Glassy Time-Scale Divergence and Anomalous Coarsening in a Kinetically Constrained Spin Chain

Peter Sollich[1,*] and Martin R. Evans[2]
[1]*Department of Mathematics, King's College London, Strand, London WC2R 2LS, United Kingdom*
[2]*Department of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom*
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We analyze 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 $t_{\rm eq} = \exp(\text{const}/T^2)$ (popular as an alternative to the Vogel-Fulcher law), while the average domain length grows with a temperature-dependent exponent, $\bar{d} \sim t^{T\ln 2}$. We show that the equilibration time $t_{\rm eq}$ also sets the time scale 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., [1–3]). One of the main features of glassy systems is that their relaxation time τ increases quickly as the temperature T is lowered. A popular representation of this increase (for so-called "fragile" glasses [2]) is the Vogel-Fulcher (VF) law, $\tau \sim \exp[-\text{const}/(T - T_0)]$. This predicts that τ 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 time scales; both can represent the experimentally observed $\tau(T)$ in many materials [4]. Thus analytical results are desirable to shed light on this controversy. In this paper, we solve a simple dynamical model exhibiting glassy dynamics and find EITS behavior.

To model relaxation in glassy systems theoretically, one can postulate some type 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 [5,6] or energy barrier distributions [7,8]). So far the main theoretical justification for either VF or EITS behavior comes from the latter approach; the EITS law, for example, is motivated by considering activated dynamics in a landscape of Gaussian distributed energy barriers [7].

The alternative approach is to consider simple models whose *dynamics* directly induce glassiness. Examples include systems with kinetic constraints [1] or entropic barriers [9], and driven diffusive models [10]. 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 [11]. The present paper provides a first example of EITS behavior emerging directly from a *microscopic* model *without* imposed quenched disorder; instead, energy barriers arise naturally from dynamical constraints.

We consider a chain of spins in a uniform field, whose dynamics is nontrivial due to an asymmetric kinetic constraint. This model was introduced by Jäckle and Eisinger [12] and has recently been rediscovered [13]. 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 $t_{\rm eq} \sim \exp(1/T^2 \ln 2)$ (EITS behavior). Secondly, before equilibrium is reached, the average domain length grows as $\bar{d} \sim t^{T\ln 2}$, 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 $t_{\rm eq}$ is not just the time scale for equilibration after a quench, but in fact is also the time scale 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 $1 \le i \le L$; 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

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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 are interested mainly in the behavior after a quench from equilibrium at some high initial temperature $T_i \gtrsim 1$ to $T \ll 1$. The basic objects which we use for the description of the system are *domains*. As shown by the vertical lines in $\ldots 1|0001|1|1|01|001|1|1|01|0\ldots$, a domain consists of an up spin and all of 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

$$P_{\mathrm{eq}}(d) = \epsilon/(1+\epsilon)^d, \qquad \bar{d}_{\mathrm{eq}} = 1 + 1/\epsilon. \quad (1)$$

Now consider what happens after a deep quench to $T \ll 1$, $\epsilon \ll 1$. The equilibrium concentration of up spins at the final temperature T is $c = 1/\bar{d} = \epsilon + \mathcal{O}(\epsilon^2)$; hence the equilibrium probability of finding an up spin within a chain segment of *finite* length d is $\mathcal{O}(d\epsilon)$ and tends to zero for $\epsilon \to 0$. In this limit ($\epsilon \to 0$ 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 neighboring domains into one large domain. During such an irreversible coarsening process, no correlations between the lengths of neighboring domains can build up if there are none in the initial state [14]. For the present model the equilibrated initial state consists of domains independently distributed according to (1). Therefore a "bag model" [14] 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).

