Structure and dynamics of the t154 lattice glass

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We revisit the t154 variant of the Biroli-Mezard lattice glass, complementing previous studies by studying statics and dynamics under periodic boundary conditions as well as systems confined in cavities with amorphous boundaries. We compute the point-to-set correlation and relaxation times under the different boundary conditions. Results point to a scenario with dynamics ruled by structural correlations.

I. INTRODUCTION

The physical mechanism behind the dramatic slowing down of dynamics close to the empirically defined glass transition has been subject of continued interest and debate [1,2]. Due to the somewhat limited amount of information available from experiments and simulations (limitations due in large part to the difficulties that arise from the very phenomenon under study, i.e. the slowdown), different theoretical proposals have been able to rationalize observed behaviors often starting from completely divergent viewpoints [3,4]. It is thus natural that models have been sought that display the main phenomenology with a bare minimum of ingredients, so as to allow for a more detailed analysis (either theoretically or numerically), and lattice models have been considered good candidates in this category [5,6,7].

Here we revisit a lattice glass model, the t154 [10], a variation of the Biroli-Mézard lattice glasses [10]. Lattice glasses are defined through an energy (which may be infinite) uniquely assigned to every configuration, and glassy behavior follows from a “natural” dynamics (Metropolis Monte Carlo, for instance). This is opposed to kinetically constrained models [13], where there are no or few constraints to possible configurations, and glassy dynamics results from rules that forbid certain transitions between configurations. A detailed study of dynamical heterogeneities of the t154 was carried out in ref. [10], where it was found that it is stable against crystallization, and that it has the main characteristics of a fragile liquid, showing in particular Stokes-Einstein violations and signs of a growing dynamic length scale as measured by a four-point correlation function. In this respect, the t154 is phenomenologically similar to kinetically constrained models. Here we focus on an aspect left out of this previous study, which is the determination of a static correlation length and its possible relationship with the dynamical behavior.

We use the approach of studying small or confined systems to put the relevant length scales in evidence. To find a static (structural) length scale we compute point-to-set (PTS) correlations [17,18], which are computed by studying systems confined in cavities with amorphous boundary conditions (ABCs) (explained below) [19]. PTS correlations were the first to be used successfully to detect a growing correlation length in supercooled liquids [20,21], a result confirmed also with other approaches [22,23]. For our dynamical analysis we use both ABCs and the usual periodic boundary conditions (PBCs), looking for changes in the relaxation times in small systems [24,25]. The goal is to extend the study of the t154 to its structural aspects, and to establish whether the structural properties are relevant for the dynamical features.

We present the model and details of our simulations in sec. II. Sec. III A summarizes our structural findings, sec. III C is devoted to our dynamical results, and we conclude in sec. IV.

II. MODEL AND SIMULATIONS

The Biroli-Mézard lattice glasses [10] are defined on a d-dimensional lattice. It’s sites can be empty or occupied by one and only one particle of class \( \ell = 1, 2, \ldots \). To this hard excluded volume, a hard density constraint is added: at most \( \ell \) of the neighbouring sites are allowed to be occupied. Different variants of the model arise when specifying the number of classes and the proportion among them. Here we focus in particular on the t154 variant [10], where \( \ell = 1, 2, 3 \) and the proportions of each class are 0.1, 0.5 and 0.4 respectively. Since the constraints are hard, temperature is irrelevant and the control parameter is the density \( \rho \) or the Lagrange multiplier \( \beta \mu \) of the particles of the first class (\( \alpha_2 \) and \( \alpha_3 \) being fixed by the composition). The relationship between chemical potential and composition can be written

\[
\beta \mu_\ell = \ln \left( \frac{p_\ell}{p_\ell} \right),
\]

