Jamming and glass transition in mean-field theories and beyond

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1 Introduction

In the last years the study of glassy materials at low temperature has attracted significant interest, both from a theoretical and an experimental point of view [1, 2, 3, 4]. Much attention has concentrated on systems formed by an athermal assembly [1] of repulsive particles with finite-range interactions, where one can observe - upon increasing density - a *jamming transition*, corresponding to a rigid arrangement of particles which cannot freely move and flow. This kind of transition properly consists in a passage from a loose, floppy state to a mechanically rigid state. However, it remains a challenging field to tackle since this phenomenon appears inside the glassy phase at $T = 0$ and its critical parameters seem to depend on the experimental or numerical protocol.

One might wonder why the points J (where such a transition locates, associated with a divergent pressure) are important to real glass forming liquids, where there are not only finite-range repulsive interactions but also longer ranged attractions. In the case of long-range repulsions, it is not possible to find any point J, the threshold where the energy changes from zero to a finite value. For long-ranged attractions, the jamming line should not even exist, lying inside the vapor-liquid coexistence curve [5, 6], at least for binary Lennard-Jones mixtures. This is a bit difficult issue to deal with and many research groups, studying experimentally or numerically attractive colloidal particles, have proposed an unifying description based on a highly universal jamming phase diagram. This would lead to a non trivial connection between glass transition, gelation and aggregation [7].

In this context the jamming transition is a fundamental theoretical paradigm for constructing a low-energy theory of glasses, which properly incorporates the complexity and evolution of the phase space. First principle theories describe quite well glassy states but not at low enough temperatures and high pressures. Studying a glass former far below the glass transition is tricky, because of the emergence of a new critical transition associated with a fractal landscape (the *Gardner transition*) [9, 10, 11], an activated dynamics and the presence of strong corrections to take into account. Moreover the inherent marginal mechanical stability characterizing jammed states generates strongly non-linear and sometimes divergent responses. A full theory further exploring and explaining these low energy excitations is still *in fieri*. Indeed, compared to an ordinary solid with long range crystalline order, the spectrum of low-energy excitations in jammed materials exhibits several anomalies. Typical vibrations in ordered materials are plane wave sound modes, giving rise to the Debye scaling of the vibrational density of states $D(\omega) \sim \omega^{d-1}$, in d dimensions [12]. A striking feature characterizing amorphous solids is the violation of the expected

[1] Working at zero temperature is appropriate for granular systems and foams, where the energy of even small rearrangements of configurations is orders of magnitude greater than the thermal energy at room temperature. This picture however fails for molecular glasses, where the temperature is a control parameter.

Debye law, showing a plateau above a cut-off frequency ω^{*2}. A related question concerns the properties of these normal modes, which are highly heterogeneous and resonant near ω^* and become quasi-localized upon decreasing the frequency. This aspect has also non-trivial implications in the thermal conductivity and the specific heat from several points of view.

Given these premises, it is now crucial to achieve a better theoretical understanding at all levels, in order to efficiently analyze the jamming transition and to bridge the gap between different scenarios. The replica method and a detailed study of the dynamics have been already used, then the missing piece is a rigorous derivation of the Thouless-Anderson-Palmer (TAP) equations [16].

2 Ongoing research

2.1 The negative perceptron and the soft spheres

In this thesis we derive the aforementioned equations, using the Plefka expansion [17] (or Georges-Yedidia expansion, in a more recent formulation) in two examples of disordered systems, the negative perceptron [21] and the soft spheres. Instead of performing a diagrammatic approach to expand the partition function, we rephrase the problem in terms of an equivalent power expansion of the Gibbs potential in a fictive interaction parameter. The two models cited above are defined by the following Hamiltonian as a function of the so-called *gap* among particles, which takes a different form depending on the case:

$$\mathcal{H}[x] = \frac{1}{2}\sum_{\mu=1}^{M} h_\mu^2 \theta(-h_\mu) \tag{1}$$

In the perceptron the gap reads: $h_\mu(x) = \xi^\mu \cdot x - \sigma$, while in the soft sphere case it is replaced by $h_{\alpha\beta}(x) = |x_\alpha - x_\beta| - \sigma$, where α, β label two identical spherical particles at a certain distance and σ is the diameter of the particle. In the soft version we consider continuous variables x on the unitary $N-$dimensional sphere, satisfying the constraint $\sum_{i=1}^N x_i^2 = N$, while the random vectors ξ^μ are i.i.d variables 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. In machine learning the attention is generally focused on positive values of σ [14], but in terms of jamming also negative values are legitimate and more interesting.

