JAMMING AND GLASS TRANSITION IN MEAN-FIELD THEORIES AND BEYOND

Ada Altieri

Supervisors: Prof. Giorgio Parisi, Prof. Silvio Franz

Dipartimento di Fisica, "Sapienza" Università di Roma
&
Laboratoire de Physique Théorique et Modèles Statistiques, Université Paris-Sud

February 4, 2016

SAPIENZA
UNIVERSITÀ DI ROMA

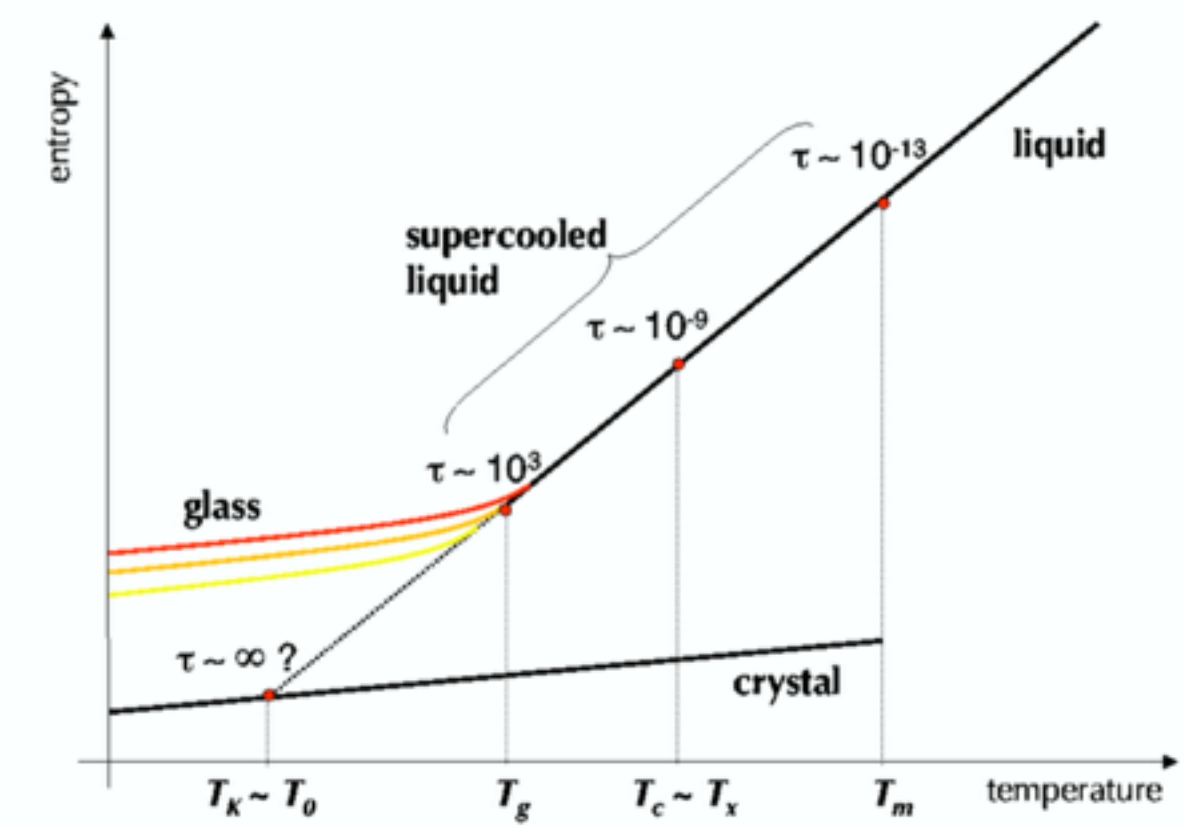
UNIVERSITÉ PARIS SUD
université PARIS-SACLAY