where \( p_\ell \) is the fraction \( \ell \)-holes, i.e. empty sites with enough free neighbours that a particle of class \( \ell \) can be placed on it without violating the constraints. Then, for
of the region at time \( t_0 \) with itself at time 0 (with the spatial structure and the dynamical behavior, so we study the effects of the boundary layer on the statics and dynamics of the cavity. Under these conditions the asymptotic value of the overlap will not necessarily be the uncorrelated value \( \rho^2 \). The asymptotic value of the overlap at the center \( q_{\infty} \) is the point-to-set correlation, and is a measure of the influence of the boundary of the cavity on the structure at its center. To measure the PTS correlation we use a cube of side 3, and averaged over 50 realizations of the boundaries. When reporting ABC results, the global overlap \( Q(t) \) is computed only within the cavity (mobile particles).

To ensure that our runs are long enough that the asymptotic value of the PTS, \( q_{\infty} \), represents the equilibrium value and is not the result of running the simulation for too short times, we perform a β-initial condition (BIC) test [29]. For this we initialize two identical cavity samples in a configuration \( \gamma \) that will serve as the reference against which the instantaneous overlap is computed. In one configuration the cavity particles are replaced by those of a different configuration \( \delta \) with very low overlap with \( \gamma \). If \( q(t) \) reaches the equilibrium value we should see \( q_{\gamma\delta}(t) \) decrease toward \( q_{\infty} \), while \( q_{\gamma\gamma}(t) \) will increase up to \( q_{\infty} \). If the two samples do not reach the same \( q_{\infty} \), thermalization of the sample has not been achieved (negative BIC test). In practice, it is easy to do the test in the GC case by simply emptying the cavity after taking the initial configuration as reference.

III. RESULTS

Our aim is to establish possible connections between the spatial structure and the dynamical behavior, so we measure space and time correlations of the density, as encoded in the overlap (Eq. 2). We start showing a (generalized) Arrhenius plot of the relaxation time vs. the density for both canonical (C) and grand canonical (GC) dynamics (Fig. 2). The relaxation times \( \tau \) were extracted from a stretched-exponential fit of the time decay of the translation-invariant distribution is \( \rho^2 \), and this is the value reached for \( t \to \infty \) with PBCs, indicating that correlation is lost. For the region \( R \) we take the whole lattice, the ABCs cavity (see below), or a small cube in the center of the cavity (in which case we name the overlap with a lowercase \( q(t) \)).

In amorphous boundary conditions the system is subject to a surface field applied at its boundaries, which is created by particles of the same kind placed outside the boundaries and held fixed in random positions drawn from the equilibrium distribution. In other words, one studies a cavity of mobile particles surrounded by particles frozen at equilibrium positions. In practice this is achieved by taking an equilibrium configuration obtained in a run with PBCs and artificially freezing the particles outside a cubic cavity (but allowing the frozen particles to interact with the mobile ones). We use a system of size \( L^3 = 30^3 \), in which we define a cubic cavity of size \( K^3 \). By varying the size \( K \) one can study the effects of the boundary layer on the statics and dynamics of the cavity. Under these conditions the asymptotic value of the overlap will not necessarily be the uncorrelated value \( \rho^2 \). The asymptotic value of the overlap at the center \( q_{\infty} \) is the point-to-set correlation, and is a measure of the influence of the boundary of the cavity on the structure at its center. To measure the PTS correlation we use a cube of side 3, and averaged over 50 realizations of the boundaries. When reporting ABC results, the global overlap \( Q(t) \) is computed only within the cavity (mobile particles).

