Mean-Field Theory:
from glassy systems to inference problems

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School on "Information, Noise and Physics of Life"

Serbia, September 2022

Moving through statistical physics of disordered systems

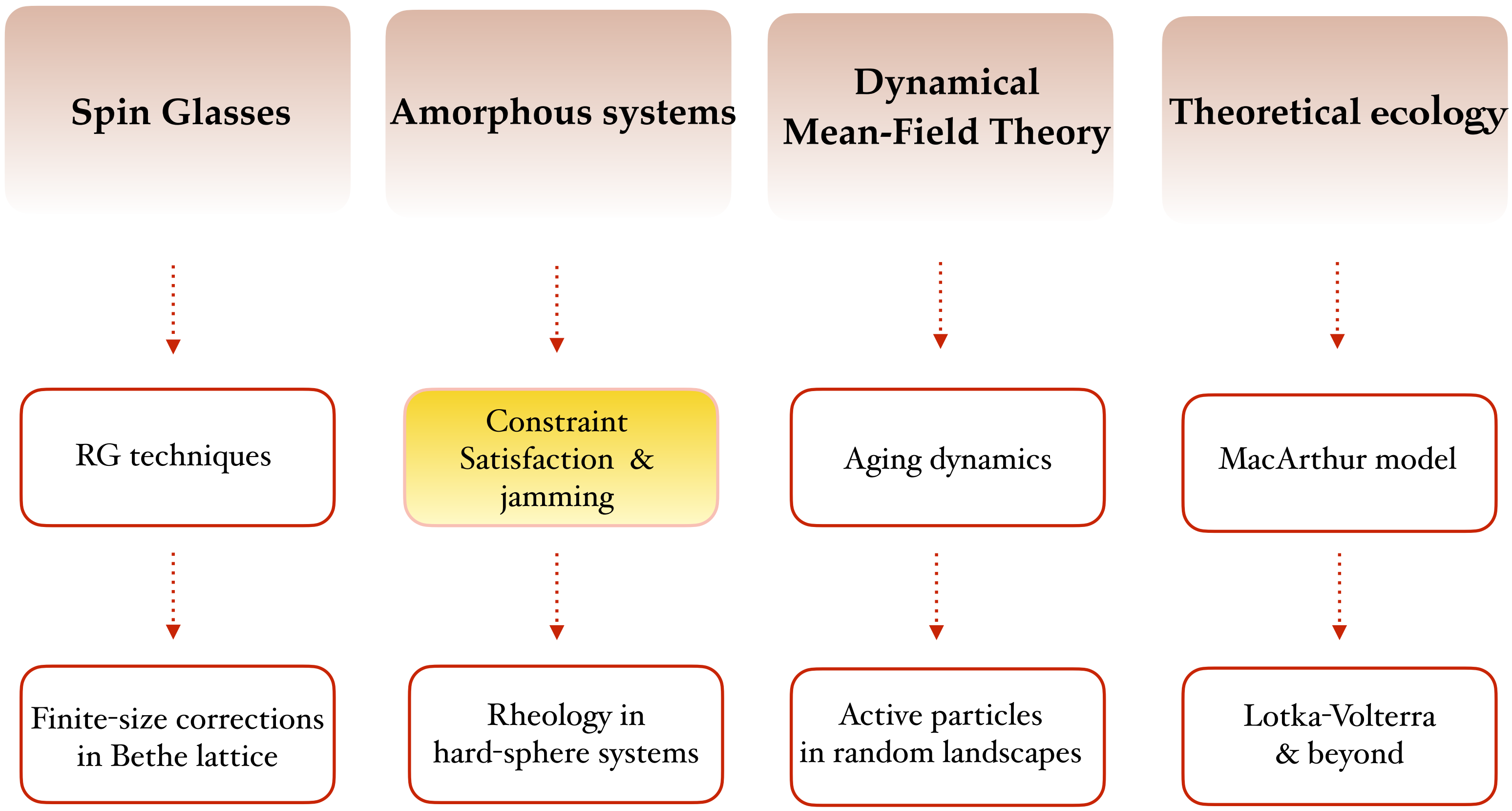
Spin Glasses

Amorphous systems