OUTLINE

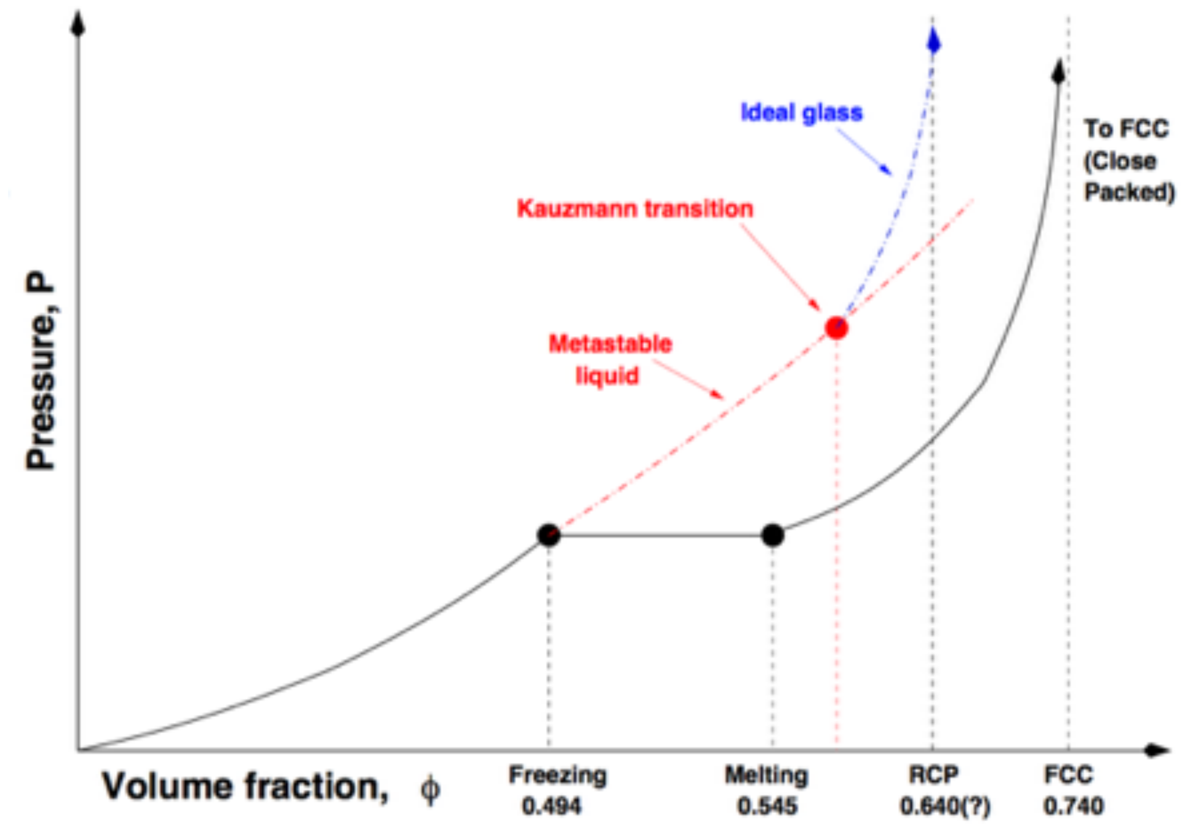
- **Introduction to glassy systems**
- **Jamming transition**
- **Perceptron and hard sphere models**
- **Recent results**
- **Conclusions and perspectives**

Glassy systems

Glasses are disordered materials that lack the periodicity of crystals but behave mechanically like solids. The most common way of making a glass is by cooling a viscous liquid fast enough to avoid crystallization.



Standard glassy plot for a soft potential (Lennard-Jones)