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 a "clamped" up spin ($s_0 = 1$) added on the left. Starting from the state $(s_0, s_1, \ldots, s_d) = 10\cdots01$, $\Gamma^{-1}(d)$ is the typical time needed to reach the empty state $10\cdots00$, where spin s_d has "relaxed." Any instance of this relaxation process can be thought of as a path connecting the two states. We call the maximum number of "excited" spins (up spins, except s_0) encountered along a path its height h. One might think that the relaxation of spin s_d needs to proceed via the state $11\cdots1$, giving a path of height d. In fact, the minimal path height $h(d)$ is much lower and given by

$$h(d) = n + 1 \text{ for } 2^{n-1} < d \le 2^n, \quad (2)$$

where $n = 0, 1, \ldots$. This result is easily understood for $d = 2^n$ [15]. To relax the 2^n-th spin s_{2^n}, one can first flip up $s_{2^{n-1}}$ and use it as an "anchor" for relaxing s_{2^n}. The corresponding path is (with $s_{2^{n-1}}$ and s_{2^n} underlined) $1\ldots\underline{0}\ldots\underline{1} \to 1\ldots\underline{1}\ldots\underline{1} \to 1\ldots\underline{1}\ldots\underline{0} \to 1\ldots\underline{0}\ldots\underline{0}$ and reaches height $h(2^n) = h(2^{n-1}) + 1$; the $+1$ arises because the anchor stays up while the spin 2^{n-1} to its right is relaxed. Continuing recursively, one arrives at $h(2^n) = h(1) + n$, but $h(1) = 1$ because the only path for the relaxation of s_1 is $11 \to 10$. To prove (2) more generally, define $d(h)$ as the length of the largest single domain that can be relaxed by a path of height $\le h$. Because of detailed balance, any relaxation path can be reversed, yielding a path of the same height from the empty state to the state $10\cdots01$. In the same way, let us define $l(h)$ to be the maximal length of *any* spin configuration (ending in an up spin) that can be reached from the empty state by a path of height $\le h$. One then has $d(h+1) = l(h) + 1$ because to relax $s_{d(h+1)}$ one needs to flip up its left neighbor while exciting no more than h additional spins. A second relation is obtained from the relaxation of a configuration realizing the bound $l(h)$. Such a configuration contains h excited spins (due to its maximal length). To relax the first of these, no extra excitations are allowed (because of the ceiling h on path height); for the relaxation of the 2nd, 3rd, ..., hth spin, a maximum of $1, 2, \ldots, h-1$ excitations are available. Summing the maximal length change at each step then gives $l(h) = \sum_{h'=0}^{h-1} d(h'+1)$. The above two recursions for $l(h)$ and $d(h)$, combined with $d(1) = l(1) = 1$, yield $l(h) = 2^h - 1$ and $d(h) = 2^{h-1}$, proving (2).

At this stage we already see the key feature of the dynamics: the energy barrier for the relaxation of spin s_d is $h(d) - 1$ (the -1 comes from the one excited spin (s_d) in the initial state). The rate for this relaxation is therefore $\Gamma(d) = \mathcal{O}(\exp[-(h(d)-1)/T]) = \mathcal{O}(\epsilon^{h(d)-1})$ [16]. Then Eq. (2) tells us that the relaxation rate for domains of size d is $\Gamma(d) \sim \exp(-\ln d/T\ln 2)$. Thus the energy barrier for the growth of domains increases logarithmically with domain size, giving a typical domain size growing as $\bar{d} \sim t^{T\ln 2}$. Also, since $\bar{d}_{\mathrm{eq}} \sim \exp(1/T)$ the equilibration time will grow according to an EITS law $t_{\mathrm{eq}} \sim \exp(1/T^2\ln 2)$.

From the scaling of $\Gamma(d)$, the coarsening dynamics in the limit $\epsilon \to 0$ naturally divides into stages distinguished by $n = h(d) - 1 = 0, 1, \ldots$. During stage n, the domains with lengths $2^{n-1} < d \le 2^n$ disappear; we call these the "active" domains. This process takes place on a time scale of $\mathcal{O}(\Gamma^{-1}(d)) = \mathcal{O}(\epsilon^{-n})$; because the time scales for different stages differ by factors of $1/\epsilon$, we can treat them separately in the limit $\epsilon \to 0$. 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 $d > 2^n$,