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FIG. 1. \( \alpha \) vs \( \rho \) obtained from canonical simulations @ \( L = 30 \).
Since the model is defined with hard constraints (as the hard spheres model for instance), at high densities the dynamics will start to become sluggish because to relax a configuration the system must find a path that goes through allowed configurations (otherwise the energy price is infinite). However, these configurations are becoming less numerous because the constraints are harder to fulfill the higher the density or the stronger the confinement. At still higher densities, groups of configurations can become completely disconnected (i.e. separated by infinite-energy barriers), and the system becomes nonergodic. On the other hand, the (nonphysical) dynamics of the GC ensemble allows destruction and creation of particles at arbitrary locations, thus effectively lowering barriers by adding connections between configurations. In particular, the loss of ergodicity is avoided, because in the worst case scenario two configurations could be joined by a path that first destroys all particles and then creates them in the required locations. Thus one expects shorter relaxation times with respect to the canonical dynamics, at least at relatively high densities where the canonical dynamics start slowing down because many trial moves lead to forbidden configurations. This expectation is fulfilled, but the GC times are appreciably smaller only for $\rho \gtrsim \rho_0 \approx 0.51$. We take this as an indication that the structure has important influence on the dynamics only for densities greater than $\rho_0$, which would indicate the start of “landscape influenced” dynamics.

The plot reveals the fragile character of the model, and the curves can be fitted by (generalized) Vogel-Fulcher-Tamman function $\tau = \exp[A/(\rho - \rho_K)]$, yielding $\rho_K^{GC} = 0.595$ and $\rho_K^C = 0.588$.

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All the results of this section were obtained in the GC ensemble, where the dynamics are faster and allows us to equilibrate systems with densities up to \( \rho = 0.54 \). Dynamics in the canonical ensemble are too slow and it is impossible to equilibrate even moderately confined cavities in canonical runs (see sec. III C). However, the choice of dynamics is irrelevant for the structural results (provided the system can be thermalized). Given that we have found some size dependence of the chemical potential, we have checked that the composition of the cavities stays at the 1-5-4 proportion. We have found some fluctuation in the composition of the smallest cavities, but in no case larger than 3%.

When the structure can decorrelate completely (as when thermalized under PBCs), we know the asymptotic limits of the overlaps \((\rho)^2\) for both \(g(t)\) and \(Q(t)\), see Fig. 3 inset. The presence of structural correlations is revealed by the fact that the asymptotic value for the cavity is higher than the PBCs case. Of course, a simulation that is too short to thermalize the system could produce a spurious high value of the asymptotic overlap. To check that the system has indeed equilibrated (and that we are measuring the actual equilibrium PTS), we perform \(\beta\) initial condition (BIC) tests \(\cite{33}\) (see sec. III). One such test is shown in Fig. 6; the same value of the overlap is reached starting from independent (low overlap) configurations. We then compute the asymptotic values \(q_\infty\) and \(Q_\infty\) averaging the overlap starting from the time when the two curves of the BIC test coincide.

From both \(Q(t)\) and \(q(t)\) it is clear that in small cavities the border is exerting a significant influence on the particles inside. We will use the values \(q_\infty(K)\) and \(Q_\infty(K)\) to extract a correlation length.

As a measure of how far the local structure influences the arrangement of other particles, \(\xi_{PTS}\) is found to increase steeply for cavities of size \(K^3 = 10^3\) and \(K^3 = 15^3\). We can see how the test renders a positive result, since both reach the same asymptotic values. Therefore we conclude that both configurations have thermalized.

### B. Correlation length

Both \(Q_\infty(K)\) and \(q_\infty(K)\) contain information about the structural correlations, but although the former is less noisy, it is more difficult to interpret. We start with the PTS correlation \(q_\infty(K)\) (Fig. 5). We find that a simple exponential can adequately fit the decay of the PTS, from which we extract a correlation length \(\xi_{PTS}\):

\[
q_c(K) - q_0 = (q_1 - q_0) \exp[-K/\xi_{PTS}],
\]

where \(q_0 = \langle \rho \rangle^2\) and \(q_1\) and \(\xi_{PTS}\) are fit parameters. When \(K \gg \xi_{PTS}\), the center of the cavity is free to rearrange as if it were subject to PBCs, thus \(\xi_{PTS}\) measures how far the local structure influences the arrangement of other particles. \(\xi_{PTS}\) is found to increase steeply for
\( \rho > 0.53 \). However, we find no sign of the nonexponential behavior described in refs. \(^{20,21}\) and \(^{34}\), explained invoking the appearance of the multiple metastable states of the Random First-Order theory of liquids. In that picture, large cavities can explore all metastable states as the liquid does, but small cavities are locked into one state by surface tension \(^{17}\).

