Jamming Percolation and Glass Transitions in Lattice Models

Cristina Toninelli*
Laboratoire Physique Théorique, Ecole Normale Supérieure, 24, rue Lhomond, 75005 Paris, France

Giulio Biroli†
Service de Physique Théorique, CEA/Saclay-Orme des Merisiers, F-91191 Gif-sur-Yvette Cedex, France

Daniel S. Fisher‡
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
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A new class of lattice gas models with trivial interactions but constrained dynamics is introduced. These models are proven to exhibit a dynamical glass transition: above a critical density ρ_c ergodicity is broken due to the appearance of an infinite spanning cluster of jammed particles. The fraction of jammed particles is discontinuous at the transition, while in the unjammed phase dynamical correlation lengths and time scales diverge as $\exp[C(\rho_c - \rho)^{-\mu}]$. Dynamic correlations display two-step relaxation similar to glass formers and jamming systems.

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In the majority of liquids dramatic slowing down occurs upon supercooling. In a rather small temperature window, typically from the melting temperature T_m to about $2T_m/3$, the viscosity increases by 14 orders of magnitude and the relaxation becomes complicated: nonexponential and spatially heterogeneous [1]. Similar features are observed in soft materials, such as colloidal suspensions and more generally in nonthermal "jamming" systems [2]. Despite a great deal of effort, these remarkable phenomena, associated with "glass transitions" are still far from understood. Even the most basic issues remain open: Is the rapid slowing down due to proximity to a phase transition? Is this putative glass transition static or purely dynamic [3]? Experimental results make it clear, however, that if an ideal glass transition does exist it should have some peculiar features: the density autocorrelation function $C(t)$ should exhibit a lengthening plateau that, at the transition, extends out to infinite times. Thus, the Edwards-Anderson order parameter, defined as the infinite time limit of $C(t)$, will be discontinuous at the transition. But this discontinuity should be accompanied by a critical divergence of the relaxation time. And, contrary to usual critical slowing down, the relaxation time should diverge exponentially, as in the Vogel-Fulcher law [1]. Long-range spatial correlations, if they exist at all, must be very subtle. These unusual properties present major theoretical challenges: whether or not there is a true transition there is no "standard" framework to start from. There are promising results for models on Bethe lattices [4] and for some with long-range interactions [5]. But the quest for models with short range interactions and no quenched disorder that are simple enough to be analyzed and can be shown to have a glass transition, namely, a transition with the basic properties discussed above, is still open, in spite of much effort.

In this Letter we introduce the first examples of such models [6,8]. These are kinetically constrained models (KCMs): stochastic lattice gases with no static interactions, except hard core, but constrained dynamics [7]. The elementary moves are particle jumps for conservative models and birth or death moves for nonconservative models. Whether a move can occur depends on the nearby configuration and is nonzero only if some local constraints are satisfied. These kinetic constraints can radically change the dynamical behavior and typically induce glassy phenomenology [7,9,10]. For some KCMs the dynamics becomes so slow at high density or low temperature that they have been conjectured to undergo a true glass transition. The simplest examples are Kob-Andersen models on a square lattice (SKA) [9], where particles can move if and only if they have no more than two nearest neighbors both before and after the move. Although the analogous model on a Bethe lattice [11,12] does have a jamming transition, we have shown previously in [11] that the SKA and a broad class of generalizations on hypercubic lattices cannot have ergodicity breaking transitions: in any finite dimension the relaxation time diverges—in many cases in a super-Arrhenius way—only at the close packing density ($\rho = 1$).

But this is not the only possible behavior. We here introduce a new class of KCMs that do exhibit a jamming transition at a nontrivial critical density, ρ_c on finite dimensional lattices.