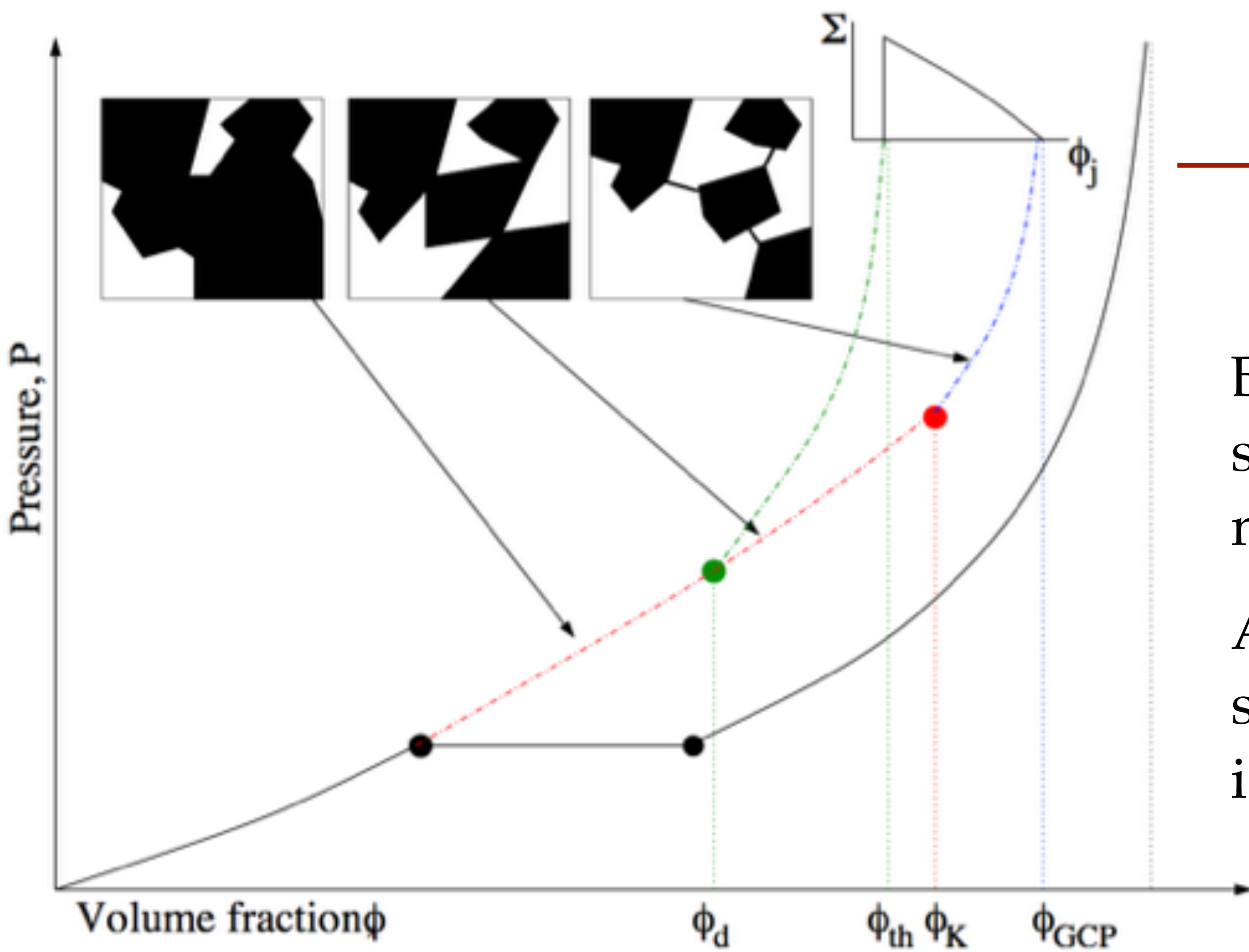


Mean-field phase diagram of hard-spheres in 3D

- The pressure diverges at a point where the system cannot be further compressed → **Random Close Packing density**

- Let us assume the existence of a ***Kauzmann transition*** (a.k.a. *ideal glass transition*), signaled by a jump in compressibility →
  - predicted by mean-field models
  - dynamically, an ergodicity breaking occurs in the MCT scenario

Mean field picture



full black line: equilibrium phase diagram

Below ϕ_d : metastable liquid made by a single state. Above, it is a superposition of many glassy states.

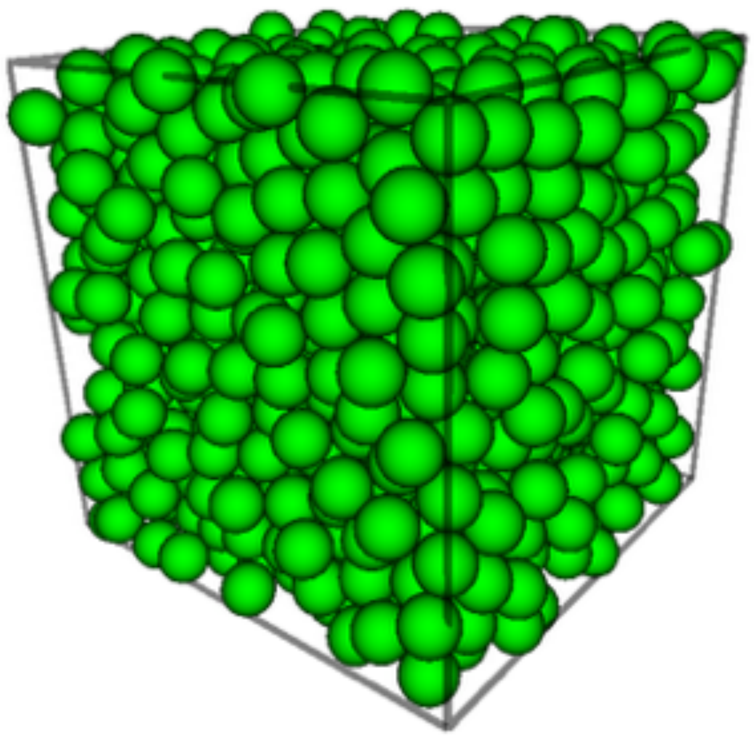
At ϕ_K : the system reaches the most dense states. If further compressed enters the ideal glass state.

