Mean Field Spin Glasses: modelling the low-energy excitations of glasses

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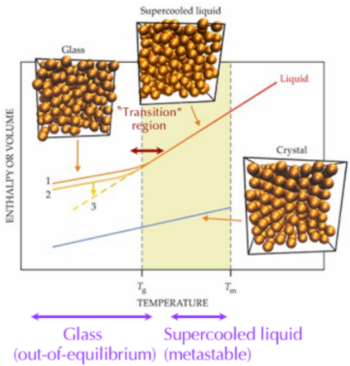
Presentation of the Physical Problem

Hello Guys, I am a Glass

Macroscopically I look like a solid, but microscopically I am totally different from any crystal you can imagine! Here some generalities

	Crystal	Glass
Structure	Spatially Homogeneous	**Spatially Heterogeneous**
Relaxation to Equilibrium	Fast	**Extremely Slow**
I depend on preparation protocol	No	**Yes**

Here's how I am created $\Longrightarrow$



(a) Credits: Berthier and Ediger, Physics Today (2016)

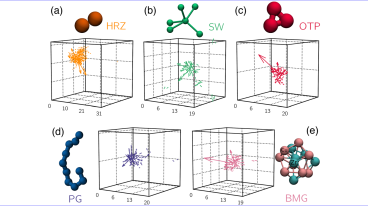
If you excite me a little, I will surprise you

At very low temperatures, I display anomalous thermodynamical properties (with respect to the crystalline ones) in the low frequency part of the normal modes spectrum! These are ascribable to the following[1]:

- My DOS (Density of States) $D(\omega)$ is different from that of my cousin Crystal:

$$D(\omega) \underset{\omega \to 0}{\sim} \overbrace{A}^{\text{not universal}} \underbrace{\omega^4}_{\text{universal}}$$

- Corresponding eigenvectors **localised** in the glass structure (see on the right).



(a) Credits: D.Richard, K. Gonzalez-Lopez, G. Kapteijns, R. Pater, T. Vaknin, E. Bouchbinder, and E. Lerner. "Universality of the Nonphononic Vibrational Spectrum across different classes of Computer Glasses". In: Physical Review Letters 125 (2020), p. 085502.

	Crystal	Glass
Low frequency spectrum	$D(\omega) \sim \omega^{d-1}$	$D(\omega) \sim \omega^4$
Localisation	No	Yes

[1] Low energy phonon modes must be removed from the glass: this can be done by putting pinning nodes in the glass that act as scatterers at fixed distance, so imposing an upper bound on the wavelengths of these modes.

Statistical Mechanics for disordered systems

Glasses are part of a more generic ensemble of thermodynamic systems called **disordered systems**: here some tools useful for the following slides

$$H = H[\boldsymbol{x};\boldsymbol{J}], \qquad \begin{cases} \boldsymbol{x} \text{ configuration} \\ \boldsymbol{J} \text{ disorder parameters} \end{cases}$$

$$Z_J = \sum_{\boldsymbol{x}} \exp\left(-\beta\, H[\boldsymbol{x};\boldsymbol{J}]\right), \qquad \beta = \frac{1}{k_B\, T}, \qquad P_J(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-\beta\, H[\boldsymbol{x};\boldsymbol{J}]\right)$$

$$\overline{(\cdot)} = \sum_{\boldsymbol{J}} (\cdot) P[\boldsymbol{J}], \qquad \text{Average over the disorder}$$

$$q_J(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{N}(\boldsymbol{x}\cdot\boldsymbol{y}), \qquad \text{Configurations overlap}$$

$$P_{MF}(\boldsymbol{x}) = \prod_{k=1}^{N} P_x(x_k), \qquad \text{Mean Field Approximation}$$

$$P_{MF}(\boldsymbol{x}) = \sum_a w_a\, P_a(\boldsymbol{x}), \qquad \text{Decomposition in pure states (MF)}$$

$$P_f(\boldsymbol{x}) = \frac{1}{2}\, P_+(\boldsymbol{x}) + \frac{1}{2}\, P_-(\boldsymbol{x}), \qquad \text{e.g.: the ferromagnet}$$

Pure states a identified by magnetization profiles $\{\boldsymbol{m}\}_a$

What is a Spin Glass?

