Glasses, Jamming and Fractal Energy Landscapes

Fractal free energy landscapes in structural glasses
P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani and F. Zamponi, Nat. Com. **5** 3725 (2014).

Recommended with a commentary by Ariel Amir, Harvard University

Glasses are all around us – literally – yet our understanding of the glass phase is still far from complete [1,2]. Upon cooling, structural glasses are characterized empirically by a viscosity that shoots up at a finite temperature for the so-called "fragile" glasses. Close to the transition, the relaxation timescales diverge. This is illustrated by the "pitch-drop" experiment of the University of Queensland [3]: pitch has been slowly flowing out of a container since 1930, with a drop falling every decade or so - the ninth of which dropped last April. Despite its sluggish flow, the pitch shatters when hit by a hammer, much like a solid. Close to the glass transition the relaxations are not only slow but also non-exponential. In fact, non-exponential relaxations characterize a broad class of glassy materials, including spin-glasses (magnetic materials where the interactions of spins can be either positive or negative [4]) and electron glasses (where an electronic system stays out-of-equilibrium for many days [5]). The connections between all these systems are only now beginning to be elucidated.

The statics and dynamics of glasses are often considered in terms of a large number of metastable states with energies close to the true ground state, which would then lead to slow relaxations and memory effects as the system explores this energy landscape. This has led to the development of the theory of random-first-order-transition of structural glasses, in a set of pioneering works by Kirkpatrick, Thirumalai and Wolynes [6]. It turns out, however, that even simplified models of glasses can show dramatically more complex behavior: an important model is the Sherrington-Kirpatrick (SK) model [7], introduced in 1975, in which spins are coupled via a random (positive or negative) interaction, and every spin is connected to all other spins. This mean-field limit of spin-glasses was shown to be much richer than originally anticipated: in a seminal work by Parisi [8] it was shown that the naïve picture of a glass described above does not hold for the SK model, and that so-called replica symmetry breaking leads to a fascinating energy landscape known as "ultrametricity", where basins are ordered hierarchically. Remarkably, the ideas and theories discussed above have led to amazing breakthroughs in solving hard computational problems [9].

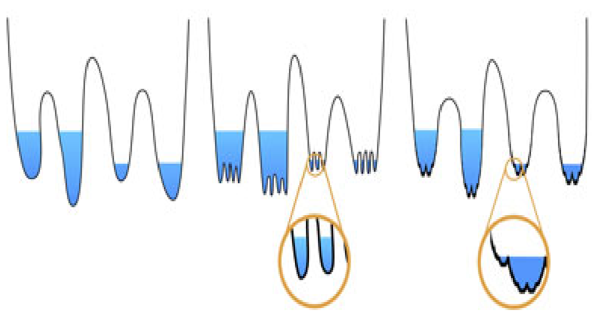

Figure 1: A rugged energy landscape (credit: Duke U.) The study by Charbonneau et al. shows that even in one of the simplest model systems for glasses, the structure of the energy landscape is incredibly complex, with basins within basins. As one approaches the jamming transition where the pressure diverges, the landscape becomes fractal.

Charbonneau et al. study a hard sphere system as a model system for glasses. While the interaction between particles in a structural glass is often modeled using a smoothly varying potential (such as the Leonard-Jones potential, where $(r) \propto r^{-12} - r^{-6}$) , using a hard-spheres model system implies that there is no energy scale associated with the potential. Hence, the potential energy contribution to the free energy is constant; Nevertheless, the contribution of the entropy to the free energy, combined with the constraints that the spheres cannot overlap, leads to a complex energy landscape in terms of the packing fraction and the pressure (see Figure 2). This landscape appears to have similar phenomenology to other glasses. In light of the insights obtained from the SK model for the complexity of glasses, the strategy of the work is to obtain analytical results for system dimension $d \to \infty$, and show that the predictions are relevant also for low dimensional systems by comparing them with numerics. Using this method the authors come up with a number of elegant results which agree extremely well with their numerical simulations. One of their key novel findings is that deep enough into the glass phase (upon reaching another phase transition discovered by Gardner [10]), the landscape is organized into a hierarchy of basins, with power-law scaling governing various observables. They are able to connect the properties of this fractal energy landscape with the physics of the jamming transition: imagine putting a large number of spheres in a box (with slightly different diameters, to avoid crystallization), and compressing them adiabatically. At a certain point, the spheres jam and the pressure one would have to exert will diverge – this is the jamming transition, which has been intensively studied over the last decade [11]. An elegant prediction of this work is that as one approaches the jamming transition, the size of the smallest basin-within-basin in the aforementioned complex energy landscape scales as p^{-k}, with $k \approx 1.4$. The authors numerically simulate athermal hard spheres in low dimensions, finding excellent agreement between their simulations and this analytical result. It should be noted that obtaining analytic results for the physics of jamming is extremely challenging, and the majority of work in this field has been numerical.

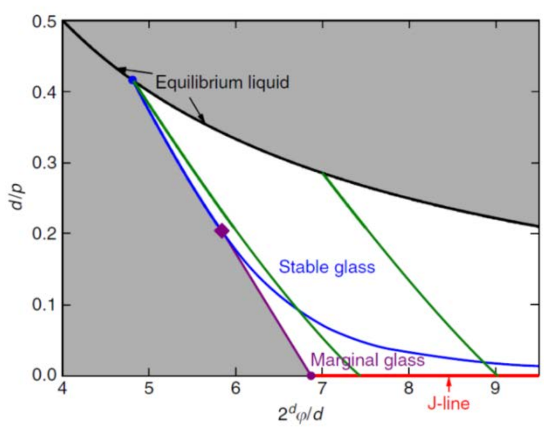

Figure 2: Phase diagram of hard spheres at high dimension *d*, as a function of the packing fraction φ and the pressure *p*. As one goes deep into the glass phase, the glass becomes “marginally stable”, and inequalities arising from demanding mechanical stability become equalities. Finally, the system “jams” at the jamming transition, where the pressure diverges.

From previous work it is known that as one approaches the jamming transition, the network of forces between neighboring particles has fascinating properties – "force chains" develop near jamming [10] and recently it was shown that the distribution of forces between neighboring spheres P(f) decays as a power law for small forces, i.e., $p(f) \sim f^{\theta}$ [12]. This phenomenon is reminiscent (and mathematically related) to similar "soft gaps" known to occur in the distribution of local magnetic fields in the SK model and in the distribution of on-site energies in electron glasses. Using their approach, Charbonneau et al. are able to capture these recent observations, as well as compute the Fourier transform of the force distribution, $F(\lambda)$, again finding remarkable agreement with numerics in low dimensions. They also corroborate a scaling relation between different exponents associated with this force network, which has been derived in Ref. [12] from considerations of mechanical stability, thus providing a useful check of their results. While our understanding of structural glasses (as well other glasses) is far from complete, this work shows that studying simplified models for glasses can provide deep insights into their physics, as well as testable and quantitative predictions. In particular, the method should be applicable also for the study of soft spheres, and to the physics of aging in glasses. According to the authors, it could also be expanded to yield a first-principles understanding of the quantum physics of two-level-systems in low temperature glasses [13], which for decades has eluded a fundamental understanding.

References

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