Local energy approach to the dynamic glass transition

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We propose a new class of phenomenological models for dynamic glass transitions. The system consists of an ensemble of mesoscopic regions to which local energies are allocated. At each time step, a region is randomly chosen and a new local energy is drawn from a distribution that self-consistently depends on the global energy of the system. Then, the transition is accepted or not according to the Metropolis rule. Within this scheme, we model an energy threshold leading to a mode-coupling glass transition as in the $p$-spin model. The glassy dynamics is characterized by a two-step relaxation of the energy autocorrelation function. The aging scaling is fully determined by the evolution of the global energy and linear violations of the fluctuation-dissipation relation are found for observables uncorrelated with the energies. Interestingly, our mean-field approach has a natural extension to finite dimension, that we briefly discuss.

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Recent numerical studies have shed new light on the close connection between the dynamical slowing down of supercooled liquids and the topography of the underlying potential energy surface. In particular, a topological interpretation of the so-called mode-coupling temperature $T_M$ has been confirmed. That is, for temperatures $T$ smaller than $T_M$, the long-time relaxation is governed by activated processes between basins of potential energy minima. For $T > T_M$, the thermal energy is larger than the potential energy barriers, which allows the system to freely explore its configuration space.

On the other hand, the (mean-field) mode-coupling approximation for liquids is exact for some disordered models such as the $p$-spin model. The spherical version of the latter, endowed with a Langevin dynamics, gives a clear illustration of the interplay between the dynamics and the topography of the energy landscape. The picture is the following. The stationary points whose energy is above the so-called threshold value $E_t$ are mainly saddles, i.e. the minimum value of the Hessian eigenvalues, $\lambda_m$, is negative. Those whose energy is below are mainly minima, i.e. $\lambda_m > 0$, and at $E_t$ the energy minima look flat: $\lambda_m = 0$. At low temperature, the expected equilibrium value of the energy is smaller than $E_t$. Therefore, starting from high temperature conditions, the system does not manage to reach the equilibrium because the phase space becomes flatter and flatter in the vicinity of $E_T$. In the thermodynamic limit, the energy slowly drifts toward $E_T$ but never reaches it, which leads to aging. The mode-coupling temperature corresponds to an equilibrium energy equal to $E_T$. In a finite size system, the energy can cross the threshold so that the dynamics becomes activated. In this situation, the phenomenological trap models give a fair description of the aging behavior. In particular, the regime just before the thermalization is expected to be well described by the activated trap model.

The present Letter proposes a phenomenological mod-
unit is set to one. Starting from an energy $e$ at time $t$, the dynamics consists in drawing a new energy $e'$ following a connectivity function $f_e(e \to e')$, and then, accepting it or not according to the Metropolis rule. The function $f_e$ depends on the mean energy per site $\epsilon = \sum e_i/N$ and reflects the topological properties of the energy surface at the global energy $N\epsilon$. Roughly speaking, $\epsilon$ can thus be thought of as an analog of the self-consistent magnetization in the ferro-magnetisme à la Curie-Weiss.

We shall endow $f_e$ with a specific dependence on $\epsilon$ to model the effect of an energy threshold. In this case, we find at low temperature a spin/energy relaxation with two time-sectors (see Fig. 4). The aging scaling is fully determined by the evolution of $\epsilon$ and the spin observable gives linear fluctuation dissipation relations (FDR) that lead to effective temperatures larger than $T$. The energies have non-linear and non-monotonic FDR's.