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

The term in square brackets is the rate at which active domains disappear; $d' \leq 2^n$ because inactive domains do not disappear. We use the rescaled time $\tau = t\epsilon^n$; 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 (3) is the domain length distribution at the end of stage $n-1$ of the dynamics, which we call $P_n(d) = P(d, \tau \to 0)$. To calculate $P_{n+1}(d) = P(d, \tau \to \infty)$, introduce the generating function, $G(z,\tau) = \sum_{2^{n-1}<d} P(d,\tau) z^d$, and its analog for the active domains, $H(z,\tau) = \sum_{2^{n-1}<d\leq 2^n} P(d,\tau) z^d$. From (3), 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 $[1 - G(z,\infty)]/[1 - G(z,0)] = \exp[H(z,0) - H(z,\infty)]$. However, at the end of stage n, all domains that were active during that stage have disappeared, and so $H(z,\infty) = 0$. Defining the initial condition for G as $G_n(z) \equiv G(z,0) = \sum_{2^{n-1}<d} P_n(d) z^d$ and similarly for the active generating function $H_n(z) \equiv H(z,0)$, we then have finally

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

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 (4) directly in terms of the probability distributions; the exponential is thus expanded into a series of convolutions of increasing order. Figure 1 shows the results for the case where $P_0(d)$ is the equilibrium distribution (1) 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 $x = d/2^{n-1}$, converge to a limiting distribution $\tilde{P}(x)$ which is independent of the initial condition. Invariance under (4) gives an equation for the corresponding Laplace transforms $g(s)$ and $h(s)$ of $\tilde{P}(x)$,

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

We find a self-consistent solution

$$\tilde{P}(x) = \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m!} \int_1^\infty \prod_{r=1}^{m} \frac{dx_r}{x_r}\, \delta\Big(\sum_{s=1}^{m} x_s - x\Big) = \Theta(x-1)\frac{1}{x} - \Theta(x-2)\frac{\ln(x-1)}{x} + \ldots, \qquad (5)$$

where $\Theta(x)$ is the Heaviside step function. This series has singularities in the kth 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 (4) (Fig. 1). 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 γ is Euler's constant.

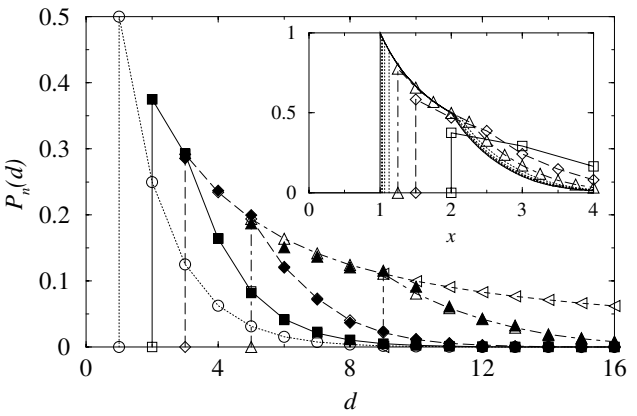

FIG. 1. Domain length distributions $P_n(d)$ at the end of stage $n-1$ of the low T coarsening dynamics, for initial temperature $T_i = \infty$. Open symbols and lines: theoretical results, calculated from (4), for $n = 0$ (○; initial condition), 1 (□), 2 (◇), 3 (△). Solid symbols: simulation results for a chain of length $L = 2^{15}$ and $\epsilon = 10^{-4}$ ($n = 1, 2$) and $\epsilon = 10^{-3}$ ($n = 3$). Inset: scaled predictions $2^{n-1}P_n(d = 2^{n-1}x)$ vs x for $n = 1, \ldots, 8$. Bold line: predicted scaling function (5).