For simplicity we focus on one of the simplest: a square lattice model without particle conservation; vacancies can loosely be thought of as "free volume" which need only be conserved on average. At the end, we discuss generalizations to both higher dimensional and conservative models. The stochastic dynamics is as follows: An occupation variable at site x cannot change if x is blocked along either of the diagonal directions, as defined below. Unblocked sites change from occupied to empty and from empty to occupied with rates $(1 - \rho)$ and ρ, respectively. Thus detailed balance is satisfied with the trivial product measure with density ρ. The blocking is determined by the eight fourth-nearest-neighbor sites of x. Denote pairs of these the north-east (NE), north-west (NW), south-east (SE), and south-west (SW) pairs as in [Fig. 1(b)]. Site x is blocked if either at least one of the NE sites and at least one of the SW sites is occupied, or at least one of the SE sites and at least one of the NW sites is occupied. Blocking can thus be along either the NW-SE or the NE-SW diagonals. As the distance to the blocking neighbors resembles a knight's move in chess, we call this the "knights model."

If a site cannot be unblocked even by first emptying with allowed moves an arbitrarily large number of other sites, we call the site frozen. Any finite cluster of particles cannot be frozen: one can always unblock all sites by emptying from the perimeter in [see Fig. 1(c)]. A crucial question is whether an infinite spanning cluster of frozen sites exists in infinite systems. We call this problem jamming percolation; it is akin to bootstrap percolation [13].

We show the following results (which can be proved [14]): (i) with blocked or periodic boundary conditions on $L \times L$ squares, there exist configurations with system-spanning clusters of frozen sites; (ii) on infinite lattices, below a critical density, ρ_c, there are no infinite frozen clusters; while (iii) above ρ_c, there is an infinite cluster of frozen particles that occupies a nonzero fraction, ϕ_∞, of the area; (iv) ρ_c coincides with the critical density for directed site percolation (DP) on a square lattice; (v) ϕ_∞ is discontinuous at ρ_c; (vi) below ρ_c, there is a crossover length $\Xi(\rho)$: squares of size $L \ll \Xi$ are very likely to have a frozen cluster, while for $L \gg \Xi$, the probability of a frozen cluster falls off exponentially; (vii) as ρ increases to ρ_c, Ξ diverges exponentially rapidly, as $\log\Xi \sim (\rho_c - \rho)^{-\mu}$ with $\mu \cong 0.64$ related to DP exponents; (viii) the relaxation time diverges as Ξ or faster. Thus even though the critical density is the same as for DP, the behavior is completely different.

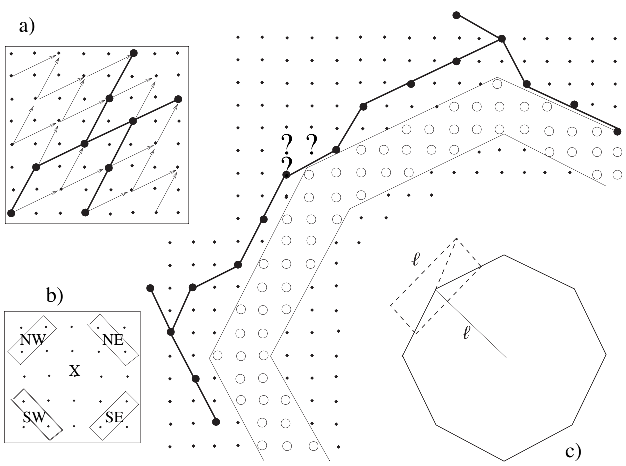

FIG. 1. (a) Sites connected by arrows form one of the graphs on which directed percolation can form frozen clusters: e.g., the set of occupied sites (big dots) shown. (b) Site X and its NE, NW, SW, SE pairs of neighbors. (c) Portion of an empty octagonal annulus. The interior of the annulus, as any finite region surrounded by a double frame of vacancies, can be eaten away. Whether the vacant region can expand is determined by the three key sites indicated by question marks. If one of these belongs to an occupied DP path in the NE direction, which is anchored on two perpendicular DP paths as shown, it blocks the expansion. Inset: the full octagon. A necessary condition for the octagon not to be expandable of one step in the NW direction is that a DP path spans the dotted rectangle.