**Mimicking a dynamic glass transition** $f_e$ is constrained by the following topological relation:

$$\rho(e)f_e(e \to e') = \rho(e')f_e(e' \to e)$$  \hspace{1cm} (1)

This is the reciprocity property of the connectivity. It says that the connection from a state $A$ to a state $B$ is identical to the connection from $B$ to $A$. In the following, we consider a Gaussian/δ function (see Fig. 2):

$$f_e(e \to e') = \left((1 - \frac{\epsilon}{\epsilon_d})^\alpha\right)\frac{1}{\sqrt{2\pi} \epsilon_d^\alpha} e^{-\frac{1}{2\epsilon_d^2}(e-e')^2} \quad \text{if} \quad \epsilon > \epsilon_d$$  \hspace{1cm} (2)

$$f_e(e \to e') = \delta(e' + \epsilon) \quad \text{if} \quad \epsilon \leq \epsilon_d$$  \hspace{1cm} (3)

which verifies (1) if $\alpha = \sqrt{1 - (1 - \epsilon/\epsilon_d)\nu}$. $\epsilon_d$, an energy that does not depend on the temperature and $\nu$, a positive exponent, are free parameters.

To justify this choice, let us consider the Monte-Carlo evolution of some disordered spin model $S$ where the spins are Ising-like. At each step, a spin is chosen with probability $1/N$ and flipped or not according to the Metropolis rule. At infinite temperature, $\epsilon = 0$ in our case, any transition is accepted. Then, between two successive flips of the same spin, the global energy, and hence the local energy, strongly fluctuate. We then expect a random choice for the local energies, which corresponds to $f_{\epsilon=0}(e \to e') \sim \exp(-\epsilon^2)$ in our formalism. Close to a ”mode-coupling” energy threshold, the scenario is different. For instance, in the p-spin model the closer to the threshold, the longer the system stays in the same region of the phase space (4). In other words, fast fluctuations do not drift the system away from an initial configuration. In the spin model $S$, fast fluctuations correspond to spin-flips and a configuration can be labeled by the data of its local energies. Therefore, close to the energy threshold, between two flips of the same spin, the corresponding local energy, $\epsilon$, should not change much. A way to include this effect is to consider a trapping into a two-state process (TSP) with energies $\{e, -e\}$. This justifies that $f_e(e \to e')$ becomes more and more peaked around $-e$ as $\epsilon \to \epsilon_d$, $\epsilon_d$ thus playing the role of the threshold—see Eq. (2) and Fig. 2. At the energy threshold, the system consists of an ensemble of TSP’s that are described by the $\delta$-function (3).

At high temperature, the Boltzmann equilibrium is recovered and $\epsilon = -1/2T$. Thus, after a temperature quench below $T_d = 1/2|\epsilon_d|$, the energy first rapidly decreases toward $\epsilon_d$ and then, is slowed down by the trapping of the TSP’s. At low temperature, we numerically find that the time needed to reach $\epsilon_d$ (measured in number of sweeps) is larger than $N$ when $\nu \geq 2$, so that it diverges in the thermodynamic limit.

**Correlation functions** We have numerically investigated the connected energy/spin autocorrelation functions, $C_e(t_w, t) = \sum_i(\langle e(t_w)e_i(t)\rangle - \langle e(t_w)\rangle\langle e_i(t)\rangle)/N$, and $C_s(t_w, t) = \sum_i(\langle s_i(t_w)s_i(t)\rangle - \langle s_i(t_w)\rangle\langle s_i(t)\rangle)/N$ respectively. The brackets stand for an average over the noise history. The initial conditions are always taken at infinite temperature and the waiting time before measurements is noted $t_w$. The simulations reported here were done with $\nu = 4$ although similar results are obtained for different $\nu \geq 2$.

Fig. 3 shows the spin autocorrelation at different temperatures. Three regimes must be distinguished. At high $T$ (data not shown), the system exponentially relaxes and the evolution is time translational invariant (TTI). At lower $T > T_d$ (Fig. 3a), the autocorrelation develops a plateau that becomes TTI at finite time (not diverging with $N$). At further lower $T \leq T_d$, the system enters in the so-called aging regime (Fig. 3b). Then, we observe a short-time regime $(t - t_w \ll t_w)$ that becomes TTI as $t_w$ increases whereas for long times $t - t_w \gg t_w$, the relaxation depends on $t_w$.