In the perceptron, we are actually replacing the interaction between spheres with a random background and considering that a single particle cannot overlap with spherical obstacles placed in random positions. In the second case (soft spheres) one can approach the problem from two different sides: i) considering both the radius of the smaller spheres and that of the background sphere large enough to be sent to infinite at the end; ii) assuming the radius of single spheres enormously smaller than that of the bigger one. Anyway, there are no new and inexplicable phenomena that can induce to change formalism. This is properly due to the aforementioned strong repulsive force between particles.

Analyzing the distribution of forces and gaps, it has been shown [21] that the perceptron is described by the same critical exponents of high dimensional hard spheres. 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 becomes sharp in the thermodynamic limit, since the probability of a random problem to be satisfiable becomes zero or one when N and M go to infinity at fixed ratio α. It corresponds in a statistical mechanics approach to an equilibrium jamming transition associated to a fast shrinking to zero of the space volume allowed to the constrained variables.

[2] This cut-off frequency corresponds to the emergence of the so-called Boson peak.

Random constraint satisfaction problems have been widely studied in the last years in the case of discrete variables: one of the most known example is the random K-SAT problem [18] where a solution has been recently founded for large values of K. Here the situation is different, depending on the continuous nature of the variables which adds a new dimension to the problem.

The perceptron model can be exactly solved from an analytical point of view and presents two different regimes [21, 22]: 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. In the region of non-convex optimization, ergodicity is broken

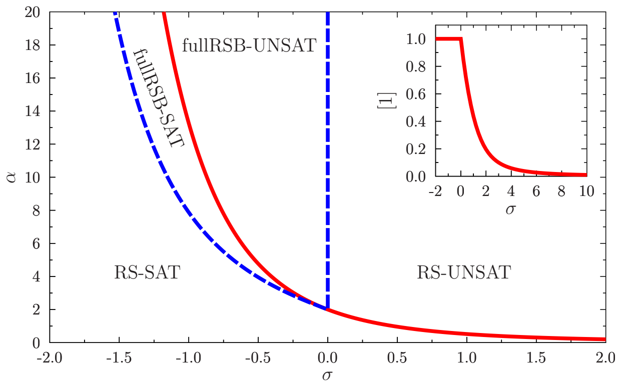

Figure 1: Phase diagram of the perceptron. The dashed blue line signals the RSB region, for $\sigma < 0$ and $\alpha > \alpha_c(\sigma)$. The full red line separates the SAT from the UNSAT phase. The plot is taken from [22].

at low temperature and large α. The direct consequence is that the RS solution becomes unstable and the structure of the overlap matrix q_{ab} must be parametrized by a function $q(x)$ defined in the interval $x \in [0, 1]$ encoding the values of the overlaps that populate different metastable states of the system [19]. This *full replica symmetry breaking* (fullRSB) ansatz implies that at $T = 0$ there are many quasi-degenerate minima in the Hamiltonian. In general the fullRSB equations can be only solved numerically, but good predictions of the typical scaling around the jamming transition can be obtained analytically.

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 [22]. This is due to an unavoidable randomness induced in disordered systems by the positions of the particles.

$$M_{ij} = \frac{1}{N} \frac{\partial^2 H_\zeta}{\partial x_i \partial x_j} = \frac{1}{N} \sum_{\mu=1}^{M} \xi_i^\mu \xi_j^\mu \theta(-h_\mu) - \zeta \delta_{ij} \tag{2}$$

In theory one should consider the correlations between the random part and the theta function in the Hessian. However to the leading order these correlations can be neglected leading to a covariance matrix where the entries can be considered independent and Gaussian distributed, simply multiplied by a *quality factor* that counts the effective number of non vanishing contributions:

$$M_{ij} \sim \frac{1}{N} \sum_{\mu=1}^{N[1]} \xi_i^\mu \xi_j^\mu - \zeta \delta_{ij} = [1] W_{ij} - \zeta \delta_{ij} \ . \tag{3}$$

Hence, the next challenging topic to focus on consists in studying in detail the SAT phase, where the gaps are positive and all the elements of the Hessian are trivially 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 TAP formalism is a very powerful method which allows us to approach the jamming line, in particular from the SAT phase.

