Are Mean-Field Spin-Glass Models Relevant for the Structural Glass Transition?

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Abstract

We analyze the properties of the energy landscape of finite-size fully connected $p$-spin-like models whose high temperature phase is described, in the thermodynamic limit, by the schematic Mode Coupling Theory of super-cooled liquids. We show that finite-size fully connected $p$-spin-like models, where activated processes are possible, do exhibit properties typical of real super-cooled liquid when both are near the critical glass transition. Our results support the conclusion that fully-connected $p$-spin-like models are the natural statistical mechanical models for studying the glass transition in super-cooled liquids.

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1 Introduction

In recent years a significant effort has been devoted to the understanding of glass-forming systems. Recent theoretical and numerical results clearly show that the slowing down of the dynamics near the glass transition is strongly

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connected to the potential energy landscape geometry. The trajectory of the representative point in the configuration space can be viewed as a path in a multidimensional potential energy surface [1]. The dynamics is therefore strongly influenced by the topography of the potential energy landscape: local minima, barriers heights, basins of attraction and other topological properties all influence the dynamics.

The potential energy surface of a super-cooled liquid contains a large number of local minima, called inherent structures (IS) by Stillinger [2]. All states that under local energy minimization will flow into the same IS define the basin of the IS (valley). With this pictures in mind the time evolution of the system can be seen as the result of two different processes: thermal relaxation into basins (intra-basin motion) and thermally activated potential energy barrier crossing between different basins (inter-basin motion). When the temperature is lowered down to the order of the critical Mode Coupling Theory (MCT) temperature $T_{MCT}$ the inter-basin motion slows down and the relaxation dynamics is dominated by the slow thermally activated crossing of potential energy barriers [3,4]. If the temperature is further reduced the relaxation time eventually becomes of the same order of the observation time and the system falls out of equilibrium since there is not enough time to cross barriers and equilibrate. This define the “experimental” glass transition temperature $T_g$. The regime between $T_{MCT}$ and $T_g$ cannot be described by the MCT since it neglects activated processes responsible for barrier crossing. In MCT the relaxation time diverges at $T_{MCT}$, leading to $T_g = T_{MCT}$, and the dynamics remains confined into a single basin forever.

The essential features of MCT for glass-forming systems are also common to the high temperature phase of some fully connected spin glass models [5], the most well known being the spherical $p$-spin spin glass model [6,7]. We shall call these models mean-field $p$-spin-like glass models. As a consequence at the critical temperature $T_{MCT}$, called $T_D$ in $p$-spin language, an ergodic to non-ergodic transition takes place. Below this temperature the system is dynamically confined to a metastable state (a basin) [8] since relaxation to true equilibrium can only take place via activated processes, absent in mean-field models. For these systems, nevertheless, it is known that the true equilibrium transition to a low temperature phase occurs below $T_D$ at the static critical temperature $T_c$, also denoted by $T_{1rsb}$ [6]. This is the analogous of the Kauzmann temperature $T_k$ for liquids. The glass transition temperature $T_g$ of real systems sits somewhere in between $T_c$ and $T_D$. This transition, obviously, cannot be reached even on infinite time in mean-field models.

Despite these difficulties mean-field models, having the clear advantage of being analytically tractable, have been largely used to study the properties of fragile glassy systems, especially between the dynamical temperature $T_D$ and the static temperature $T_c$. The picture that emerges is however not complete
since activated process cannot be captured by mean-field models. Therefore
the relevance of mean-field results for real systems cannot be considered com-
pletely stated.

Only recently activated processes in mean-field-like models have been inves-
gigated in extended numerical investigation of finite-size fully-connected $p$-spin-
like models [4,9]. Comparing the results with the observed behavior of super-
cooled liquids near $T_{MCT}$ we can conclude that, once activated process are
allowed, mean-field $p$-spin-like models are highly valuable for a deep under-
standing of the glass transition in real systems.