<u>In the inset</u>:

the complexity (i.e. the logarithm of the number of glassy states) as a function of the jamming density.

References:
G. Biroli, M. Mézard, Phys. Rev. Lett. **88**(2), 025501 (2001)
J.P. Bouchaud, G. Biroli, J. Chem. Phys. **121**, 7347 (2004)

The jamming transition

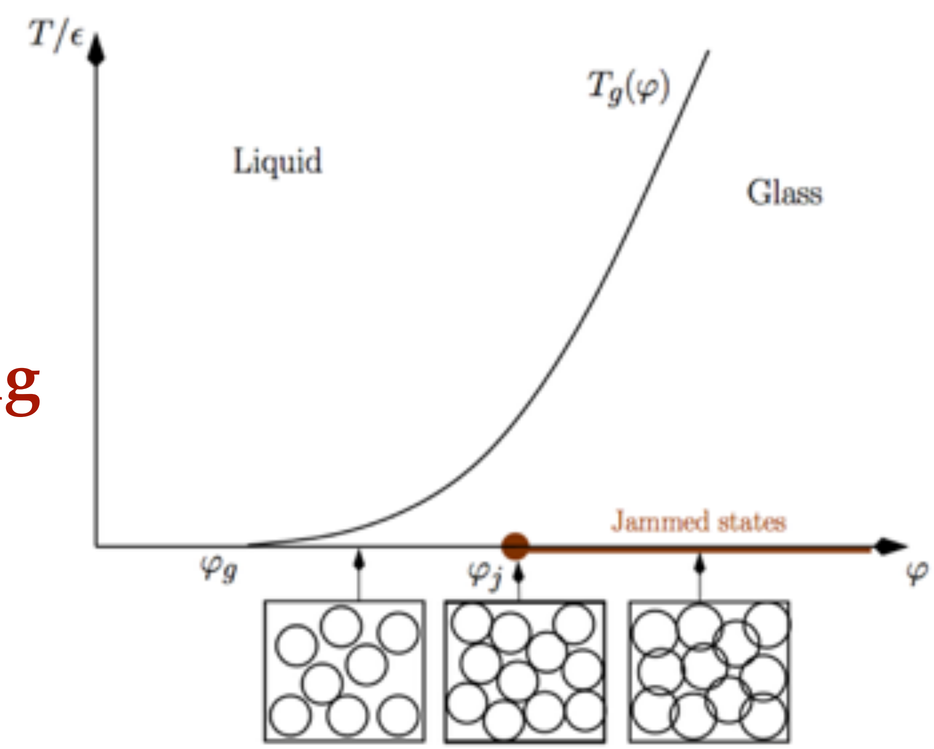


This transition occurs in a huge class of materials such as granular matter, emulsion droplets, powders and colloidal suspensions.

The jamming point is reached when - under equilibrium or off-equilibrium conditions - the size of cages where the particles are confined shrinks to zero, making the system mechanically rigid.

- **This phenomenon is quite difficult to analyse since the jamming transition is inside the glassy phase**

- **The jamming temperature and the jamming packing fraction could depend on the numerical/ experimental protocol**



Further interdisciplinary applications $\Bigg\{$
- number theory
- optimization problems
- biophysics

Jamming versus Glass Transitions

- Important similarities, at least at rheological level.
- In both cases solidity emerges close to a “critical” volume fraction.

glass transition

the system goes from the liquid phase to an “entropically” rigid solid.
More exactly, from a fluid (high T, low density) to a glass (low T, large density).

jamming transition

transition from an “entropic“ rigidity to a mechanical rigidity.
It appears upon compressing at T=0 inside the glass.

Similar macroscopic curves

but they occur over well-separated time and stress scales

↓

qualitatively different microscopic dynamics.

