Jamming versus Glass Transitions

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Recent ideas based on the properties of assemblies of frictionless particles in mechanical equilibrium provide a perspective of amorphous systems different from that offered by the traditional approach originating in liquid theory. The relation, if any, between these two points of view, and the relevance of the former to the glass phase, has been difficult to ascertain. In this Letter, we introduce a model for which *both* theories apply strictly: it exhibits on the one hand an ideal glass transition and on the other "jamming" features (fragility, soft modes) virtually identical to that of real systems. This allows us to disentangle the two physical phenomena.

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The traditional way to introduce the glass transition is to start with a liquid of, say, hard particles at low pressures [1] and to consider a slow compression. At a given point, the viscosity increases dramatically, the dynamics becomes sluggish, and the system falls out of equilibrium. Slower compression protocols push the equilibrium regime further and make the transition sharper, and one conceives of a limit of infinitely slow annealing in which one recognizes (perhaps) a true thermodynamic change of state. An argument in favor of a thermodynamic transition was given years ago by Kauzmann, who interpreted it as a consequence of the liquid running out of configurational entropy. Although the possibility of proving the occurrence of such an ideal glass transition for a real system seems remote, there is a family of models (or approximations), for which this picture holds strictly, within the so-called "Random First Order" (RFO) scenario [2,3], a mean-field theory allowing for a complete analytic analysis.

An apparently unrelated set of ideas comes from considering amorphous assemblies of hard, frictionless particles in mechanical equilibrium. In general, such systems can be hypostatic, hyperstatic, or isostatic, depending on whether the set of contacts yields a number of conditions smaller, larger, or precisely equal to the number of degrees of freedom—just like a table with two, four, or three legs touching a floor. A polydisperse system of spheres will be isostatic with probability one [4,5], much in the same way that a four-leg table will only have three touching a rough floor. Because breaking one single contact already destabilizes an isostatic system, one can then argue that such systems are *marginal* [5–7]: they have large responses and a spectrum of vibrations with finite density of very low frequency "soft" modes. One is then in the presence of a "Jammed" configuration that is *critical*, with diverging lengths, nontrivial exponents, etc. [7].

A natural question is whether this critical "Jamming" phenomenon is in some way a finite-dimensional (beyond mean-field) manifestation of the glass transition [7] or, in other words, whether the diverging length associated with the soft modes of an amorphous packing is a manifestation of the order underlying the glass transition in finite dimensions. In this Letter, we propose to answer such questions by constructing a family of models having both theories written side-by-side with a "J-point" isostatic equilibrium with a spectrum of soft modes virtually identical to that of systems of hard spheres and that are by construction mean-field models with a "Random First Order" behavior [2].

The model.—Consider the usual hard-sphere model where N nonoverlapping spheres live in a cube of dimension d, with periodic boundary conditions. Following [8], we now obtain a mean-field version of this model: the idea is to let each sphere interact *only* with a set of z other ones, all the rest being *transparent* to it. The set of particles that interact with a given sphere is chosen once and for all. If $z = N - 1$ for each particle, we recover the original problem, but we shall instead work with z finite. The model is completely defined by a quenched regular random graph (see Fig. 1) with nodes labeled by the particle number and bonds that denote interaction.

This model presents a number of advantages: first, since interactions are set through a random treelike graph—or Bethe-Lattice—it is by construction a mean-field glass model that can be studied exactly with the cavity method [9] which is an extension of the well-known work of Bethe

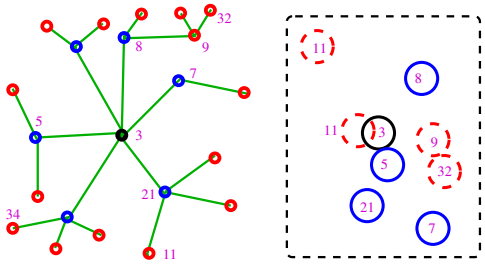

FIG. 1 (color online). The model: Particles evolve in a d-dimensional space (right), but are only able to "see" a preestablished subset of the rest. Which particle interacts with which is encoded in the quenched graph (left).

