Jamming and glass transition in mean-field theories and beyond

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The behavior of glasses at low temperatures is one of the most active fields of research in condensed matter physics both from a theoretical and an experimental point of view. It is well known that in the so-called glassy systems upon decreasing the temperature the relaxation time increases of several orders of magnitude, from picoseconds to days. However in some specific cases such a divergence is associated to a real thermodynamic transition, which is not so evident in structural glasses leading to heated debates on the correctness of specific laws to describe fragile and strong glasses [1, 2, 3]. Beyond these controversies, there are some points globally accepted in the community of glasses: by looking at a glassy system on a time scale much smaller than the relaxation time, a collective phenomenon occurs consisting in a freezing of "particles" inside cages due to their neighbors. If one of them tends to escape, this process involves a cooperative movement of a few particles whose number increases when decreasing the temperature.

In the past years different methods have been proposed to study these phenomena, like the Mode-Coupling Theory (MCT) [4, 5], which explains quite well how the phase space can split into many smaller regions below a critical temperature, defined as *dynamical temperature* or *mode-coupling temperature*. This is a phenomenological theory but using replicas one can show that the MCT temperature corresponds to an ergodicity breaking temperature. Indeed from an analytical point of view such a phenomenon of fragmentation in disconnected regions is related to a *one step replica symmetry breaking* (1RSB). In mean-field description, the temperature reduction process implies different steps: i) a replica symmetric phase, where the space is totally connected (*i.e.* the liquid phase); ii) a one step replica symmetry broken phase; iii) finally, a continuously broken phase, where disconnected subbasins arise but each of these regions is organized according to a hierarchical ultrametric structure [7, 8, 10]. The project will be mainly focused on the last more interesting phase hunched forwards a cautious application of the full-RSB equations [7].

Much attention has been devoted to the fast increase of the correlation time associated to cages formation and in this direction a fundamental understanding has been achieved in the study of hard spheres: the potential is simply described by a hard-core constraint where the only interaction is an excluded volume effect. In this context it has been proven that in the infinite pressure limit these systems develop a *jamming transition* which corresponds to a vanishing size of the cages, both under equilibrium and off-equilibrium conditions, and to a rigid arrangement of particles which cannot freely move and flow.

Jamming is thus a novel theoretical paradigm for constructing a low-energy theory of glasses, which properly incorporates the complexity and evolution of the phase space [11]. Because of the inherent marginality of these states, low-energy excitations exhibit strongly non-linear and even divergent responses. A full theory explaining these properties and how idealized models apply to real materials in a broad range of experimental conditions is needed. We propose to develop a complete theory of jammed states in both infinite and finite dimensions, unifying real-space scaling pictures to exact analytical approaches. Questions to be asked concern in particular the exact computation of the upper critical dimension (below which great deviations from the mean-field theory predictions occur), a detailed analysis of harmonic oscillations for soft and hard sphere models in the zero temperature limit (a good starting point could be the study of the spectral density of the Hessian matrix of the potential, which has its roots in the Random Matrix Theory) and a deeper understanding of the presence of an excess of zero modes far to be in agreement with the Debye predictions for solids, but supposed to have a connection with the emergence of the so-called *Boson peak* [12]. A remarkable issue is also the analysis of the specific heat and the thermal conductivity which deviate from the just mentioned Debye law: they turn out to be affected by a strange dependence on the temperature. An efficient approach could request the two-level systems theory for quantum glasses starting from the assumption of considering the whole object as a collection of non-interacting two-state systems [13].

In order to go into details, we are currently studying a simple model of jamming, known as *perceptron* and defined by the following Hamiltonian as a function of the gap h_μ:

$$H[x] = \frac{1}{2}\sum_{\mu=1}^{M} h_\mu^2 \theta(-h_\mu) \ , \qquad\qquad h_\mu = \xi^\mu \cdot x - \sigma \tag{1}$$

In the soft version we consider continuous variables x on the unitary $N-$dimensional sphere and the vectors ξ^μ are i.i.d with zero mean and unit variance. The sum is extended up to $M = \alpha N$, where N represents the total number of variables in the system and M the number of constraints, both of them to be sent to infinity keeping fixed the ratio α.

This model can be exactly solved from an analytical point of view and presents two different regimes [14, 15]: a first convex optimization regime where σ is positive, characterized by non-critical features and a non-convex regime, for negative values of σ, where isostaticity (i.e. the number of contacts strictly equal to the number of the degrees of freedom) and criticality become fundamental on the jamming line. It is a well established model in machine learning and neural networks [16, 17] exploited for decades as a linear signal classifier. By analyzing the distribution of forces and gaps, it has been demonstrated [14] that this model can be described by the same critical exponents computed in high dimensions for hard spheres. In a certain sense there should exist an universality class to which non-convex constrained satisfaction problems belong: by varying the number or the type of satisfied/violated clauses one could jump between two different phases, from a satisfiable region (SAT phase, with at least one configuration in agreement with all the requested constraints) to an unsatisfiable one (UNSAT phase, where all the constraints cannot be verified simultaneously). This SAT/UNSAT transition corresponds from a statistical mechanics point of view to an equilibrium jamming transition associated to a fast shrinking to zero of the space volume allowed to the constrained variables. The most interesting features of such a model arise when we consider the replica symmetry broken case: critical behaviors emerge at the jamming point, like power-law singularities in the pair correlation function and in the probability distribution of forces and gaps.

By applying the Plefka method [19] (or Georges-Yedidia expansion, in a more recent formulation), we can find out the TAP equations [20] and consequently a more manageable expression for the Hessian matrix. The UNSAT phase, characterized by a non vanishing fraction of negative gaps, has been already studied obtaining for the Hessian the typical form of a random matrix from a modified Wishart ensemble [15]. The most challenging aspect to focus on will consist in studying the SAT phase where the gaps are positive and all the elements of the Hessian are equal to zero. Since the constraints are not in contact and all the second derivatives are zero - beyond this apparent stumbling block - it is necessary to elaborate a more sophisticated procedure to obtain worthy physical results. The next step should lead to a proper reconstruction of the density of states close to the jamming line. In the whole glassy phase the lower edge of the spectrum is identically zero as a consequence of the marginality, however, we would like to have a global control of the spectrum and to understand the typical behavior of the replicon mode, which usually plays the dominant role in the correlation functions [8, 9].

Moreover, in terms of anharmonicity and elastic properties, much effort has been devoted to study theoretically and numerically the microscopic cause of the rigidity of hard sphere glasses near the maximum packing. A heuristic argument presented in [21] suggests to describe the hard sphere interaction at the random close packing through an effective logarithmic potential just by exploiting isostaticity and classical mechanics considerations. We would like to formulate a rigorous mathematical evidence of the fact that at the jamming point the effective potential describing the perceptron has the same logarithmic behavior as the hard sphere model.

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