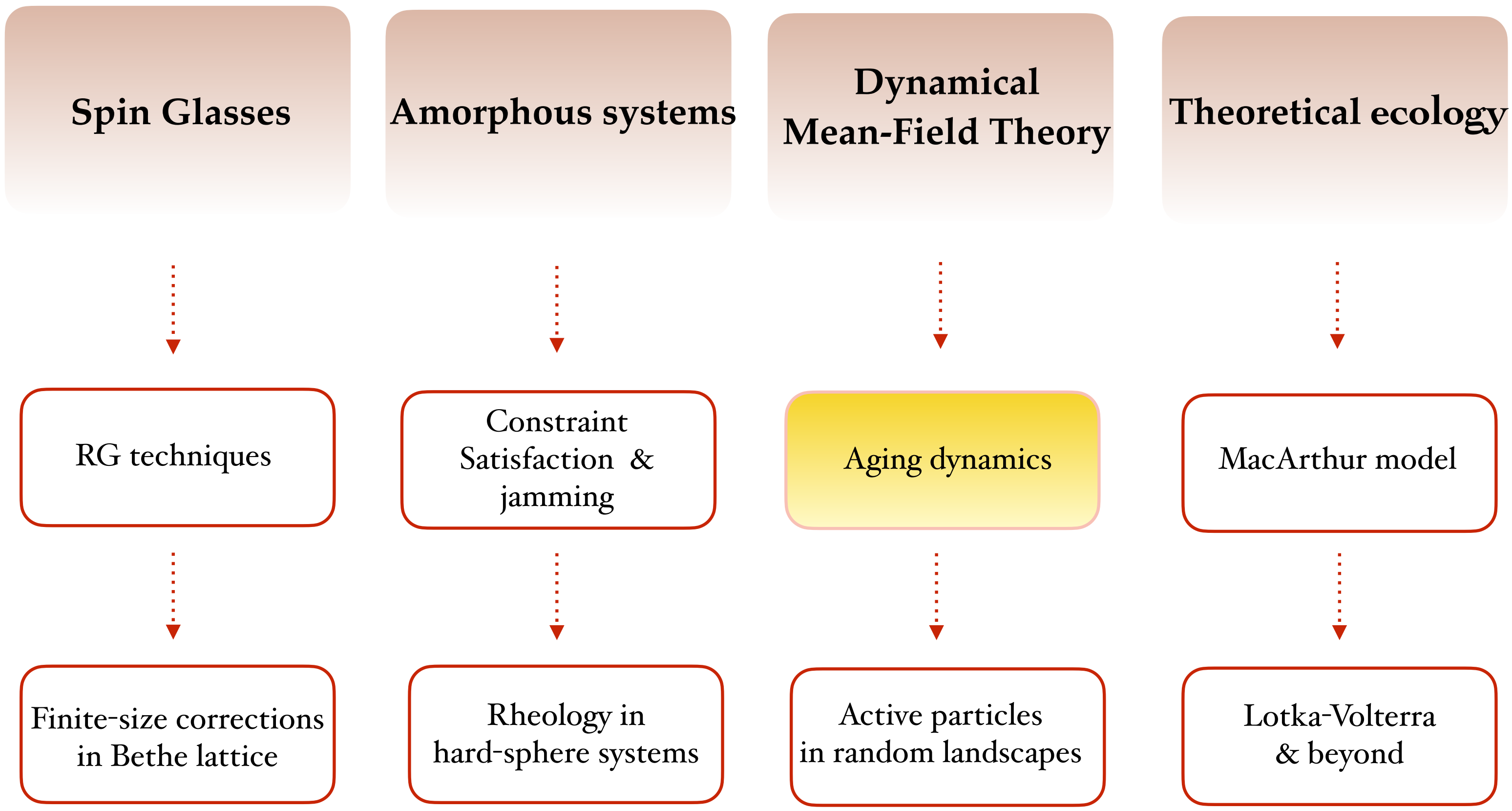
Dynamical Mean-Field Theory

Theoretical ecology

Moving through statistical physics of disordered systems



Moving through statistical physics of disordered systems



Optimization problems

Aiming to **FIND LOW-ENERGY CONFIGURATIONS**.

It's a fundamental problem in theoretical physics but also in computer science.