The partition function is given by:

$$Z = \int d\mathbf{x} e^{-\beta H(\mathbf{x})} \; , \tag{4}$$

where the Hamiltonian of our system has the expression reported in Eq.(1). In such a way we can define an effective Hamiltonian, in terms of the space variables x_i, the gaps h_μ and their conjugated variables $\hat{h}_\mu$:

$$\beta\mathcal{H}_{\text{eff}}[x, h, \hat{h}] = \sum_{\mu=1}^{M} \left[\frac{\beta}{2} h_\mu^2 \theta(-h_\mu) + i\eta \hat{h}_\mu (h_\mu - h_\mu(x)) \right] \tag{5}$$

We apply a Plefka-like expansion with respect to the quantity $\hat{h}_\mu h_\mu(x)$, introducing a fictive interaction parameter η, which will be set to one at the end of calculations. Useful compact notations to construct our framework are reported in the following, representing respectively the Edwards-Anderson parameter (a.k.a. the *self-overlap*) and the first two momenta of the average variable $\hat{h}_\mu$, conjugated to h_μ:

$$q = \frac{1}{N} \sum_i m_i^2 \; , \quad r = \frac{1}{\alpha N} \sum_{\mu=1}^{M} g_\mu^2 \; , \quad \tilde{r} = \frac{1}{\alpha N} \sum_{\mu=1}^{M} \langle \hat{h}_\mu^2 \rangle \tag{6}$$

where we have adopted the notation: $m_i = \langle x_i \rangle$, $g_\mu = \langle \hat{h}_\mu \rangle$. The variable g_μ plays the role of a generalized force. The corresponding Gibbs potential takes the following form, where the first terms enforce the average value of the magnetization and the average value of $\hat{h}_\mu$ by means of Lagrange multipliers:

$$G(m_i, g_\mu) = \sum_i m_i u_i + \sum_\mu i g_\mu v_\mu - \log \sum_{x, h_\mu, \hat{h}_\mu} e^{S_\eta(x_i, h_\mu, \hat{h}_\mu)} \tag{7}$$

The sum over $x, \hat{h}_\mu, h_\mu$ has to be intended as an integral over the spherical degrees of freedom x_i and over $h_\mu \hat{h}_\mu$. The generic TAP expression of the Gibbs potential reads:

$$G(m_i, g_\mu) = \sum_i f(m_i) + \sum_\mu \Phi(g_\mu) + \left. \frac{\partial G}{\partial \eta} \right|_{\eta=1} \eta + \frac{1}{2} \left. \frac{\partial^2 G}{\partial \eta^2} \right|_{\eta=1} \eta^2 + \mathcal{O}(\eta^3) \; . \tag{8}$$

where the first piece can be easily derived from a saddle-point condition, expected to be proportional to $log(1-q)$ as in an usual spherical p-spin model, while the second one depends only on g_μ and its related Lagrange multipliers. We are entitled to neglect higher order terms except for the first two ones: this argument appears clearer taking into account the strict equivalence between our approach and a $1/d$ diagrammatic expansion, where further corrections become irrelevant in the thermodynamic limit. The first-order derivative with respect to η reads:

$$H = i \sum_{i,\mu} \frac{\xi_i^\mu m_i g_\mu}{\sqrt{N}} \tag{9}$$

while the second derivative can be regarded as an *Onsager reaction term* in the TAP formalism.

As anticipated above, our method can be directly applied to soft sphere models, where the *gap* $h_\mu \to h_{\alpha\beta}$ becomes a dot product between the given positions of two identical spherical particles:

$$h_{\alpha\beta} = \frac{x_\alpha \cdot x_\beta}{\sqrt{N}} \tag{10}$$

with the usual spherical constraint on $x_{\alpha,\beta}$. The effective Hamiltonian now reads:

$$H = i \sum_{\langle \alpha, \beta \rangle} \frac{\hat{h}_{\alpha\beta} x_\alpha \cdot x_\beta}{\sqrt{N}} \tag{11}$$

Anyway the expression for the generalized free energy is very similar to the previous case. We only expect a different scaling in αN. Moreover, if third-order terms in the expansion provide a subleading contribution with respect to the first two momenta, we shall be entitled to replace our framework with an equivalent disorder model where the displacement $h_{\alpha\beta}$ can be written in terms of a random matrix, such as $\sum_{ij} \xi_{ij}^{\alpha\beta} x_i^\alpha x_j^\beta$. This means that we are considering our model as a fully connected disorder system (analogous to a Mari-Kurchan model [27]), with an infinite coordination number.

2.2 Effective thermodynamic potential near random close packing density

A really interesting issue to highlight in our framework consists is the emergence of a logarithmic interaction, if analyzing the Gibbs potential in a proper scaling regime. A recent argument [23] proposed by Brito and Wyart based on this idea considers a hard sphere glass with elastic interactions among particles. As in the jamming limit the integration in the displacements can be exactly mapped in an integration in the gaps, they can compute the single gap isobaric partition function. If the set of distances between particles in contact can be assumed to be formed by independent degrees of freedom, the partition function can be rewritten as a product of terms each of them corresponding to an individual contact, which implies that $f_{ij} = \langle h_{ij} \rangle^{-1} \beta^{-1}$.