We report the main results obtained for the Ising-spin Random Orthogonal
Model (ROM) [10,11], defined by the Hamiltonian [10,11],
\[ H = -2 \sum_{ij} J_{ij} \sigma_i \sigma_j \]
where $\sigma_i = \pm 1$ are $N$ Ising spin variables, and $J_{ij}$ is a $N \times N$ random symmetric
orthogonal matrix with $J_{ii} = 0$. For $N \to \infty$ this model has the same thermo-
dynamic properties of the $p$-spin model: a dynamical transition at $T_D = 0.536$,
with threshold energy per spin $e_{th} = E_{th}/N = -1.87$, and a static transition
at $T_c = 0.25$, with critical energy per spin $e_{1rsb} = -1.936$ [10,11].

2 Thermodynamics of Inherent Structures: How to evaluate the
configurational entropy

The free energy analysis (TAP) [8,11] reveals that the phase space is com-
posed by an exponentially large (in $N$) number of different basins, separated
by infinitely large (for $N \to \infty$) barriers. Each basin is unambiguously la-
belled by the value of the energy density $e$ of the local minimum contained
within it, i.e. the IS of the system. In this picture the dynamical transition is
associated with IS having the largest basin of attraction for $N \to \infty$, while
the static transition with IS with the lowest accessible free energy (vanishing
configurational entropy) [12,8].

In the mean-field limit, the allowed values of $e$ are between $e_{1rsb}$ and $e_{th}$. 
Solutions with $e$ larger than $e_{th}$ are unstable (saddles), while solutions with $e$
smaller than $e_{1rsb}$ have negligible statistical weight. Moreover in the $N \to \infty$
limit IS with $e = e_{th}$ attract most (exponentially in $N$) of the states and
dominate the behavior of the system. Other IS are irrelevant for $N \to \infty$. For
finite $N$ the scenario is different since not only the basins of IS with $e < e_{th}$
acquire statistical weight, but it may happen that solutions with $e > e_{th}$ and
few negative directions (saddles with few downhill directions) become stable,
simply because there are not enough degrees of freedom to hit them.

To get more insight the IS-structure of finite systems we follow Stillinger and
Weber [13] and decompose the partition sum into a sum over basins of different
IS and a sum within each basin. Collecting all IS with the same energy $e$, denoting with $\exp[Ns_c(E)]de$ the number of IS with energy between $e$ and $e + de$, and shifting the energy of each basin with that of the associated IS, the partition sum can be rewritten as [13]

$$Z_N(T) \simeq \int de \exp N \left[ -\beta e + s_c(e) - \beta f(\beta, e) \right]$$

(1)

where $f(\beta, e)$ can be seen as the free energy density of the system when confined in one of the basin associated with IS of energy $e$. The function $s_c(e)$ is the configurational entropy density also called complexity. From the partition function we can compute the average internal energy density $u(T) = \langle e \rangle + \partial(\beta f)/\partial\beta = \langle e(T) \rangle + \langle\Delta e(T)\rangle$. The first term is the average energy of the IS relevant for the thermodynamics at temperature $T$, while the second is the contribution from fluctuations inside the associated basins. In the limit $N \to \infty$ only IS with $e = e_{th}$ contribute and $\lim_{N \to \infty} \langle e(T) \rangle = e_{th}$ for any $T > T_D$. For finite $N$, and $T$ not too close to $T_D$, the thermodynamics is dominated by IS with $e > e_{th}$ and $\langle e(T) \rangle > e_{th}$ [4]. This is more evident from the (equilibrium) probability distribution of $e$ since it is centered about $\langle e(T) \rangle$ indicating that IS with $e \simeq \langle e(T) \rangle$ have the largest basins. This scenario has been also observed in real glass-forming systems [14–18].

From the knowledge of IS-energy distribution we can reconstruct the complexity $s_c(e)$ since from eq. (1) the probability that an equilibrium configuration at temperature $T = 1/\beta$ lies in a basin associated with IS of energy between $e$ and $e + de$ is: $P_N(e, T) = \exp N \left[ -\beta e + s_c(e) - \beta f(\beta, e) \right]/Z_N(T)$. In the temperature range where this applies, the curves $\ln P_N(e, T) + \beta e$ are equal, except for a temperature dependent factor $\ln Z_N(T)$, to $s_c(e) - \beta f(\beta, e)$. If the $e$-dependence of $f(\beta, e)$ can be neglected, then it is possible to superimpose the curves for different temperatures, see Fig. 1 (a). The data collapse is rather good for $e < -1.8$. Above the curves cannot be superimposed anymore indicating that the $e$-dependence of $f(\beta, e)$ cannot be neglected. In liquid this is called the anharmonic threshold [19,20].