We first show that both an unfrozen and a frozen phase exist. At sufficiently low densities, the occupied sites do not percolate via connections up to fourth neighbors: the resulting finite clusters can always be unblocked from their perimeters. Thus at low densities, frozen clusters do not occur. In contrast, at high densities, spanning frozen clusters occur. Consider site directed percolation with directed links that connect a site to its two NE (fourth) neighbors as in [Fig. 1(a)]. Infinite directed paths of occupied sites exist for $\rho \geq p_c^{\mathrm{DP}} \cong 0.705$ (the critical threshold for conventional site DP on a square lattice [15]). These clusters of sites are frozen since each has at least one occupied fourth neighbor in both NE and SW directions. Thus, $\rho_c \leq p_c^{\mathrm{DP}}$.

For the above argument it was sufficient to use blocking along just one of the two diagonal directions. But, because of blocking in the perpendicular diagonal direction, typical frozen configurations do not resemble DP clusters: they consist of short DP paths that terminate at each end in a T junction with a DP path in the perpendicular direction. Thus large regions can be frozen even if they are not spanned by DP clusters.

An explicit construction is instructive. Consider a structure built of DP paths of length s intersecting at T junctions as in Fig. 2(a). This structure does not contain any long DP cluster, yet it is frozen. And, crucially, there exists a similar frozen cluster as long as each DP path remains inside a nearby rectangular region of size $s \times s/6$ [see Fig. 2(a)]. Therefore the probability of the system being frozen is bounded from below by the probability that all these rectangles are spanned. This is substantial if the DP spanning probability of each such rectangle is very high.

The crucial needed property follows from the anisotropy of critical DP clusters: a cluster of length s typically has transverse dimensions of order s^ζ with ζ (often called $1/z$), the anisotropy exponent, $\zeta \cong 0.63$ [15]. Therefore an $s \times bs$ rectangle with s in the parallel direction can be cut into slices of width s^ζ such that for each slice the probability of DP spanning paths is substantial for $\rho \geq p_c^{\mathrm{DP}}$. Therefore, even at p_c^{DP}, the probability $r_b(s)$ of not having any DP crossing in a large $s \times bs$ rectangle is $r_b(s) < \mathcal{O}[\exp(-2Cbs^{1-\zeta})]$ (with C a constant).

What happens just below p_c^{DP}? The above argument still holds for rectangles that are of order the DP parallel correlation length, $\xi_\parallel$. This, together with the previously explained construction of a frozen structure, implies that an $L \times L$ square is likely to have a frozen structure built of DP clusters of length $\xi_\parallel$ if $r_{1/6}(\xi_\parallel)L^2/\xi_\parallel^2 \ll 1$. For

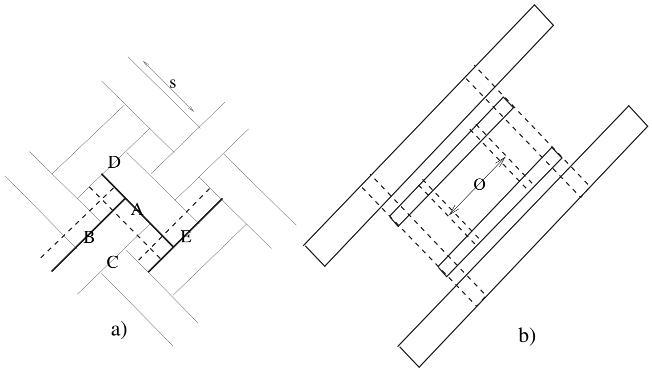

FIG. 2. (a) Frozen structure made of DP paths of length s (represented by straight continuous lines) intersecting at T junctions. The A path anchors one end of the B and C paths, while its ends are anchored by the D and E paths. This anchoring is retained if path A is displaced until the nearby dotted line, even if the B and E paths are similarly displaced no further than their corresponding dotted lines. Thus the structure is frozen if all the rectangles—shown and unshown—formed by the solid and dashed lines are spanned lengthwise by DP paths. (b) Two sequences of intersecting rectangles, $\mathcal{R}_i$, that, when spanned lengthwise by directed paths, make the central site, O, frozen. For clarity, the rectangles in one direction are shown with dashed lines.