These behaviors can be rationalized within a master equation (ME) approach. As $\epsilon \to \epsilon_d$, the distribution $f_e$ can be expanded in powers of $(1 - \epsilon/\epsilon_d)\nu$. Keeping only the first terms, the ME for the energy $e$ reads

$$\partial_t P(e, t) = -w(e \to -e)P(e, t) + w(-e \to e)P(-e, t) - (1 - \epsilon(t)/\epsilon_d)\nu F_1(P(\pm e), P^\prime(-e), P^\prime\prime(-e))(4)$$

with $\epsilon(t) = \int de P(e, t)$. $F_1(\cdot)$ is a functional of $P(x, t)$. 

![FIG. 2: $\epsilon$-dependence of the connectivity function. For $\epsilon \to \epsilon_d$, the evolution is essentially trapped within the TSP's $\{-e, e\}$. The greater the exponent $\nu$, the more narrow $f_e$, i.e. the more efficient the trapping within the TSP's. $e < 0$ in this figure.](image-url)
and \( w \) is the Metropolis rate.

When dealing with the above two-time autocorrelation functions, the initial conditions in Eq. (4) must be taken at time \( t_w \). Thus, the two first terms of the right hand side, that account for the relaxation within the TSP’s, contribute to the fast relaxation toward the plateau. The last term allows the system to further relax with a typical timescale \((T - T_d)^{-\nu} \) as \( T \to T_d \) since the closer to \( e_d \), the sharper the timescale separation in (4). Fig. 3a confirms this scaling law once normalized the plateau values.

For \( T \leq T_d \), \( e(t) \) drifts toward \( e_d \) without reaching it. In the limit \( t_w \to \infty \) (rigorously taken after \( N \to \infty \)), fast and slow timescales totally decouple. First, the TSP’s locally equilibrate, which leads to \( P(e, t)w(e \to e) = P(-e, t)w(-e \to e) \). Next, under these conditions the ME (4) reduces to:

\[
\frac{\partial}{\partial t} P(e, t) = -(1 - \epsilon(t)/e_d)^\nu F_2(P(e), P^*(e), P'(e))
\]

where \( F_2 \) is a functional different than \( F_1 \). This gives the dynamical evolution of \( P(e, t) \) during the decay from the plateau. The timescale \((1 - \epsilon(t)/e_d)^{-\nu} \) is now time-dependent. Furthermore, considering the decoupling of fast and slow timescales, the spin autocorrelation function in the aging regime can be written as [20]:

\[
C_s(t_w, t) = \int \int \int \int d\phi d\hat{z} \phi(t) C_s(\phi, \hat{z}, t_w) (e_d - e) G(e, t) (e_d - e) G(e, t)
\]

In this relation, \( G(e, t) \) is the energy density of the TSP’s and is given by \((P(e, t) + P(-e, t))/2\). \( G(e, t) \) is the corresponding propagator with the initial condition \( P(\pm e, t) = \delta(e \mp e_d)(t - t_w) \). \( p(e) \) is the Boltzmann weight restricted to the TSP \( \{e, -e\} \). Thus, the relation [19] means that the decay from the plateau comes from the decorrelation of the TSP’s \( \{e, -e\} \) due to a diffusion of the energy \( e \) governed by the equation [20].

Denoting \( \phi_{w}(x) = \int_{t_w}^{t} d\phi' (1 - \epsilon(t')/e_d)^{-\nu} \), Eq. (4) calls for a solution \( G(e, t|w_w, t_w) = \tilde{G}(e, \phi_{w}(t)|e_w, 0) \). Inserting this relation into (3) and noticing that \( G(e, t_w) \) becomes stationary as \( t_w \to \infty \), the aging scaling reads:

\[
C_{s,e}(t_w, t) = \tilde{C}_{s,e}(\phi_{w}(t))
\]

the reasoning for the energies being identical. This scaling is numerically well verified (see Fig. 4), which corroborates our treatment of the aging regime. Moreover, in this scope, the plateau value for the spins at time \( t_w \) is equal to \( \int e G(e, t_w)(p(e) - p(-e))^2 \), that is also numerically well verified (see Fig. 3). The Edwards-Anderson parameter \( q_{EA} \) is given by this quantity when \( t_w \to \infty \).