The perceptron

The Hamiltonian is defined by a quadratic confining potential associated with a constraint on the *gaps:*

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

$$h_\mu \equiv \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\xi_i^\mu x_i - k > 0 \qquad \forall \mu = 1, \ldots, M$$

positive:
convex optimization regime

↓

the space of allowed configurations is the intersection of convex domains

negative:
non-convex, critical optimization regime

↓

space divided in disconnected smaller domains

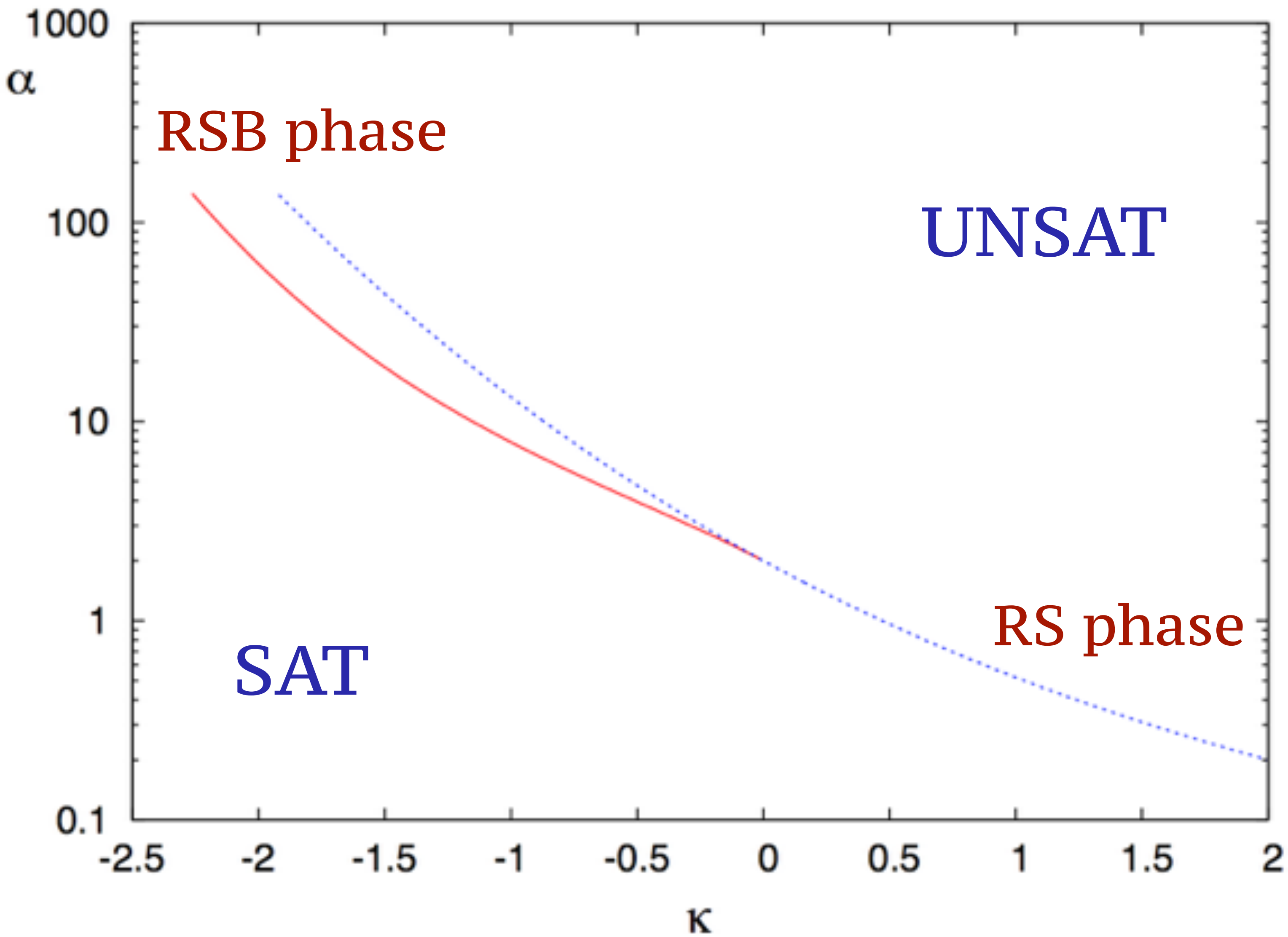
Packing fraction maximization in hard sphere problems ↔ Maximization of k once fixed the ratio M/N.