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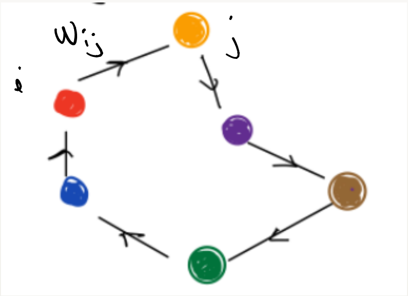

TYPICAL INSTANCE:

Suppose you know a set of cities $1, 2, \ldots N$ and a cost w_{ij}

QUESTION: What is the path $i_1, i_2, \ldots, i_N$ that passes **one and only one** through all the cities and minimises the total cost?

$$E(i_1, i_2, \ldots, i_N) = \sum_k w_{i_k, i_{k+1}}$$

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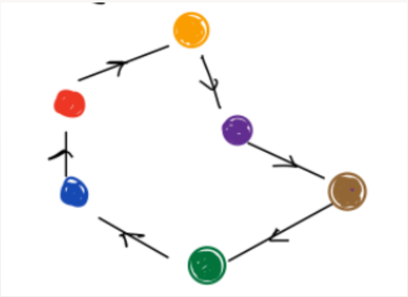

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$$E(i_1, i_2, ..., i_N) = \sum_k w_{i_k, i_{k+1}} \longrightarrow$$

Travelling salesman problem

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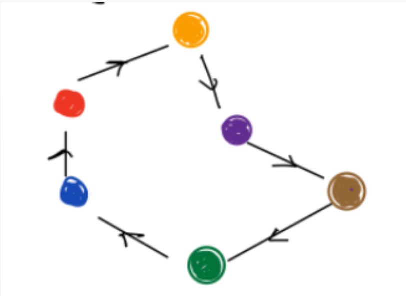

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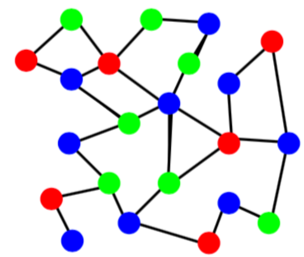
→ Travelling salesman problem

Generalization of this problem ⇒ DECISION PROBLEM

Is there a path such that the total cost is below a given threshold?

$$E(i_1, i_2 \ldots i_N) = \sum_k w_{i_k, i_{k+1}} < E_0$$

Discrete variable instance: the random colouring



A special class of optimization problem obtained when the cost function is a sum of LOCAL TERMS.

Each node $i=1,\dots,N$ can be colored with

q colors : $\sigma_i = 1,2\dots q$ "Potts spins"

$$E(\underline{\sigma}) = \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}$$

cost function (counting how many monochromatic edges connect 2 nodes with the same color).

↓

$= 0$ if the two variables are different

> 0 if the two variables have the same color.

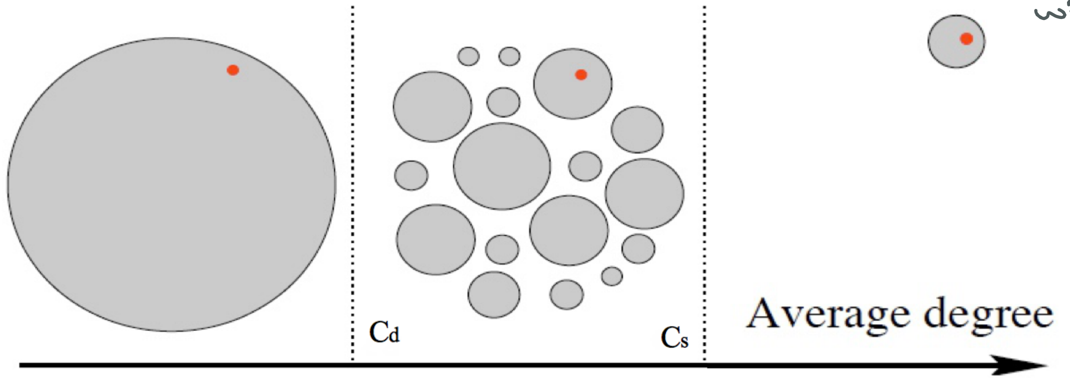
Typically studied on

- Erdös - Renyi graph (connectivity is a RANDOM VARIABLE, $\langle c \rangle = 2M/N$).
- Random Regular graph (connectivity c fixed).

The random colouring problem: phase diagram

$c = M/N$

Considering the *random coloring problem*, the control parameter is the average connectivity. $M, N \to \infty$ with c fixed.