The structural information contained in \( Q_\infty(K) \) is encoded in a more complicated way: even for cavities several times larger than \( \xi_{PTS} \) (i.e. for distances over which there is no correlation as measured by the PTS), \( Q_\infty \) will be higher than the PBCs value due to the pinning effect of the frozen border on particles near the edge of the cavity. That is, even when the center of the cavity is completely uncorrelated with the border, the global overlap is picking up the influence of the border over the nearby particles. If one makes the simple “one state” assumption (i.e. there are no metastable states such that the cavity is always in the only liquid state, and the overlap decays exponentially from a value of 1 at the border to a value \( q_0 \) well inside the cavity) one gets \(^{33}\)

\[
Q_{1S}(K) = 3(1 - q_0) \left[ \frac{1 - 2}{x} + \frac{2(1 - e^{-x})}{x^3} \right] + q_0, \tag{6}
\]

with \( x = K/\xi \), where the penetration length \( \xi \) should be proportional to \( \xi_{PTS} \) in this scenario. A fit of this expression, shown in Fig. 7, yields a penetration length that behaves as shown in Fig. 8. Comparing the evolution of \( \xi_{PTS} \) and \( \xi \) with density, both show qualitatively similar behavior up to \( \rho \approx 0.53 \), increasing approximately two-fold from \( \rho = 0.48 \). At higher densities their behavior differs markedly: while \( \xi \) stays constant, \( \xi_{PTS} \) increases steeply (approximately three times from \( \rho = 0.53 \) to \( \rho = 0.54 \)).

\[
\frac{\rho}{\rho} \approx \exp(-\langle t/\tau \rangle^\beta + q_\infty) \tag{5}
\]

We now compute the relaxation times \( \tau \) under various conditions. In all cases it was extracted from a stretched-exponential fit \( g_c(t) = A \exp(-\langle t/\tau \rangle^\beta + q_\infty) \) of the time decay of the local overlap \( g_c(t) \). The aim is to study size effects on \( \tau \), to see whether a dynamically relevant length scale can be detected. As opposed to the statics study of sec. III A, here the choice of canonical or grand-canonical ensemble can make a big difference. The hard constraints of the model are hard to fulfill the higher the density or the stronger the confinement, thus we expect confined systems with canonical dynamics will have larger relaxation times as the cavity is made smaller, and eventually become completely jammed \(^{32}\). On the other hand, the (nonphysical) dynamics of the GC ensemble lowers barriers and avoids ergodicity breaking as discussed above.

\[
\frac{\rho}{\rho} = 0.53\text{, increasing approximately two-fold from } \rho = 0.48. \quad \text{At higher densities their behavior differs markedly: while } \xi \text{ stays constant, } \xi_{PTS} \text{ increases steeply (approximately three times from } \rho = 0.53 \text{ to } \rho = 0.54).}
\]
Thus one expects shorter confined systems with GC dynamics to be faster, but also the shape of the relaxation time vs. size curve could be qualitatively different.

1. GC dynamics

From the decay of $q(t)$ for GC dynamics in ABCs cavities we obtained the relaxation times shown in Fig. 10 with a stretching exponent $\beta$ taking values in $0.45 < \beta < 0.85$ for the smaller cavities ($K \leq 10$), whereas for larger cavities ($K > 10$) $\beta$ smoothly shifted to the $0.50 < \beta < 0.65$ region. There are no discernible size effects up to $\rho \approx 0.53$ (the density at which $\xi_{\text{PBC}}$ starts to grow rapidly). Beyond this density, scatter among the curves is seen, with smaller cavities seemingly faster than larger ones. Unfortunately there are small variations in $\rho$ as $K$ is varied, which forbids from plotting $\tau$ vs $K$ at constant density (because although the fluctuations in $\rho$ are small $\tau$ is extremely sensitive to $\rho$).