References:

S. Franz, G. Parisi, *The simplest model of jamming*, arXiv:1501.03397 (2015)

E. Gardner, B. Derrida, *Optimal storage properties of neural network models*, J. Phys. A: Math. Gen. **21** (1988).

The phase diagram



The de Almeida-Thouless line (red) of instability of the RS solution in the SK model plotted together with the jamming line (blue).

Especially the case with a negative bias appears quite interesting:

- replica symmetry is broken ;
- criticality emerges at the jamming point with associated power law singularities.

Future aims: studying the SAT phase and bridging the gap between the scaling properties at criticality and the computation of associated soft modes.

Spectrum of low energy excitations

Elastic anomalies with respect to the Debye law are associated with the Boson peak.

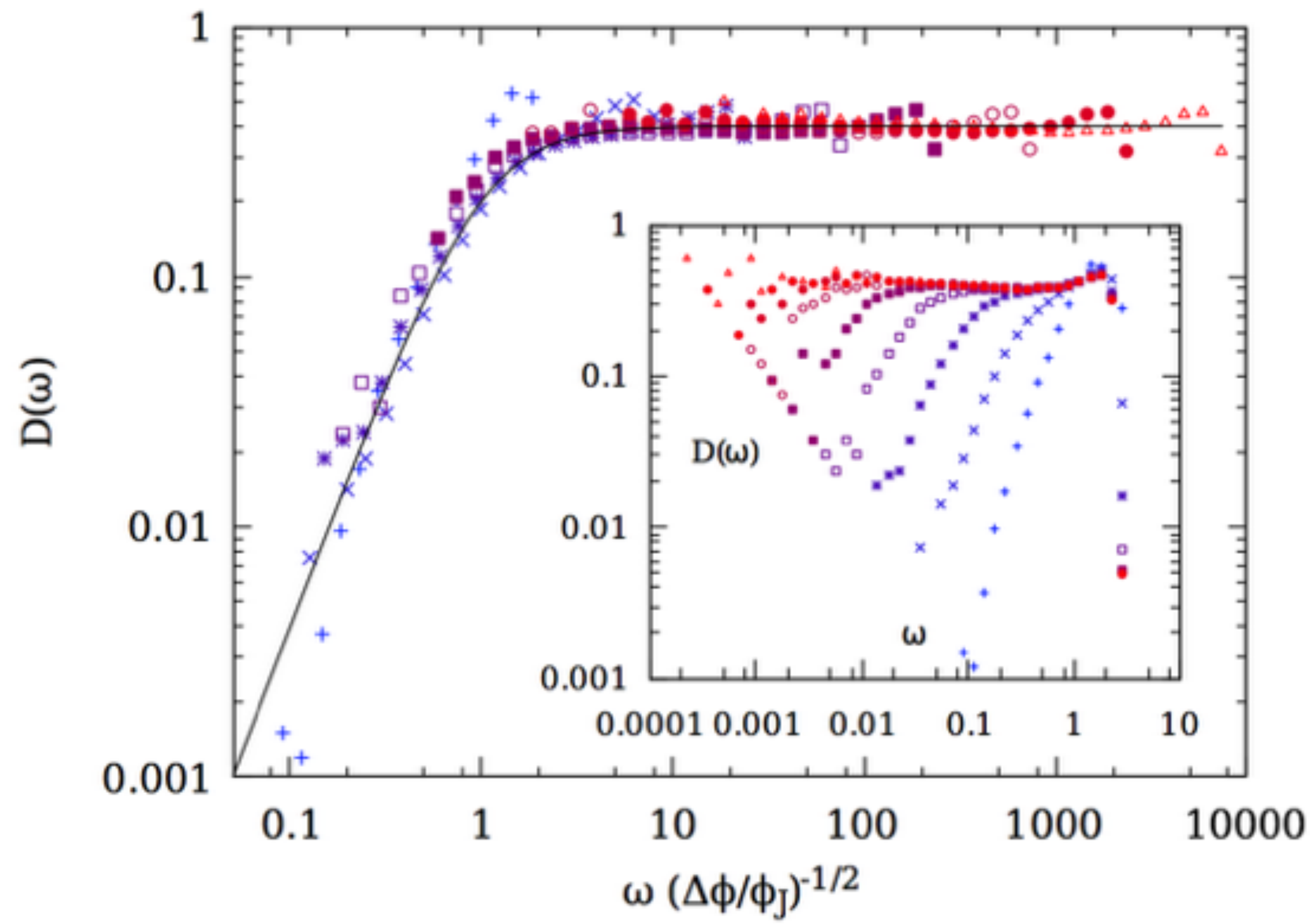
$$D(\omega) = \rho(\lambda)\frac{d\lambda}{d\omega} \quad \Rightarrow \quad D(\omega) = \omega^{d-1}$$ ▶ crystals