and Peierls on trees. Secondly, our model can be seen as a constraint satisfaction problem (CSP) defined on a random graph, where the constraint on each node is that the position within the cube of the sphere on that node be such that it does not overlap with any of the other z interacting spheres (that are linked on the graph). This model bridges the gap between the field of random discrete CSP such as the coloring problem [10,11] and disordered hard-sphere packings [8]. Our approach thus provides an original way to attack packing problems within mean-field theory. In this Letter, we take the first steps in this direction by studying numerically the model in $d = 2$ and restrict ourselves to the question of determining the differences between the Jamming and the glass transition.

Glassy behavior.—The low pressure or low density "liquid" state can be discussed easily within the cavity method. It just corresponds to considering the model on a tree in the usual Bethe-Peierls way and ignoring long-range correlations. A straightforward computation shows that the entropy of the liquid state on a random graph of connectivity z is $S_{\text{liquid}} = z \log(1 - \pi D^2)/2$, where D is the diameter of the spheres. Using a pressure $-P$ conjugated to the sphere "volume" [8] $V = D^2$, this yields the equation of state for the liquid $P = (z\pi/2)(1 - \pi D^2)^{-1}$. However, this equation is inconsistent at large pressures: indeed for $P = \infty$, it yields a limiting value independent of the connectivity z, which is unphysical, and where each sphere is in contact with all its neighbors; this requires not only the number of contacts to be much larger than the isostatic value, but also the presence of a 2 coloring of the graph [8] and thus violates rigorous results in graph theory: this proves that a phase transition must occur at a finite pressure. It is indeed possible to prove within the cavity method [12] that the liquid phase is unstable towards a glass phase at some finite pressure, and ongoing analytic work in this direction shows that the system has a glass phase [12] of the Random First Order kind for z sufficiently large, as usual with frustrated models on such structures [9–14]. This is illustrated on Fig. 2 in a system with a slight polydispersity [15] (in which case one should compute the averaged $S_{\text{liquid}} = \overline{z \log[1 - \pi(R_1 + R_2)^2]/2}$ over the distribution of radii $P(R)$): a clear signal of glass transition with its compression rate dependence is observed.

Jamming.—We now turn to jammed configurations obtained following the procedure of [7]: starting from small particles, we "inflate" them infinitesimally and adjust their positions to eliminate any (infinitesimal) overlap, until a jammed state is obtained. At very large pressure, particles are found to be either locally blocked by their neighbors (in which case they have at least three contacts), or are "rattlers" that can be displaced without moving the others [16]. The locally blocked particles have a subset that cannot be displaced even with collective rearrangements–except global translations. For our polydisperse system, this subset turns out not to have redundant contacts, and hence constitutes an *isostatic core* (see left panel of Fig. 3). We

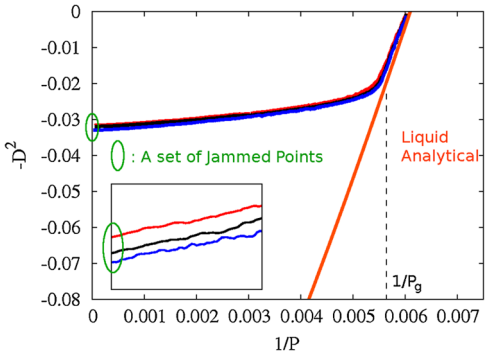

FIG. 2 (color online). Volume versus inverse pressure for a system of $N = 4000$ particles with $z = 100$ and 9% polydispersity. The choice of variables for the axes is to stress the analogy with the more usual energy-temperature annealing plots. The annealing curves follow the liquid analytical solution at low pressures, but break away at the glass transition pressure P_g, which is clearly visible.

find many states with slightly different densities, all of which are isostatic and have indiscernible properties.