$L < \Xi_< \sim \xi_\parallel \exp(C_< \xi_\parallel^{1-\zeta})$—a lower bound on Ξ—squares thus contain frozen clusters with high probability in spite of the rarity of DP clusters with length larger than $\xi_\parallel \ll \Xi$.

We now need to show that below p_c^{DP}, sufficiently large squares are unlikely to contain frozen clusters. Again, this can be done by construction—now of unfrozen regions. Consider an infinite system within which is an octagonal annulus of radius (center to NW) ℓ that is completely empty. Whether or not this empty region can be expanded depends crucially on three key sites in each diagonal corner, say, the NW corner, as shown in Fig. 1(c). If all three key sites are empty or emptyable—i.e., unfrozen—the empty annulus can be expanded along its two adjacent (NNW and WNW) sides. A necessary condition to have a key site frozen is that it belongs to a DP cluster in the NE direction that is anchored at both ends, as in Fig. 1(c). Furthermore, in order for this anchorage to occur, it is necessary that the NE path spans the rectangular dotted region of size $\ell \times b\ell$ (with b a constant) in Fig. 1(c). For $\rho < p_c^{\mathrm{DP}}$ DP clusters with length ℓ much larger than the DP correlation length, $\xi_\parallel$, are exponentially rare and the rectangle spanning probability is $\sim \exp(-\ell/\xi_\parallel)$ [15]. Thus, if $\rho < p_c^{\mathrm{DP}}$, the probability that the annulus can be expanded out to infinity by successive expansions is high for $\ell \gg \xi_\parallel$ [7,11,13]. Since the infinite system contains a nonzero density of these empty regions, which can be expanded to unblock the whole system, we conclude that $\rho_c = p_c^{\mathrm{DP}}$.

Estimating how rare the unblocking regions are near ρ_c yields an upper bound on the crossover length Ξ. Starting with a small empty nucleus the—small—probability δ that it can be expanded out to size $\sim \xi_\parallel$ (and hence readily to infinity) is the product of many small terms. This is dominated by $\ell \sim \xi_\parallel$: from $r(\xi_\parallel)$, we obtain $\delta > \exp(-2C_> \xi_\parallel^{1-\zeta})$. Since in an $L \times L$ square there are $(L/\xi_\parallel)^2$ roughly independent positions for such empty nuclei, some are likely to occur if $\delta L^2/\xi_\parallel^2$ is not small. Thus we find that $\Xi \le \Xi_> \sim \xi_\parallel \exp(C_> \xi_\parallel^{1-\zeta})$. We have found upper and lower bounds for the crossover length, Ξ, of similar form; hence

$$\log \Xi \sim \xi_\parallel^{1-\zeta} \sim (\rho^c - \rho)^{-\mu} \quad \text{with } \mu = (1-\zeta)\nu_\parallel \cong 0.64,$$

with $\nu_\parallel \cong 1.73$ the correlation length exponent for DP [15].

We now discuss another peculiarity of this transition: the nature of the frozen clusters implies that the density, ϕ_∞, of the infinite frozen cluster jumps at ρ_c. To analyze the probability that a site is frozen, consider an occupied site, e.g., the origin, which belongs to a DP cluster that extends to a (small) distance $\ell_0/2$ in both the NE and SW directions: this occurs with some probability p_0. Now focus on two infinite sequences of rectangles $\mathcal{R}_i$ of increasing size $\ell_i \times \ell_i/12$ with $\ell_1 = \ell_0$, $\ell_i = 2\ell_{i-2}$ and intersecting as in (Fig. 2). If each of these rectangles is spanned lengthwise by a DP cluster, the origin is frozen. The probabilities of perpendicular DP paths are positively correlated. Thus $\phi_\infty \ge p_0 \prod_i [1 - r_{1/12}(\ell_i)]^2$. Since $\xi_\parallel$ is infinite at ρ_c, as shown above, $r_b(\ell)$ decays exponentially to zero as $\exp[-Cb\ell^{1-z}]$. Therefore, the infinite product is nonzero, giving a strictly positive bound on $\phi_\infty(\rho_c)$ for any ℓ_0. Thus, in contrast to DP or conventional percolation, the infinite frozen cluster of jamming percolation is "compact"—i.e., with dimension $d = 2$—at the transition.