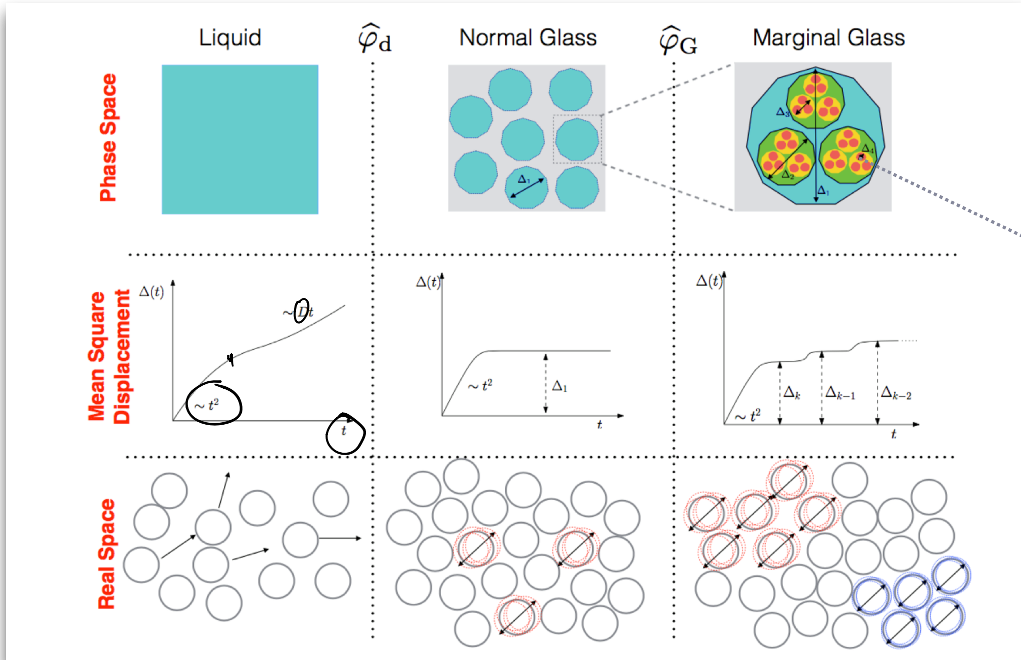
$\Sigma_i \sim \exp(N)$

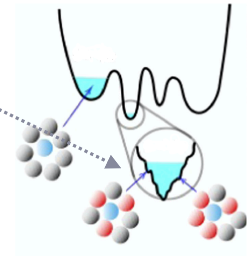
- For low enough degree, all solutions belong to a single Gibbs state.
- Above a critical connectivity the space of solutions splits into exponentially many different clusters.
- Above Cs, no solutions exist anymore. The ground state energy is zero before and then grows continuously above this threshold.

F. Krzakala, J. Kurchan, Phys. Rev. E **76** (2007)

F. Krazakala, L Zdeborová, Phys. Rev. Lett. **102** (2009)

From discrete to continuous degrees of freedom





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P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, Nature Communications **5**, 3725 (2014)

Liquid phase: single smooth basin, reflecting the unbroken symmetry (ergodic phase);

Stable glass phase: many smooth and distinct basins characterizing the landscape

Marginal glass: infinitely broken phase → each basin breaks up into many (hierarchically organised) sub-basins.

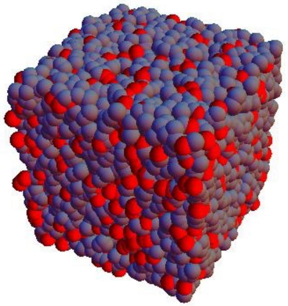
Glass transition

from the liquid to an ***entropically* rigid solid**.
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**.

qualitatively different microscopic dynamics (well-separated time and stress scales)



Jamming: a fundamental theoretical paradigm to investigate low-energy phases of glasses.

emergence of anomalous (soft) modes

marginal stability condition:
any small perturbation will push the glass into a new state ~ equivalent

interdisciplinary applications:

- neural networks
- optimization problems
- ecology

Physical implication of jamming

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

$$D(\omega) = \rho(\lambda)\frac{d\lambda}{d\omega} \Rightarrow D(\omega) = \omega^{d-1} \longrightarrow \text{ordinary solids}$$

$$D(\omega) \sim const. \longrightarrow \text{jammed materials}$$

2. Highly universal behavior related to marginal stability

- a power law in the distribution of forces at small values $P(f) \sim f^{\theta}$ $\theta = 0.42311$
- a similar scaling for the gaps between the particles: $g(h) \sim h^{-\gamma}$ $\gamma = 0.41269$

3. Quantum fluctuations in low-temperature glasses

M. Wyart, Ann. Pays. Fr. **30** (2005); M. Wyart, SR Nagel, TA Witten, Europhys. Lett. **72** (2005)
P. Charbonneau, E. I. Corwin, G. Parisi, F. Zamponi, PRL **109** (2012);
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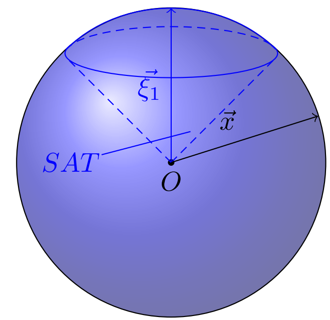
How to define an appropriate model for describing glassy phases?