The jammed configurations have a spectrum of modes that is strikingly similar to those found in the finite-dimensional system [6,17,18]. In Fig. 3, we show the vibration modes obtained by considering a soft potential and a small superposition of particles that follows from inflating the particles slightly beyond the jammed configuration, as in [17]. A second, perhaps more satisfactory way to study the vibrations of a hard-sphere ensemble is to consider the very high pressure dynamics of hard particles around a jammed state, and computing the displacement correlations $\langle A_{ij} \rangle$ with $A_{ij} = x_i(t)x_j(t) - \langle x_i \rangle \langle x_j \rangle$ where $\langle \bullet \rangle$ denotes average over a time that is long yet insufficient for escaping the vicinity of the jammed configuration. The displacements fall into two classes: the many-particle vibrations that scale as P^{-1}, and the rattlers that do not, because the cages are roughly independent of the pressure. The role of the frequencies in a potential is played by the eigenvalues of $P^{-1}A^{-1/2}$. The spectrum of these eigenvalues is shown in Fig. 3: at infinite pressure, there is a proliferation of soft modes, but as the volume fraction φ is lowered, and the pressure becomes finite, the system interacts, due to collisions and rattling, with more particles than what is imposed by the isostaticity condition, and the isostaticity-related soft modes start disappearing. Again, this is in perfect agreement with the usual systems [6].

Jamming versus glass.—Having discussed the isostatic packings with the standard J-point phenomenology [6,7,17,19], as well as the mean-field glassy nature of our model, we can now distinguish the "Jammed" and the "Glass" features as follows (Fig. 4). There is a liquid equilibrium line, which terminates at the equilibrium glass transition pressure P_K. Below P_K, the Gibbs measure is dominated by a few of the deepest glassy states [3]. There are also metastable ones (indicated by the horizontal lines), which are stable (only) within the mean-field picture. As in

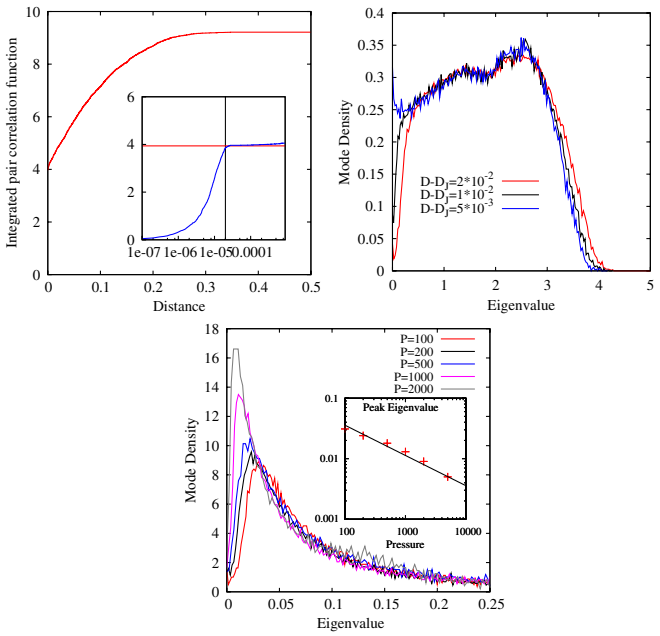

FIG. 3 (color online). *Left:* Integrated pair correlation function restricted to the collectively jammed core. The average number of neighbors is four, as one expects from an isostatic system in two dimensions. The inset shows a zoom in the small distance region, the horizontal line is the isostaticity condition, while the vertical line is the gradient descent step used to jam the system. *Right:* Vibration modes with small overlaps (here noted $D - D_J$, difference between actual diameter of the particles and diameter particles should have to be at jamming). The resulting spectrum is almost identical to that of a particle system (cf. Fig. 1 of Ref. [17]). *Bottom:* Hard particles: vibration modes of the isostatic core, rescaled with the pressure. In the inset, gap in the spectrum versus pressure scales as $P^{-1/2}$. The curves are virtually identical to those of a finite-dimensional system, as obtained by Brito and Wyart [6]. These curves correspond to a configuration with $N = 1000$ and $z = 13$.