To summarize, two distinct timescales appear at low temperature. A fast one coming from the relaxation within the TSP’s, and a slower one that increases as \( e(t) \) drifts to \( e_d \). Notice that a full aging regime \((t/t_w) \to \infty \) is expected only if \((1 - \epsilon(t)/e_d)^{-\nu} \) decreases as \( t \) increases, then \( \phi_{w} \propto \log(t/t_w) \). However, we have never seen this regime in our simulations.

Response to a field \( h \) \( T \) \( T \)

The two-time magnetic susceptibility corresponding to the spin autocorrelation function reads \( \chi_s(t, t) = \partial(\xi_s(t))/\partial h(t) \). \( \xi_s(t) \) is measured a time \( t - t_w \) after having switched on, at time \( t_w \), a small constant field \( h \) coupled to \( s \). The \( \xi_s \)’s are quenched random variables that take values \( \pm 1 \). At low temperature and in the long-time limit, a piecewise relation between \( \chi_s \) and \( C_s \) has been found in the p-spin model [17]:

\[
\chi_s(t_w, t) = (1 - C_s(t_w, t))/T \text{ if } C_s > q_{EA}
\]
FIG. 5: FDR. $N = 1000$, $e_d = -0.7$. The solid line is the equilibrium relation. The responses have been computed using $h = 0.1$.

$$= \frac{(q_{EA} - C_s(t_w, t))}{T_e} \text{ if } C_s < q_{EA} \quad (9)$$

The relation (8) is the usual equilibrium relation and is due to a local equilibrium property of the system. The linear relation (9) in the aging regime leads to an effective temperature $T_e \geq T$ that shares the thermodynamic properties of canonical temperatures $T_h$ and $T_m$. Interestingly, such a behavior has been later observed in numerical simulations and in experiments as well [21], which prevents any artifact of the mean-field treatment.

We computed $\chi_s$ in our system by adding to $E_{i}$ a magnetic energy $e_m = -\frac{h}{T_e} z_i s_i$. Fig. 5 shows, for different $t_w$, the plot $T_h(t_w, t) = u(C(t_w, t))$ obtained in the linear regime of the response. We see that it can be divided into two sectors corresponding to the fast relaxation and the aging regime respectively. The former gives an equilibrium-like relation. This directly results from the local equilibrium within the TSP’s (see above). The interesting results come from the aging part since it seems that we have a linear FDR for which we can define an effective temperature $T_e \geq T$. As in the $p$-spin models, $T_e$ slightly increases as $T$ decreases.

We have also investigated the response of the local energies. We found non-monotonic behaviors in the aging regime similarly to the results of [25] in finite dimensional kinetic constrained models. Thus, our results suggest that even in mean-field situations, local energies may respond non-monotonically which may lead in some case to negative $T_e$’s [25].

**Conclusion** We have considered the stochastic dynamics of $N$ independent local energies. At each Monte-Carlo step, the new energies are drawn from a distribution $f_\varepsilon$ whose properties self-consistently depend on the global energy $N \varepsilon$ of the system. The dependence is chosen in order to model an energy threshold in the spirit of the $p$-spin model. Given this mode-coupling scenario, we obtain at low temperature the typical properties of aging. In particular, our approach gives a rather intuitive (and simple) illustration of how two time-sectors may appear in a mean-field situation. The linear violation of the fluctuation dissipation relation, for observables uncorrelated with the energies, further confirms the similarity between our phenomenological description and the microscopic disordered models.

Interestingly, one can generalize this mean-field approach to finite dimension replacing $\varepsilon$ by a local energy $\epsilon_i = \frac{1}{2} \sum_{j < z} \epsilon_j$ where the sum is taken over the $z$ nearest neighbors. In this case, one expects $T_e$ to become a crossover below which dynamical heterogeneities should play an important role.

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