A path from computer science to jamming: the perceptron

- Let us consider a vector $\mathbf{x} = \{x_1, x_2, ..., x_N\}$ such that $\sum_{i=1}^{N} x_i^2 = N$

- Take additionally $M = \alpha N$ random vectors ξ^μ with $\mathcal{N}(0,1)$

- Define the *gaps* as: $h_\mu \equiv \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \xi_i^\mu x_i - \sigma > 0 \qquad \forall \mu = 1, ..., M$



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S. Franz, G. Parisi, J. Phys. A: Math. Theor. **49**, 145001 (2016)

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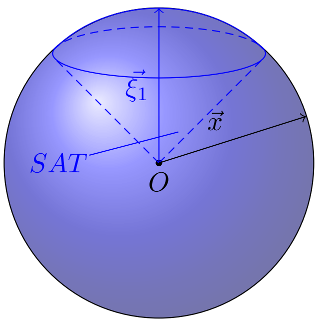

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positive bias:
convex optimization regime

usual perceptron classifier
in machine learning and computer science

negative bias:
non-convex, critical regime

same universality class of hard spheres (HS)

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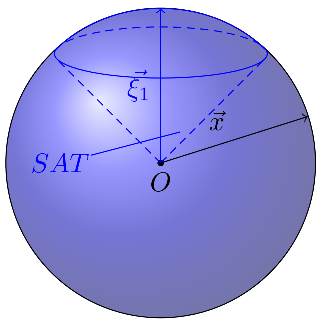

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The energy cost due to the violated/satisfied clause is $\mathcal{H} = \frac{\epsilon}{2} \sum_{\mu=1}^{M} h_\mu^2 \theta(-h_\mu)$

E. Gardner, B. Derrida, J. Phys. A: Math. Gen. **21** (1988)
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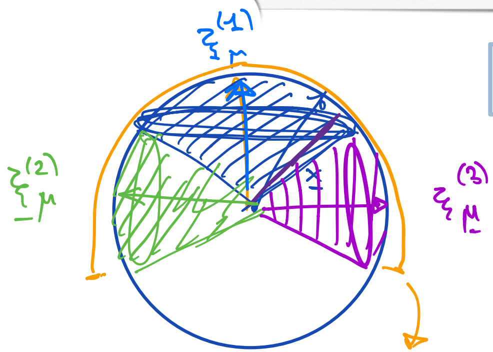
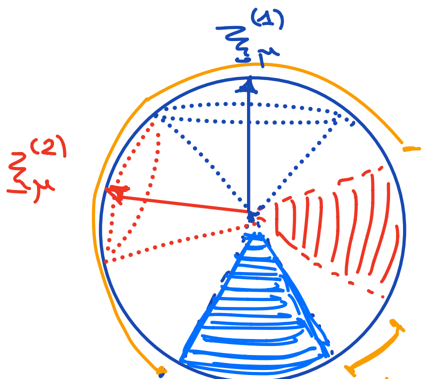
How to sketch the allowed space of solutions?



$\sigma > 0$ CONVEX OPTIMIZATION REGIME

because the space of configurations is a simple intersection of CONVEX DOMAINS.

ALLOWED CONFIGURATIONS.



$\sigma < 0$ NON-CONVEX OPTIMIZATION REGIME

→ Disconnected islands of solutions.

→ intersection of non-convex domains of ALLOWED SOLUTIONS.

Back to the spherical model: connections with sphere systems

Towards a new interpretation

SOFT SPHERES

- $\{x_i\}$ **positions of the spheres**
- $h_{ij} = x_i \cdot x_j - \sigma$ **gap between two spheres**
- $\mathcal{H}[\{x_i\}] = \frac{\epsilon}{2} \sum_{\langle i,j \rangle} h_{ij}^2 \theta(-h_{ij})$ **Energy**