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 $T \ll 1$ 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 nth 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 (4). The average domain length $\bar{d}$ will follow a "staircase" function, jumping at $\nu = n$ from $\bar{d}_n = \sum_d P_n(d) d$ to $\bar{d}_{n+1}$. In the large ν scaling regime, this tells us that $2^{\nu-1}\bar{x} \leq \bar{d} \leq 2^\nu \bar{x}$ (where $\bar{x} = 1.78\ldots$ from above), or $\frac{1}{2} \leq \bar{d}/(\bar{x} t^{T\ln 2}) \leq 1$ 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 $\bar{d}_{\rm eq} = \exp(1/T) + \mathcal{O}(1)$, we then also show that the dominant divergence of the equilibration time of the system for $T \to 0$ is $t_{\rm eq} = \exp(1/T^2 \ln 2)$.

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 [17] 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 ϵ 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 $(d/d\nu)\bar{d}(\nu)$ with regard to ν. These are shown in Fig. 1 for the cases $n = 1, 2, 3$, and are again in good agreement with our theory.

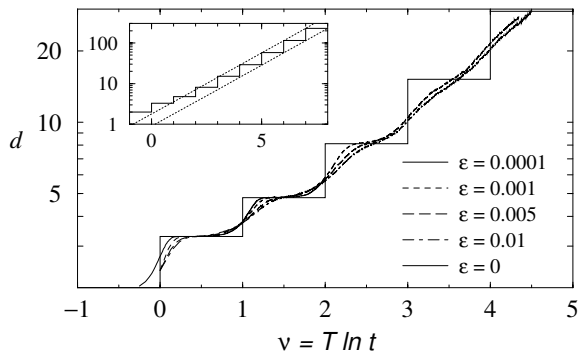

FIG. 2. Evolution of average domain length $\bar{d}$ after quench from $T_i = \infty$ to T at $t = 0$, plotted on a log scale vs $\nu = T \ln t$. Simulation results for four values of $\epsilon = \exp(1/T)$ are shown, obtained from a single run for a spin chain of length $L = 2^{15}$. Bold line: theoretical prediction for $T \to 0$. Inset: theory for larger ν and $\nu \to \infty$ asymptotes.

Our result for the equilibration time $t_{\rm eq} = \exp(1/T^2 \ln 2)$ is based on the extrapolation of the finite-$\bar{d}$ coarsening behavior $\bar{d} \sim t^{T \ln 2}$ into the equilibrium region $\bar{d} = \mathcal{O}(1/\epsilon)$, where it is no longer strictly valid. We now show, however, that the same time scale 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, $\langle [s_i(0) - c][s_j(t) - c]\rangle = \delta_{ij} c[R(t) - c]$ [12,18]. 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 time scales $t = \mathcal{O}(\epsilon^{-\nu})$ for finite ν and $\epsilon \to 0$. For $\nu = n + 0$, all domains of length $d \le 2^n$ will have disappeared. Therefore only up spins that bounded longer domains at $t = 0$ will have an $\mathcal{O}(1)$ 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 $R(\nu = n + 0) \simeq 1 - 2^n \epsilon + \mathcal{O}(\epsilon^2)$ [19]. Neglecting corrections of $\mathcal{O}(\epsilon^2)$, the quantity $-\ln R(\nu)$ thus lies between $2^{\nu-1}\epsilon$ and $2^\nu \epsilon$ (for $\nu > 0$). Reverting to ordinary time, we have $1/2 \le -[\ln R(t)]/(t/t_{\rm eq})^{T \ln 2} \le 1$ for short times $(t/t_{\rm eq})^{T \ln 2} \ll 1$. The relevant time scale that enters here is exactly the equilibration time $t_{\rm eq} = \exp(1/T^2 \ln 2)$ 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 discuss briefly the spin-spin autocorrelation function for longer times $(t/t_{\rm eq})^{T \ln 2} = \mathcal{O}(1)$, where the analysis becomes more involved [12,15,18]. 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 time scale. Combining this with a plausible hypothesis for the behavior of the relaxation time scales $\Gamma^{-1}(d)$ for $d = \mathcal{O}(1/\epsilon)$, the following scenario seems likely [20]: In the limit $T \to 0$, $R(t)$ first decays linearly with the rescaled time variable $\delta = (t/t_{\rm eq})^{T \ln 2}$. 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 δ. (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 $D > 1$ [21].

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*Email address: peter.sollich@kcl.ac.uk

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