To supplement our predictions, we have studied $L \times L$ systems numerically. The distribution of the densities, ϕ_L, of the frozen clusters shows two peaks with weak size dependence as found at conventional first order transitions. This is consistent with the predicted discontinuous behavior. The probability that there exists a frozen cluster is substantial for ρ 15% below ρ_c even in our largest systems ($L = 1600$): it is thus hard to study the asymptotic critical behavior (see [16] for an analogous problem in the context of bootstrap percolation). But in a slightly different model one can get closer to the transition [14]: these data are consistent with the predicted $\ln \Xi \sim (\rho_c - \rho)^{-\mu}$ with $\mu \cong 0.64$, but the small range of $\ln L$ available makes the uncertainties in μ large.

Our results on jamming percolation have important implications for the equilibrium dynamics of the knights model. For $\rho < \rho_c$ the fact that infinite frozen clusters do not exist imply that the system is ergodic [proof can be done as in [11] (2.5)] but dynamical correlations, such as the density autocorrelation function, $C(t)$, display two-step temporal relaxation with a long plateau followed eventually by a relaxation (numerical results will be reported elsewhere [14]). The relaxation time diverges exponentially near ρ_c, at least as Ξ^z, with $z \ge 1$: This is reminiscent of the Vogel-Fulcher law found experimentally near glass transitions. Above ρ_c, the plateau stretches to infinite times with the Edwards-Anderson order parameter, $q \equiv \lim_{t\to\infty} C(t)$, discontinuous at the transition. This follows from our results, since q is related to the density of frozen sites.

We have seen that, even though the critical densities are the same, the properties of jamming percolation are strikingly different from the power-law behavior of directed percolation. Most of the physics is controlled by relatively short DP clusters joined together at T junctions. The only role of long DP clusters is to prevent very rare large unfrozen regions from unblocking their surroundings. There is substantial universality in the primary features of the jamming percolation. This extends even to the SKA model, which has frozen configurations composed of double-width occupied bars that terminate in T junctions with similar perpendicular bars, but there is no real transition because very long bars are unlikely. Yet the SKA's behavior as $\rho \nearrow 1$ is similar to the knights model as $\rho \nearrow \rho_c$ with $1/(1-\rho)$ roughly replacing powers of $\xi_{\parallel}$. Surprisingly, if the square lattice of the SKA is replaced by a particular complicated fourfold coordinated lattice, $\rho_c < 1$ and the behavior is similar to the knights model. Thus the local structure matters a lot as in real glasses. Note that cooperative models with a transition, in contrast to those without, display two-step relaxation from the dynamics within blocked regions: this is like beta relaxation in glasses [1].

Models with particle-conserving dynamics behave surprisingly similarly to those without: the nature of the transition (and in some cases the critical density) remain the same because the slowing of the dynamics is dominated by the large clusters of the underlying jamming percolation. Diffusive transport rides on top of this [14,17,18]. In three dimensions, two natural generalizations of our jamming percolation exist: one composed of DP clusters—which should slow down as a double exponential of $(\rho-\rho_c)^{-\bar{\mu}}$—and the other of directed sheetlike structures that will have exponential slowing down as we have found in 2D. The key ingredients are kinetic constraints that enable huge jammed clusters to form out of small objects without these becoming much more common or much larger.

For the future, the connection between our results and the jamming transition found for continuum particle systems [2] needs exploring. With the hope of increased understanding of the rapid liquid to glass crossover observed experimentally, one should also analyze the effects of constraint-violating processes occurring with a very low rate. For both glasses and granular materials, studying the nonequilibrium effects caused by a quench or by driving forces [14] is merited even in the simplest models that exhibit a jamming transition. After the completion of this work a new version of a preprint [8] appeared in which other models with a jamming transition are introduced and studied numerically.

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*Electronic address: cristina@corto.lpt.ens.fr
†Electronic address: biroli@cea.fr
‡Electronic address: fisher@physics.harvard.edu

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