$$\boxed{D(\omega) \sim const.}$$ ▶ jammed solids

- closeness to the jamming point
- marginal mechanical stability

This implies a power law behavior in the distribution of forces at small values: $P(f) \sim f^{\theta}$

A similar scaling also holds for the pseudo-gaps: $g(h) \sim h^{-\gamma}$



P. Charbonneau, E. I. Corwin, G. Parisi, A. Poncet, F. Zamponi, *Universal non-Debye scaling in the density of states of amorphous solid,* arXiv 1512.09100v1 (2015)

Analytical computation of the TAP equations

Let's consider a prototype of disorder system: the SK model.

$$\mathcal{H}_{\rm int} = -\frac{1}{2}\sum_{i\neq j} J_{ij} S_i S_j$$

infinitely long ranged

$$\mathcal{H}(\eta) = \eta\mathcal{H}_{\rm int} - \sum_i h_i^{\rm ext} S_i$$

The Gibbs potential reads: $\boxed{-G(\eta,\{m_i\}) = \ln \mathrm{Tr} e^{-\mathcal{H}(\eta)} - \sum_i h_i^{\rm ext} m_i}$

We can define a power expansion in terms of the fictive interaction strength η:

$$G(\eta,\{m_i\}) = G(0,\{m_i\}) + \left.\frac{\partial G}{\partial \eta}\right|_{\eta=0}\eta + \left.\frac{\partial^2 G}{\partial \eta^2}\right|_{\eta=0}\eta^2 + \mathcal{O}(\eta^3)$$

Gibbs potential of non-interacting spins

For $\eta = 1$, this is exactly the TAP expression if higher-order terms are irrelevant.

Formally equivalent to perform a $1/N$ <u>diagrammatic expansion</u> and sum up all relevant diagrams in the thermodynamic limit.

Results: TAP equations for the perceptron

Useful definitions to construct our framework:

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

average effective Hamiltonian

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

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

$$= \sum_i f(m_i) + \sum_\mu \Phi(g_\mu) - i\sum_{i,\mu}\frac{\xi_i^\mu m_i g_\mu}{\sqrt{N}} + \frac{\alpha N}{2}(\tilde{r} - r)(1-q)$$

reaction term

T. Plefka, *Convergence condition of the TAP equation for the infinite-ranged Ising spin glass model,* J. Phys. A.: Math. Gen **15** (1982)

In our recent computation the Hessian of the potential reads:

$$M_{ij} \equiv \frac{\partial^2 G}{\partial m_i \partial m_j} = \delta_{ij}\left[\frac{1}{1-q} - \alpha(\tilde{r} - r)\right] + \frac{2 m_i m_j}{N(1-q)^2} + \sum_\mu \frac{\xi_i^\mu \xi_j^\mu}{N} \frac{1}{\Phi''(g_\mu) - (1-q)}$$

<u>What we have seen:</u>

- The coefficient multiplying the Kronecker delta vanishes at the jamming point
- The second term has a form of a projector: it gives only an isolated eigenvalue apart from the continuous band
- The last term (with an appropriate normalization) turns out to be correctly a theta-function far from the criticality

$$\boxed{M_{ij} = \frac{1}{N} \sum_\mu \xi_i^\mu \xi_j^\mu \theta(-h_\mu) - \mu \delta_{ij}}$$

A possible approach to study the spectrum: **Random Matrix theory**

Why? $\dashrightarrow$ $$M_{ij} = \frac{1}{N}\sum_{\mu} \xi_i^\mu \xi_j^\mu \theta(-h_\mu) - \mu\delta_{ij}$$

The Hessian matrix of a disordered system is a random matrix

<u>In the UNSAT phase:</u>

In principle, the random part and the theta-function could be correlated.