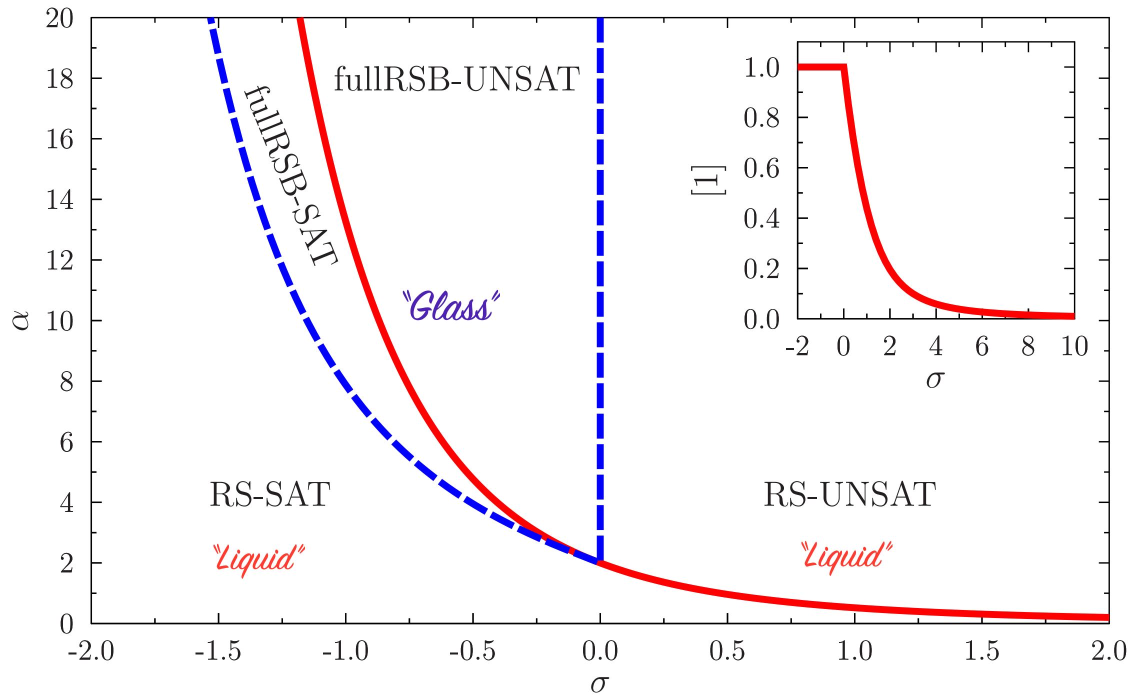
PERCEPTRON

- $\mathbf{x} = \{x_1, x_2, ..., x_N\}$ **reference position**
- $h_\mu = \xi^\mu \cdot x - \sigma$ **gap between the reference particle and spherical obstacle**
- $\mathcal{H}[\mathbf{x}] = \frac{\epsilon}{2} \sum_{\mu=1}^{M} h_\mu^2 \theta(-h_\mu)$ **Energy cost**

The tunable parameter ϵ allows us to interpolate between the hard and the soft regime.

The perceptron phase diagram

$\alpha = M/N$ ⟷ packing fraction $\qquad \sigma$ ⟷ change the pressure



Aim to investigate the effective behavior of such systems close to the jamming line & to study the vibrational spectrum as a signature of an excess of soft modes.

The effective potential in the spherical perceptron

The fundamental quantity to start with is the partition function in which additional Lagrange multipliers are embedded to enforce the average value of particle positions:

$$e^{-G(\vec{m})} = \int d\vec{x} e^{-\beta H[\vec{x}] + \sum_{i=1}^{N} u_i (x_i - m_i)}$$

Then, by extending the definition in the presence of both position variables and generalized forces, we have:

$$\Gamma(\vec{m}, \vec{f}) = \sum_{i=1}^{N} m_i u_i + \sum_{\mu=1}^{M} f_\mu v_\mu - \log \int d\vec{x}\, d\vec{h}\, d\vec{\hat{h}}\, e^{-\beta H[\vec{h}] + \sum_{i=1}^{N} x_i u_i + \sum_{\mu=1}^{M} i\hat{h}_\mu v_\mu + \sum_{\mu=1}^{M} i\hat{h}_\mu (h_\mu(x) - h_\mu)}$$

η (annotating $i\hat{h}_\mu (h_\mu(x)$)

$$G(\vec{m}) = \Gamma(\vec{m}, \vec{f}) \quad \text{evaluated in} \quad \frac{\partial \Gamma(\vec{m}, \vec{f})}{\partial f} = 0 \ .$$

How to derive an effective potential?