Direct consequence of $f(\beta, e) \approx f(\beta)$ for $e < -1.8$ is that in this range the partition function can be written as the product of an intra-basin contribution $\exp(-N\beta f)$ and of a configurational contribution which depends only on the IS energy densities distribution. The system can then be considered as composed by two independent subsystems: the intra-basin subsystem describing the equilibrium when confined within basins, and the IS subsystem describing equilibrium via activated processes between different basins. As the temperature is lowered and/or $N$ increased the two processes get more separated in time and the separation becomes more and more accurate. A scenario typical of super-cooled liquids near the MCT transition [21,3].
Fig. 1. (a) Configurational entropy as a function of energy. The data are from system sizes $N = 48$ (empty circle) and $N = 300$ (filled circle), and temperatures $T = 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$ and 1.0. For each curve the unknown constant has been fixed to maximize the overlap between the data and the theoretical result [11]. The line is the quadratic best-fit. (b) Configurational entropy density as a function of temperature. The line is the result from the best-fit of $s_c(e)$ while the symbols are the results from the temperature integration of $d s_c(T)/d \langle e(T) \rangle = T^{-1}$ for $N = 48$ (empty circle), $N = 300$ (empty triangle) and $N = 1000$ (filled circle).

3 Non-equilibrium behavior: the role of activated processes

More informations on the IS structure can be obtained from non-equilibrium relaxation processes. To study the non-equilibrium dynamics we quench at time zero the system from an initial equilibrium configuration at temperature $T_i > T_g$ to a final temperature $T_f < T_g$ and study the evolution of the average IS energy per spin $\langle e(t) \rangle$ as function of time, see Fig.2 (b). Two different relaxation processes are clear seen. A first regime independent of $T_f$, and a second regime independent of both $T_i$ and $T_f$. The final temperature $T_f$ controls the cross-over between the two regimes. A similar behavior has been observed in molecular dynamics simulations of super-cooled liquids [18]. The two regimes are associated with different relaxation processes. In the first part the system has enough energy and relaxation is mainly due to path search out of basins through saddles of energy lower than $k_B T_f$. This part depends only on the initial equilibrium temperature $T_i$ since it sets the initial phase space region. Different $T_i$ leads to different power law. In particular relaxation must slow down as $T_i$ decreases since we expect that lower states are surrounded by higher barriers, in agreement with numerical data [9].
During this process the system explores deeper and deeper valleys (basins) while decreasing its energy. The process stops when all barrier heights become of $O(k_B T_f)$. From now on the relaxation proceeds only via activated process. A first consequence is that lower the final temperature $T_f$ shorter the first relaxation, in agreement with our findings [See figures 2].

The analysis of the distance between the instantaneous system state and the corresponding IS, counting the number of single spin flip needed to reach the IS, reveals that for all times the systems stays in configurations few spin flips away from an IS. A similar study starting from equilibrium configurations at temperature $T_e(\langle e(t) \rangle)$ evaluated comparing panels (a) and (b) of figure 2 [18] leads to similar numbers. We then conclude that during relaxation the aging system explores the same type of minima (and basins) visited in equilibrium at temperature $T_e$. Direct consequence is that once the system has reached the activated regime there cannot be memory of the initial $T_i$, and all curves with different $T_i$ but same $T_f$ should collapse for large time [9].

4 Conclusions

To summarize, we have shown that finite-size mean-field $p$-spin-like models are good candidates for studying the glass transition. The key point is that near the glass transition the thermodynamics of the systems is dominated by the IS distributions, therefore all systems with similar IS distributions...
should have similar behavior. Finite-size mean-field $p$-spin-like models have the double advantage of being analytically tractable for $N \to \infty$ and easily simulated numerically for finite $N$, offering good models to analyze the glass transition.

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