To the leading order in large N these correlations can be neglected.

$$M_{ij} = [1]W_{ij} - \mu\delta_{ij}$$

Wishart matrix

Hence the eigenvalues belong to the Marchenko-Pastur distribution:

$$\rho(\lambda) = \begin{cases} (1-[1])\delta(\lambda+\mu)+\nu(\lambda) & \text{if } \ [1]<1 \\ \nu(\lambda) & \text{if } \ [1]>1 \end{cases}$$

$$\nu(\lambda) = \frac{1}{2\pi}\frac{\sqrt{(\lambda-\lambda_-)(\lambda_+-\lambda)}}{\lambda+\mu}$$

$$\lambda_\pm = (\sqrt{[1]}\pm 1)^2 - \mu$$

Generalization to hard sphere models

This approach can be formally extended to hard spheres, where the constraint is:

$$\theta(h_{\alpha\beta}(x) - \sigma) \ , \qquad h_{\alpha\beta}(x) = (x_\alpha - x_\beta)^2$$

a hard core constraint, which prevents overlaps between two different spherical particles.

The "effective Hamiltonian" in the Plefka-like expansion reads:

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

The Gibbs potential is quite similar to the previous case.

The difference lies in the dimensional scaling.

How exactly taking the infinite limit for M, N… deserves much attention.

Results in hard sphere models

Only the first two terms in the expansion are relevant.
Hence there is a formal equivalence between this framework and a Mari-Kurchan model in the fully connected limit.

$$H(\{\mathbf{x}\},\{\mathbf{A}\}) = \sum_{\langle i,j \rangle} V(x_i - x_j - \mathbf{A}_{ij}) \qquad \mathbf{A}_{ij} = \mathbf{A}_{ji}$$

quenched random variables with a certain probability distribution

As a consequence, we can define for our system a disordered equivalent model:

$$h^{\alpha\beta} = \sum_{ij} \xi_{ij}^{\alpha\beta} x_i^{\alpha} x_j^{\beta}$$

i.i.d random variables with well-defined variance

Characteristic scalings and effective potential

We can distinguish three possible regimes both in the perceptron and in the hard spheres:

- CONTACT REGIME ⟶ the average gap proportional to the contact force
- MATCHING REGION ⟶ nontrivial analytical solution
- ENTROPIC REGIME ⟶ the average gap inversely proportional to the force

In the first case, one correctly recovers the original harmonic potential.

The most interesting properties come out from the third regime (for small gaps).

Effective potential

Much debate has concentred around the microscopic cause of the rigidity in hard sphere glasses at RCP*.

Exploiting **isostaticity** and classical **mechanics considerations** on contact forces, we have recently obtained a strong evidence of the fact the thermodynamic potential for **the perceptron** displays a logarithmic correction, which becomes dominant at the jamming point.

$$\boxed{\mathcal{G}(g_\mu) \sim -\frac{1}{\beta}\sum_{\mu=1}^{M} \log(1/g_\mu) \sim -\frac{1}{\beta}\sum_{\mu=1}^{M} \log(\langle \delta h_\mu \rangle)}$$

Note: it looks like a quite general feature, independent from the microscopic details and the form of the potential energy (quadratic or not).

*C. Brito, M. Wyart, *On the rigidity of a hard sphere glass near random close packing*, Europhys. Lett . **76** (2006)

Perspectives

- Numerical resolution of the TAP equations in perceptron and hard spheres
  - to reconstruct the spectral density and the main properties in the SAT phase;
- Deeper understanding of the behavior of the correlation functions, especially related to the appearance of soft modes (*i.e.* the *replicon* mode)
  - to establish a connection between our results and the replica formalism;
- Computation of loop corrections to mean-field models
  - to determine the upper and lower critical dimensions .

Conferences and Schools:

- Workshop on "Regulation and Inference in Biological Networks", February 2015, Bardonecchia
- "XIV Workshop on Complex Systems", March 2015, Fai della Paganella
  Poster contribution
- Beg Rohu Summer School 2015 : "Statistical Physics, Biology, Inference and Networks", Saint-Pierre Quiberon (France)
- Workshop LPTMS, September 2015, Domaine du Val-Planguenoual
  Talk contribution
- Conference "The meaning of it all", December 2015, Paris

Publications:

A.Altieri, G. Parisi and T. Rizzo, *Composite operators in cubic field theories cubic and link-overlap fluctuations in spin-glass models*,
http://arxiv.org/pdf/1510.08774 (2015)
Phys. Rev. B **93**, 024422

Thank you for your attention!