Starting point to study **marginal stability** and the **landscape of states**: definition of an **effective potential as a function of a local order parameter** (average position/gap)

1. Let us write down a high temperature/small coupling expansion [1, 2] of the potential

2. In fully connected systems in the thermodynamic limit the expansion can be safely truncated after a finite number of terms

3. Once identified the minima of the potential, one can study their basin of attraction and their stability.

[1] T. Plefka, J. Phys. A: Math. Gen. **15** (1982)
[2] A. Georges, J.S. Yedidia, J. Phys. A: Math. Gen. **24** (1991)

The effective potential in the spherical perceptron

Let's start defining the effective hamiltonian of our model

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

irrelevant in the SAT phase

formal parameter of the expansion

Performing an expansion in η, we get this resulting expression at a mean-field level:

- $\eta = 0$ non-interacting degree
- $\eta = 1$ **exact model**

A. Altieri, S. Franz, G. Parisi, J. Stat. Mech. (2016) 093301

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$$\Gamma(m,f) = -\frac{N}{2}\log(1-q) + \sum_\mu \Phi(f_\mu) - \sum_{i,\mu}\frac{\xi_i^\mu f_\mu m_i}{\sqrt{N}} + \frac{\alpha N}{2}\left[(\tilde{r}-r)(1-q)\right]$$

entropic term

effective Hamiltonian

reaction term

$$\Phi(f)|_{min_{v_\mu}} = f\cdot v - \log\left[\frac{1}{2}\text{Erfc}\left(\frac{\sigma - v}{\sqrt{2(1-q)}}\right)\right]$$

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

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Message passing equations and inference

Once the effective potential is well-defined, we might want to obtain the stationary equations.

These Eqs. can be solved iteratively.

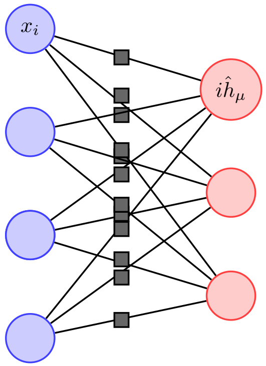
$$\frac{\partial \Gamma}{\partial m_i} = 0 \quad \Rightarrow \quad m_i \left(\frac{1}{1-q} - \alpha(\tilde{r} - r) \right) = \sum_{\mu} \frac{\xi_i^{\mu} f_{\mu}}{\sqrt{N}} \,,$$

$$\frac{\partial \Gamma}{\partial f_{\mu}} = \Phi^{'}(f_{\mu}) - \sum_{i} \frac{\xi_i^{\mu} m_i}{\sqrt{N}} + (1-q) f_{\mu} = 0$$

$i = 1 \dots N$

$\mu = 1 \dots M$

"TAP EQUATIONS"



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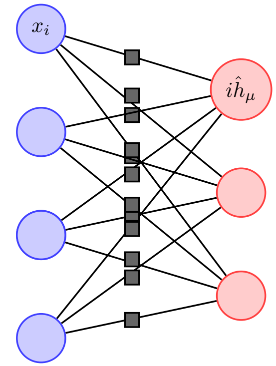

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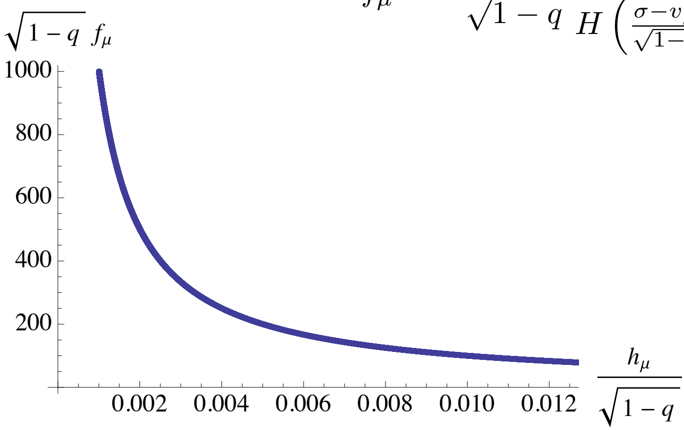
$$f_\mu = -\frac{1}{\sqrt{1-q}} \frac{H'\left(\frac{\sigma - v_\mu}{\sqrt{1-q}}\right)}{H\left(\frac{\sigma - v_\mu}{\sqrt{1-q}}\right)}$$

$$f_\mu \approx \frac{1}{h_\mu(\vec{m})} \mathcal{G}\left(\frac{h_\mu(\vec{m})}{\sqrt{1-q}} \right)$$



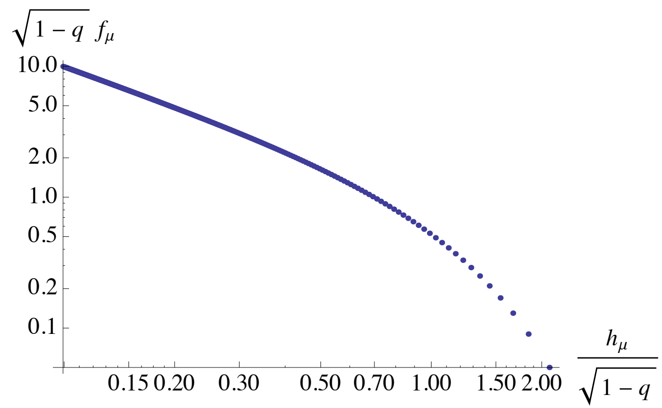


Fig: Effective forces as a function of random gaps.