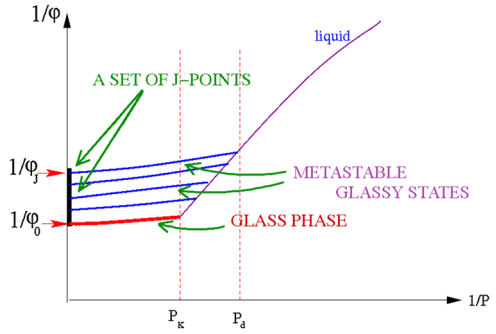

FIG. 4 (color online). A sketch of the density(φ)-pressure (P) plane in RFO models (see, e.g., [2,8,14]). Dynamic and static transition pressures are P_d and P_K. The glass phase and the "jamming line" ($P = \infty$, $\varphi_0 < \varphi < \varphi_J$) are clearly distinct. The isostaticity-related quantity χ_{EA} is finite within a state if P is finite (except perhaps for a small effect of acoustic modes in $d = 2$). In particular, it is finite within the ideal glass state, while it is infinite on the jamming line. Everywhere in the trapezoidal region delimited by the equilibrium line $0 < P < P_d$, the threshold level, and the jamming line the activation time diverges (at times exponential in N), and with it the four-point function χ_4. In finite dimensions, χ_4 would only diverge strictly at the jamming line (at finite times) and close to the glass line (at times comparable to the activation time).

any system with a dynamic transition, any compression process ending at infinite pressure leads the system into a metastable state. The "jamming line" $\{P = \infty, \varphi_0 < \varphi < \varphi_J\}$ is the set of such (out of equilibrium) blocked configurations. The slower the compression, the denser the target state is, and one needs an infinitely slow process to reach φ_0. In particular, we denote the J point φ_J as the result of the fastest compression starting from a random configuration [7], which we expect to be different from the deepest level φ_0—just as a quench to zero temperature does not terminate in the ground state of any complex system. In a finite-dimensional system, only two lines in the phase diagram are stable, apart from the liquid state: the jamming line (at infinite pressure) and the equilibrium glass phase—if it exists at all. Their only common point is $(\varphi_0, P = \infty)$.

A measure of the criticality of a state is the staggered displacement $\langle \sum_i \vec{\xi}_i \vec{x}_i \rangle / h$ produced by random forces $\vec{f}_i = h\vec{\xi}_i$, with $\vec{\xi}_i$ random unit vectors. This corresponds, in the spin-glass literature, to the quantity $(1 - q_{EA})/T$. It is proportional to $\chi_{EA} = P^2 \sum_i [\langle x_i^2(t) \rangle - \langle x_i \rangle^2] = P^2 \mathrm{Tr}(\langle A \rangle)$. If ω are the eigenvalues of $P^{-1}A^{-1/2}$ and $Q(\omega)$ the density of modes, then $\chi_{EA} \sim \int d\omega Q(\omega)/\omega^2$. Because of the soft modes [6], this quantity diverges on approaching the jamming line when normalized this way, see inset of Fig. 3. A perhaps more standard measure is the function $\chi_4(t, t') = \sum_{ij} A_{ij}(t) A_{ij}(t')$. It has a maximum which diverges as the system approaches *either* the jamming points (because of the soft modes) or the equilibrium glass line, because of the divergence of activation time (i.e., the time needed to overcome a free-energy barrier).

