x)$ we find $\bar{x} = \exp(\gamma) = 1.78 \ldots$, where $\gamma$ is Euler’s constant.

In order to compare the results to simulations, consider starting from an equilibrated state at some initial temperature, say $T_i = \infty$, quench the system to temperatures $T < 1$ at time $t = 0$ and observe its time evolution. If the results are plotted against the scaled time variable $\nu = \ln(t)/\ln(1/\epsilon) = T \ln t$, then for $T \to 0$ the $n$-th stage of the dynamics shrinks to the point $\nu = n$. In this limit we predict that, for $n-1 < \nu < n$, the domain length distribution is $P_n(d)$ as defined by the recursion (15). The average domain length $\bar{d}_n$ will follow a ‘staircase’ function, jumping at $\nu = n$ from $\bar{d}_n = \sum_{d=1}^{d_{n-1}} P_n(d)$ to $\bar{d}_{n+1}$. In the large $\nu$ scaling regime, this tells us that $2^{n-1}\bar{x} \leq \bar{d} \leq 2^n\bar{x}$ (where $\bar{x} = 1.78 \ldots$ from above), or $\frac{1}{2} \leq \bar{d}/(\bar{x} T^{1/2}) \leq 1$ when expressed in terms of ordinary time $t$.

We can therefore say that the system coarsens with an exponent that depends on temperature and is given by $T \ln 2$ to lowest order in $T$. By extrapolating this coarsening law to the equilibrium domain length $d_{eq} = \exp(1/T) + O(1)$, we then also have that the dominant divergence of the equilibration time of the system for $T \to 0$ is $t_{eq} = \exp(1/T^{1/2})$.

In Fig. 2 we show the results of simulations for a range of values of $\epsilon = \exp(1/T)$. We used a waiting time Monte Carlo algorithm (12) combined with an efficient binary tree representation for the positions of the mobile spins. This let us access far larger systems ($L = 2^{15}$) and longer times (up to $t = 10^{10}$) than in previous simulations (13). The plateaus in $\bar{d}(\nu)$ that develop with decreasing $\epsilon$ can clearly be seen, and their values are in good agreement with the predicted theoretical values. We also obtained the domain length distributions on the plateaus, by taking data at the minima of $(d/d\nu)\bar{d}(\nu)$ w.r.t. $\nu$. These are
FIG. 2. Evolution of average domain length $d$ after quench from $T_i = \infty$ to $T_t = 0$, plotted on a log scale vs. $\nu = T \ln t$. Simulation results for four values of $\epsilon = \exp(1/T)$ are shown, obtained from a single run for a spin chain of length $L = 2^{15}$. Bold line: Theoretical prediction for $T \to 0$. Inset: Theory for larger $\nu$ and $\nu \to \infty$ asymptotes.

shown in Fig. 1 for the cases $n = 1, 2, 3$ and are again in good agreement with our theory.

Our result for the equilibration time $t_{eq} = \exp(1/T^2 \ln 2)$ is based on the extrapolation of the finite-$d$ coarsening behavior $d \sim t^{T \ln 2}$ into the equilibrium region $d = O(1/\epsilon)$, where it is no longer strictly valid. We now show, however, that the same timescale is obtained from the initial decay of the spin-spin correlation function at equilibrium at low temperature $T$. It turns out that due to the asymmetric constraint the correlation function is site diagonal, $\langle s_i(0) - c \rangle (s_j(t) - c) = \delta_{ij} c R(t) - c$. Here $R(t)$ is the probability that an up-spin at $t = 0$ is also up at a later time $t$. With increasing $t$, it decays from $R(0) = 1$ to the equilibrium concentration of up-spins, $c = \epsilon/(1 + \epsilon)$. To find the initial decay of $R(t)$, consider again timescales $t = O(\epsilon^{-v})$ for finite $\nu$ and $\epsilon \to 0$. For $\nu = n + 0$, all domains of length $d \leq 2^n$ will have disappeared. Therefore only up-spins that bounded longer domains at $t = 0$ will have an $O(1)$ probability of still being up. From the equilibrium distribution (1), one sees that they constitute a fraction $(1 + \epsilon)^{-2^n}$ of the up-spins at $t = 0$, and hence $R(\nu = n + 0) \approx 1 - 2^n \epsilon + O(\epsilon^2)$. Neglecting corrections of $O(\epsilon^2)$, the quantity $-\ln R(\nu)$ thus lies between $2^{v-1} \epsilon$ and $2^v \epsilon$ (for $\nu > 0$). Reverting to ordinary time, we have $1/2 \leq -\ln R(t)/t = O(\epsilon^2) + O(1)$ for short times $(t/t_{eq})^{T \ln 2} \ll 1$. The relevant timescale that enters here is exactly the equilibration time $t_{eq} = \exp(1/T^2 \ln 2)$ found above. We can thus identify the equilibration time for coarsening after a quench, with the equilibrium relaxation time; both have an EITS-divergence at low $T$.

Finally, we comment briefly on the spin-spin autocorrelation function for longer times $(t/t_{eq})^{T \ln 2} = O(1)$, where the analysis becomes more involved. We have tackled this problem by extending the concept of domains to that of ‘superdomains’ which are bounded by up-spins that remain up on a given timescale. Combining this with a plausible hypothesis for the behavior of the relaxation timescales $\Gamma^{-1}(d)$ for $d = O(1/\epsilon)$, the following scenario seems likely: In the limit $T \to 0$, $R(t)$ first decays linearly with the rescaled time variable $\delta = (t/t_{eq})^{T \ln 2}$. This is compatible to lowest order with a stretched exponential relaxation. But then the decay becomes much faster, and $R$ actually decays to zero at a finite value of $\delta$. (For nonzero $T$, there is a crossover into a slower decay, presumably exponential in $t$, at late times.) It would also be of interest to study the relaxation times of similar models in dimension $D > 1$.

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[17] Note that only domains with $d > 2^n$ contribute to this sum, all shorter domains having disappeared during previous stages of the dynamics.
[20] With probability $O(\epsilon)$, two short domains of length $d = O(1)$ will be next to each other. The right domain may then not disappear on a timescale $\Gamma^{-1}(d)$ if the left one disappears first and thereby ‘lengthens’ it. Also, spins that have flipped down will flip up again with probability $O(\epsilon)$. We have neglected both of these effects because they only give corrections of $O(\epsilon^2)$ to $R(\nu)$.