In our work we would like to go beyond a qualitative analysis and to point out the general nature of such a prediction. We have recently proven that the perceptron is characterized by the same behavior in the small-gap regime. This is a pivotal outcome with respect to the common idea of a harmonic potential, which only holds in the other regime, where the generalized forces have a characteristic scaling proportional to the average gap. The key point is that such a result has a range of applicability beyond the microscopic details of the system and the specific form of the potential energy.

2.3 Average distribution of eigenvalues in the SAT phase

Our current objective is to numerically solve the TAP equations through a parallel or a random sequential algorithm. Fixed points of the TAP equations are stationary points of the corresponding TAP free energy.

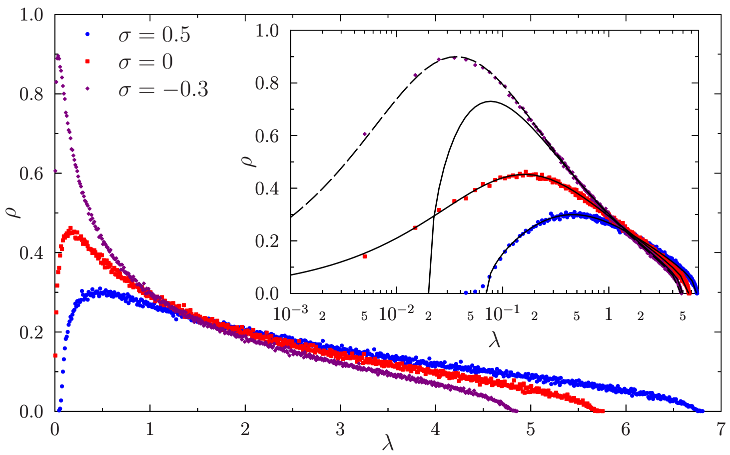

Figure 2: Spectrum of the Hessian in the UNSAT region for $N = 1600$, $\alpha = 4$ and $\sigma = 0.5, 0, -0.3$, in linear (main panel) and semilog (inset) scales. The Marchenko-pastur law with RS parameters (full lines) perfectly reproduces the data for $\sigma \geq 0$, while deviations are observed for $\sigma < 0$. The plot is taken from [22].

In such a way, TAP equations do not include any time indices and were mostly iterated in the simplest form of having time $t-1$ on all magnetizations on the right hand side, and t on the left hand side. This implies several problems to converge even when other methods, such as belief propagation (BP), work well and replica symmetry is not broken [28]. The reason behind this non-convergence lies in wrong time indices and when done correctly, convergence is restored, as nicely as BP. A recent explanation of this phenomenon is proposed in [29] and also in [30], where the authors re-derive these results as a large degree limit of BP.

Once the convergence is assured in our equations, we shall study in detail the statistics of the thermodynamic variables and reconstruct the spectrum in the SAT phase. The characteristic behavior of the spectral density for the complementary UNSAT phase is reported in Fig.(2). It is known that in the fullRSB UNSAT phase the spectrum is $\rho(\lambda) \sim \frac{\sqrt{\lambda}}{\lambda+\zeta}$ for small λ, while at jamming it has a different behavior $\rho(\lambda) \sim \frac{1}{\sqrt{\lambda}}$ with a much larger density of soft modes. The reason behind this great interest is that low energy excitations in glassy systems have important connections with thermodynamic and transport properties.

3 Perspectives and future work

- Concerning the spectral properties of these models, it is well-known that 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 at criticality [26, 25]. The marginal stability and the vanishing behavior of the replicon mode are both natural consequences of a continuous replica symmetry breaking in mean-field-like glasses. These zero modes look like Goldstone modes in systems with a broken continuous symmetry: indeed these excitations are due to the presence of many metastable glassy states which are really close to the ground state and connected to it via nearly flat directions in the energy landscape.

- Once the questions about the SAT phase will have been clarified, it will be interesting to highlight the connection between the TAP formalism and the replica method, reproducing all these results with replicas.

- Another remarkable issue is the analysis of the specific heat and the thermal conductivity, which deviate from the Debye law for solids, strongly affected by quantum effects already at temperatures of order of ten degrees Kelvin. In glassy systems the specific heat displays a linear behavior in temperature in contrast with the expected cubic behavior, which is not so simple to explore due to the presence of strong off-equilibrium phenomena. A possible method to better analyze these features could be to reproduce a continuum quantum model of perceptron. We should exploit our knowledge of the relations between mean field models and real three dimensional world to extract predictions for some specific glassy materials.

- Finally, a part of my thesis project should be carried out in collaboration with Tommaso Rizzo, mainly focused on the dynamical field theory and the glass transition topics.

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