Thinking in terms of *landscape* [8], the picture that emerges is one of a system with many glassy states, separated by high and wide free-energy barriers, as usual in RFO models. Fragility and soft modes are a property of the (infinite pressure) jammed configurations *within* each of these states, but states are not marginal in the coarse-grained view obtained as soon as temperature is nonzero and the pressure finite (at least in all but the more superficial "threshold" levels). This separation between large valleys with critical bottom is consistent with the fact that systems of frictionless particles at zero temperature are at the same time fragile (even slight shear stresses make them creep some amount) while still capable of resisting a shear stress proportional to the pressure without flowing continuously (they have *internal friction* [20].)

Jamming a crystal.—To unambiguously demonstrate that a large stable state with an internal "fragile" structure is possible in finite dimensions, and that the Jamming point is of different nature than that of the glass transition, let us finally consider an ordinary fcc crystal of spherical particles with very small (.003%) polydispersity. The crystal-

line order is hardly affected (see Fig. 5), and polydispersity becomes irrelevant at finite pressures P. However, at $P = \infty$, the system is isostatic and has a spectrum of soft modes even richer than that of an amorphous packing. In an amorphous solid, each one of the many equilibrium glass states plays a similar role to the one of the crystal state above, their very high pressure jamming properties being juxtaposed with the underlying long-range glass order, already established at finite pressure.

Conclusion.—We confront two different visions of amorphous systems: a glassy solid state with order characterized by a permanent, amorphous modulation of density—not unlike a crystal or a quasicrystal—and a jamming situation brought about by chains of force associated with actual contact between hard particles. These two phenomena may coexist but are distinct. The fact that a mean-field model reproduces both the glass transition and J-point criticality in a separate way suggests that we abandon the idea that the former is some kind of finite-dimensional realization of the latter. The mean-field picture just above the glass transition pressure is one of large basins separated by high barriers, without an excess of truly zero frequency modes except perhaps at the least deep states. The isostaticity-related marginality of the jammed configurations appears only at very large pressures, deep within a basin. This local criticality combined with absence of criticality "in the large" is attested by the paradoxical fact that amorphous matter is fragile to small stresses but may still sustain extensive stresses without flowing, a fact that can be understood easily in the example of the polydisperse crystal. Perhaps the most evident manifestation of the different nature of the jamming ($P = \infty$) and the glass lines is the fact that, although lengths such as associated to four-point function χ_4 diverge in both, the growth is astronomically slower approaching the glass line from the liquid phase, than approaching the jamming line [21].

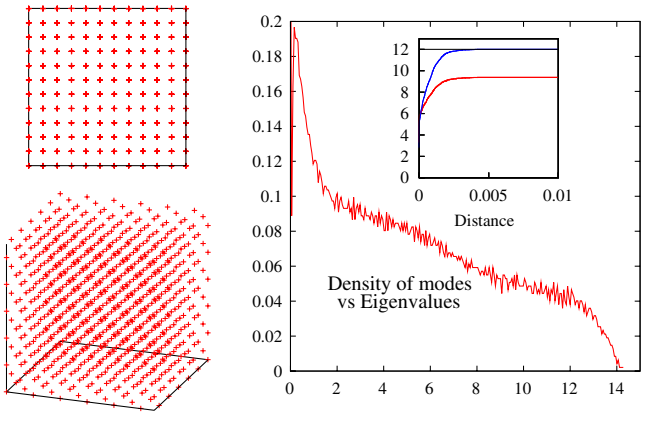

FIG. 5 (color online). *Left:* A jammed configuration in the polydisperse crystal ($N = 864$). The distortion of the crystalline order due to polydispersity is extremely weak. *Right:* Spectrum of normal modes of the polydisperse crystal, obtained in the same way as Fig. 3, central panel. There are many soft modes (to be compared with Fig. 3). In inset: integrated pair correlation function, including and excluding rattlers: the number of contacts of nonrattlers is ≈ 6.

In conclusion, we have introduced a set of new models that can be studied analytically and numerically and that provide nontrivial connections between different fields.

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