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Jamming in hierarchical networks

Xiang Cheng *, Stefan Boettcher

Department of Physics, Emory University, Atlanta, GA 30322, USA

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ABSTRACT

We study the Biroli–Mezard model for lattice glasses on a number of hierarchical networks. These networks combine certain lattice-like features with a recursive structure that makes them suitable for exact renormalization group studies and provide an alternative to the mean-field approach. In our numerical simulations here, we first explore their equilibrium properties with the Wang–Landau algorithm. Then, we investigate their dynamical behavior using a grand-canonical annealing algorithm. We find that the dynamics readily falls out of equilibrium and jams in many of our networks with certain constraints on the neighborhood occupation imposed by the Biroli–Mezard model, even in cases where exact results indicate that no ideal glass transition exists. But while we find that time-scales for the jams diverge, our simulations cannot ascertain such a divergence for a packing fraction distinctly above random close packing. In cases where we allow hopping in our dynamical simulations, the jams on these networks generally disappear.

1. Introduction

The jamming transition, as discussed by Liu and Nagel in 1998 [1], for example, has been the focus of both theoretical and experimental studies [2–4]. A granular disordered system for increasing density can reach a jammed state at which a finite yield stress develops [1,5], or at least extremely long relaxation times ensue [6,7], similar to the emerging sluggish behavior observed when the viscosity of a cooled glassy liquid seemingly diverges. Thus, a jamming transition may be induced in various ways, such as by increasing density, decreasing temperature, or/and reducing shear stress [3]. Below the jamming transition, the system stays in long-lived meta-stable states, and its progression to its corresponding equilibrium state entails an extremely slow, non-Debye relaxation [8–11]. Jamming transitions have been observed in various types of systems, such as granular media [12], molecular glasses [13,14], colloids [15], emulsions [16], foams [17,18], and some theoretical systems [4,11,19]. These systems can behave like stiff solids at a high density with low temperature and small perturbations. In these transitional processes, the systems can self-organize their own structure to avoid large fluctuations [17] and to reach a quasi-stable jammed state, characterized by an extremely slow evolution to the unjammed equilibrium state. Some studies show that the sluggishness may indicate the existence of a Gardner transition in which the energy landscape contains numerous local minima separated by high barriers [20,21]. The properties of those quasi-stable non-equilibrium states as well as their corresponding equilibrium state is the main focus of this paper.

The properties of the jamming transition have been studied extensively [2–4,12], but we still lack an essential understanding of the physics underlying the jammed state. In particular, it is still an open question whether the onset of jamming itself is associated with any (or several [19]) phase transitions, and whether any such transition in the dynamics would be associated with emerging features of the energy landscape in configuration space [20,22]. The later would indicate the possibility of linking jamming with an underlying equilibrium transition. Despite of much progress in simulating computational models of jamming, theoretical progress has been much slower than the accumulation of experimental discoveries. One of the reasons is the scarcity of theoretical models with a microscopically tractable thermodynamics that capture the complex jamming process [23,24]. In recent years, a lattice glass model proposed by Biroli and Mezard (BM) [25] has been shown as a simple but adequate means to study the jamming process in such detail. It is simple because the model follows specific dynamical rules which are elementary to implement in both simulations and analytical work. In distinction to kinetically constrained models such as that due to Kob and Andersen [26], in which particles are blocked from leaving a position unless certain neighborhood conditions are satisfied, BM embeds geometric frustration merely by preventing the neighborhood of any particles to consist of

* Corresponding author.
E-mail addresses: xcheng7@emory.edu (X. Cheng), sboettc@emory.edu (S. Boettcher).

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more than l other particles. Beyond that, it proceeds purely thermodynamically. The phase diagram can be reduced to just one (or both) of two control parameters, chemical potential and temperature. Either is sufficient to reproduce a jamming transition which is similar to that observed in off-lattice systems [25].

Using the BM-model in a mean-field network (i.e., a regular random graph), Krzakala et al. find jammed states in Monte Carlo simulations and a genuine thermodynamical phase transition (ideal glass transition) in its mean-field analytical solutions [23]. In other words, the jammed state coincides with an underlying equilibrium state that possesses a phase transition to a glassy state. Also, other recent studies in different glassy systems indicate a close relationship between the jamming transition and other phase transitions, such as random first-order transition [27], glass transition [19,28], and Gardner transition [20]. These investigations strongly indicate that a true phase transitions might be the reason for the onset of jamming. The theoretical evidence for such a connection thus far is based largely on mean-field models [20,22,23,25], as such a transition is hard to ascertain for finite-dimensional lattice glasses. Yet, it remains unclear whether mean-field solutions in disordered systems can provide an adequate conception for real-world behavior.