A. Altieri, S. Franz, G. Parisi, J. Stat. Mech. (2016) 093301

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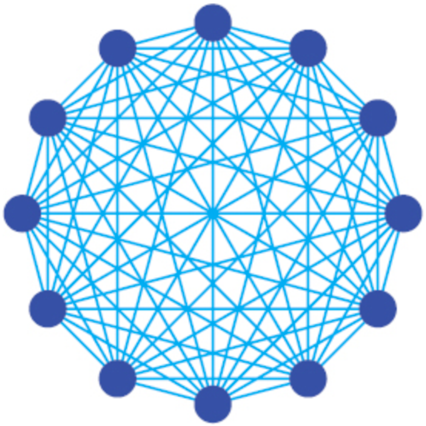
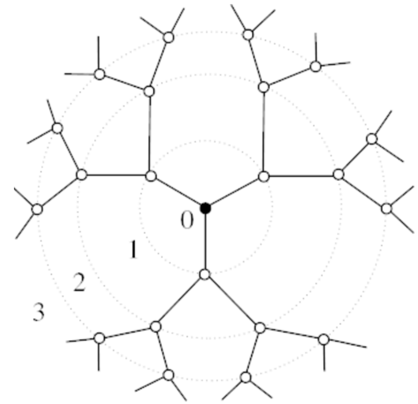
Beyond the fully-connected model

FULLY-CONNECTED MODEL



FINITE CONNECTIVITY



- Disordered systems on random lattices can mimic finite dimensional systems.

- Either in a random dilute version of the perceptron model or in finite-size systems, an analysis beyond mean-field might be relevant.

- Clearly, in the thermodynamic limit $\mathcal{F}[\text{dilute model}] = \mathcal{F}[\text{Bethe}]$

What is the actual role of higher-order corrections to the effective potential close to jamming?

Higher order corrections to the effective potential

We aim to compute further corrections to the effective potential
in order to investigate how it deviates from its critical trend upon increasing the distance from jamming.

The third order contribution in the Plefka-like approach reads:

$$\frac{\partial^3 \Gamma}{\partial \eta^3} = \langle H \rangle \frac{\partial \langle H \rangle}{\partial \eta} + \langle H \Upsilon_2 \rangle + \langle H \left(H - \langle H \rangle + \Upsilon_1 \right)^2 \rangle$$

$$\Upsilon_n = \sum_i (s_i - m_i) \frac{\partial}{\partial m_i} \left(\frac{\partial^n \Gamma}{\partial \eta^n} \right)$$

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$$\Upsilon_n = \sum_i (s_i - m_i)\frac{\partial}{\partial m_i}\left(\frac{\partial^n\Gamma}{\partial\eta^n}\right)$$

$$\frac{\partial^3\Gamma}{\partial\eta^3} = \langle H_{eff}^3\rangle + \langle H_{eff}\rangle\langle H_{eff}^2\rangle - 2\langle H_{eff}\rangle^3 - \langle H_{eff}\rangle\alpha N r(1-q) - \langle H_{eff}\rangle\alpha N q(\tilde{r} - r) +$$

$$+\left\langle H_{eff}\left(-\sum_{i,\mu}\frac{\delta x_i}{\sqrt{N}}\xi_i^\mu f_\mu\right)^2\right\rangle + \left\langle H_{eff}\left(-\sum_{i,\mu}\frac{\delta f_\mu}{\sqrt{N}}\xi_i^\mu m_i\right)^2\right\rangle +$$

$$-2\left\langle H_{eff}^2\left(\sum_i \delta x_i \sum_\mu \frac{\xi_i^\mu f_\mu}{\sqrt{N}} + \sum_\mu \delta f_\mu \sum_i \frac{\xi_i^\mu m_i}{\sqrt{N}}\right)\right\rangle$$

In the jamming limit, all these terms give a vanishing contribution, confirming that the potential is well described by **binary interaction**.

Thank you for your attention!

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Questions?

References

Introduction to glassy systems

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