We did the same analysis for PBCs (Fig. 11). In this case, although there is no clear tendency and density seems to be more scattered than in ABCs, larger systems appear to relax faster.

2. Canonical dynamics

Turning now to canonical dynamics, as discussed above one expects smaller systems to be slower and eventually completely jammed. Indeed we found that as $\rho$ is decreased, it is more and more likely to find a sample that is stuck out of equilibrium, i.e., the value of $q(t)$ or $Q(t)$ oscillates at values higher than the equilibrium value found with GC dynamics and validated with the BIC test. Sometimes this value is nearly $Q(t) = \rho$, i.e. the $t = 0$ value. The results we report here were obtained by averaging only over samples that do not block, following the logic of ref. 28. The idea is that this is a toy model with hard core interactions, which therefore artificially excludes relaxation mechanisms (like activated jumps) which a real system could use in order to relax. Thus the jammed samples would contribute to the average an exaggerated (infinite) relaxation time, so the average obtained excluding them would give a trend qualitatively similar to the behavior of a realistic model. We report only PBCs results for $L \geq 10$, since systems with $L < 10$ systems tend to block, e.g., for $\rho = 0.526$, only two out of fifty samples would relax for $L = 6$. We do not report systems confined with ABCs because in those cases the relaxation time grows very quickly and most samples end up completely jammed, even for the largest cavities.

Fig. 12 shows $\tau$ vs. $\rho$ for PBCs systems of different sizes. For $\rho < 0.53$ there are no size effects, except perhaps for the smallest ($L = 5$) system. At the two highest densities, it seems the smaller systems are slower than larger ones (i.e. the opposite from the trend observed in ABCs cavities with GC dynamics). However, a more complicated (nonmonotonic) behavior is to be expected with canonical dynamics 28 29. Some evidence of this is Fig. 13.

IV. DISCUSSION AND CONCLUSIONS

We have presented a study of some dynamic and thermodynamic properties of the t154 model that complements the analysis of ref. 16. At the static level, we have computed the point-to-set (PTS) correlation, and found it decays as a simple exponential with the size of the cavity. The corresponding correlation length $\xi_{\text{PTS}}$ shows around $\rho \approx 0.53$ a rather steep increase (about threefold between $\rho = 0.525$ and $\rho = 0.54$). Up to $\rho = 0.53$, the
Above this density, the decay of the local overlap from the wall boundary inside the cavity seems to continue to rise gently and does not reflect the steep increase of \( q_0 \). This two-parameter fit is good but yields \( q_1 \approx 0.3 \approx q_0 \), i.e. it essentially recovers the one-state fit. This together with the purely exponential relaxation of \( q_0(R) \) makes it hard to invoke a multistate scenario.

We have also performed a finite-size study of the relaxation times (as obtained from the decay of the self overlap) using both GC dynamics (where we examined systems with ABCs and PBCs) and canonical dynamics (where only PBCs systems could be studied). The GC dynamics start showing finite-size effects (or fluctuations at least) around the density \( \rho = 0.53 \) at which \( \xi_{\text{PTS}} \) starts growing steeply. This is in agreement with a structural, rather than kinetic origin of the slowdown mechanism of this model.

The analysis of canonical dynamics also shows some indication of finite-size effects around density \( \rho = 0.53 \), but this analysis is rather inconclusive, mainly because it has not been possible to reach high densities with small systems. The trend is apparently the opposite with respect to GC (i.e. smaller systems are slower rather than faster). However very small systems should eventually become faster [28], a nonmonotonicity which we have not clearly observed.

In summary, our results hint at a scenario where dynamics are ruled by structural correlations, but with little evidence for a particular theory.

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