In this paper, we propose to use the lattice glass model BM on hierarchical networks [29,30], which are small-world networks with a fixed, lattice-like geometry. They combine a finite-dimensional lattice backbone with a hierarchy of small-world links that in themselves impose a high degree of geometric frustration despite of their regular pattern. These networks can be considered as an instructive intermediary between mean-field and finite-dimensional lattice system, which may reveal more insights about real systems. Their recursive patterns and fixed structures make them computationally approachable and analytically solvable using renormalization group (RG). Moreover, these networks have been shown to possess interesting phase transitions in the Ising model [31] or for percolation [32,33], but no glassy systems have been studied on these networks. It would be interesting to see how these networks perform in the lattice glass model. More details of why using these networks are discussed in Section 3.2.

Our goal in this work is to find (1) whether the lattice glass model leads to jamming states in hierarchical networks, (2) whether there is an ideal glass transition underlying the jamming transition, and (3) whether the local dynamics affects the jamming process. To our knowledge, these questions have not been studied in any small-world systems. Our results can contribute new insights to understand jamming.

We find that BM in these networks can jam, even when there is certifiably no equilibrium transition [30]; the geometric frustration that derives from the incommensurability among the small-world links is sufficient in many cases to affect jamming. In fact, jamming is most pronounced for fully exclusive neighborhoods ($l = 0$). It disappears for more disordered neighborhoods ($l = 1$), at least for our non-regular networks, where the allowance of $l = 1$ neighbor to be occupied seems to provide the "lubrication" that averts jams. However, the packing fractions at which time-scales diverge is virtually indistinguishable from random close packing within the accuracy of our simulations.

Mean-field calculations of BM in Ref. [22] predict a kinetic transition for dynamic rules based on nearest-neighbor hopping. In our simulations, we find that such hopping, in addition to the particle exchange with a bath, can affect a dramatic change in the dynamic behavior and eliminated jamming in all cases we consider.

This paper is organized as follows. In Section 2, we describe the model, the networks, and our numerical simulations. In Section 3 we discuss the results of our simulations for each network. In Section 4 we conclude with a few summary remarks and an outlook for future work.

2. Model & methods

In this section, we describe the model and the networks on which we will study its behavior. To benchmark the equilibrium properties of the model on those networks, we implement a multi-canonical algorithm due to Wang and Landau [34,35]. We further need a grand-canonical annealing algorithm to study the dynamics of the lattice glass model on those networks.

2.1. Lattice glass model

The lattice glass model as defined by Biroli and Mezard (BM) [25] considers a system of particles on a lattice of N sites. Each site can carry either $x_i = 0$ or $x_i = 1$ particle, and the occupation is restricted by a hard, local "density constraint": any occupied site ($x_i = 1$) can have at most l occupied neighbors, where l could range locally from 0 to the total number of its neighbor-sites. In this model, the jamming is defined thermodynamically by rejecting the configurations violating the density constraint. Here, we focus on global density constraints of $l = 0$ (completely excluded neighborhood occupation) and $l = 1$ as the most generic cases. The system can be described by the grand canonical partition function

$$Z(\mu) = \sum_{\textbf{allowed}\ \{x_i\}} \exp\left[\mu \sum_{i=1}^{N} x_i\right], \tag{1}$$

where the sum is over all the allowed configurations $\{x_i\}$. Here, μ is the reduced chemical potential, where we have chosen units such that the temperature is $k_B T = 1/\beta = 1$, and $\sum_{i=1}^{N} x_i$ is the total number of particles in a specific configuration.

From the grand canonical partition function in Eq. (1), we can obtain the thermodynamic observables we intend to measure, such as the Landau free energy density $w(\mu)$, the packing fraction $\rho(\mu)$, and the entropy density $s[\rho(\mu)]$, as defined in the following equations:

$$\begin{aligned} w(\mu) &= -\frac{1}{N}\ln Z, \\ \rho(\mu) &= \frac{1}{N}\left\langle \sum_{i=1}^{N} x_i \right\rangle_{\mu} = \frac{1}{N}\frac{\partial \ln Z}{\partial \mu}, \\ s(\mu) &= \frac{1}{N}\left(1 - \mu\frac{\partial}{\partial \mu}\right)\ln Z. \end{aligned} \tag{2}$$

2.2. Hierarchical networks

In our investigations, the 3 hierarchical networks are the Hanoi networks [29]. They are small-world networks with a hierarchical, recursive structure built on a 1D lattice. There are 4 main reasons of using these hierarchical networks:

1. The recursive nature of the patterns can ultimately provide analytical solution via the renormalization group (RG) [30], which is usually impossible for most fixed-structure networks;
2. Their lattice-like structures share more similarities with regular lattices than mean-field models, which could contribute more insights about real-world systems than mean-field models;
3. These three hierarchical networks have different degrees and geometries from which we may learn the relationship between geometry and jamming;
4. The fixed structures, unlike a random geometry in many mean-field models, can significantly reduce the computational cost by avoiding averages over many random ensembles.