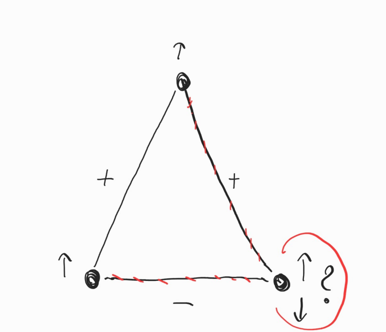
What is a Spin Glass?

$$H_{EA} = -\frac{1}{2} \sum_{i,j \text{ n.n.}} J_{ij} S_i S_j$$
$$S_i = \pm 1, \quad i = 1, \dots, N$$

- **Quenched Disorder** (typically Gaussians):

$$\overline{J} = J_0/\sqrt{N}$$
$$\overline{J^2} = J_1^2/N, \quad J_1 \neq 0$$

- **Frustration**: competing interactions.



- Historically, Spin Glasses were firstly modeled by Edwards and Anderson with the purpose of studying **disordered magnetic systems**.
- They identify, for $J_0 \ll J_1$ and $T \ll J/k_B$ a phase with non-trivial equilibrium magnetization profiles $\boldsymbol{m}_J$, and they propose as an order parameter the **overlap** $q = \frac{1}{N} \overline{|\boldsymbol{m}_J|^2} \equiv \frac{1}{N} \sum_i \overline{m_i{}^2}$.

Non-trivial Mean Field Approximation

The Mean Field approximation of the Edwards-Anderson model is the Sherrington-Kirkpatric (S-K) Model

$$H_{SK} = -\frac{1}{2}\sum_{i,j} J_{ij} S_i S_j - h \sum_i S_i$$

$$J_{ij} \overset{d}{\sim} \mathcal{N}(0, \frac{J^2}{N})$$

where we have chosen $J_0 = 0$ and $J_1 = J$ and field h to break the global inversion symmetry of the spins.

$$f = -\lim_{N\to\infty} \frac{1}{N\,\beta} \overline{\ln Z_J} = -\lim_{N\to\infty} \frac{1}{N\,\beta} \lim_{n\to 0} \frac{\overline{(Z_J)^n - 1}}{n}, \quad \text{Replica Trick}$$

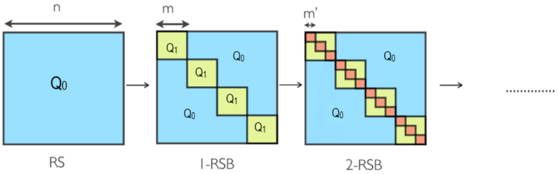
$$f = -\frac{1}{\beta} \lim_{n\to 0} \max_Q (A[Q;\beta])$$

$$Q_{ab} = \langle S_a S_b \rangle \qquad \text{Overlap Matrix}$$

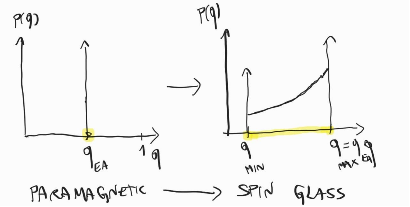
- S-K ansatz: $Q_{ab} = q$, Replica Symmetric (RS).
- Stable at high temperatures, unstable for $T < J/k_B$.

Breaking the Replica Symmetry: the Parisi-Scheme

The correct solution of the S-K model in the glass phase was provided by Parisi through the following replica symmetry breaking algorithm:



Iterating the procedure an infinite amount of time and sending $n \to 0$ in the end we get a continuous distribution of overlaps $P(q)$: the true order parameter of the Spin Glass transition is a function!



Physical Interpretation: Infinite Equilibrium States!

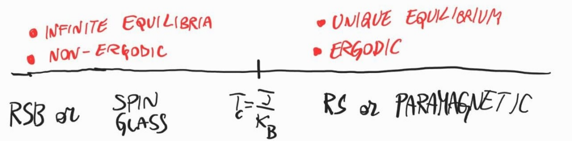
The physical interpretation of the Parisi solution is understood by making the connection between pure states and replicas explicit:

$$\boldsymbol{m}_\alpha, \qquad \text{Pure States identified by magnetization profiles}$$

$$q_{\alpha\beta} = \frac{1}{N}(\boldsymbol{m}_\alpha \cdot \boldsymbol{m}_\beta), \qquad \text{Overlap between pure states}$$

$$\overline{\sum_{\alpha,\beta} w_\alpha w_\beta \delta(q - q_{\alpha\beta})} \equiv P(q) = \lim_{n \to 0} \frac{2}{n\,(n-1)} \sum_{a,b} \delta(q - Q_{ab}^{SP})$$

Infinite pure states $\iff$ Breaking of Replica Symmetry



Modelling glassy excitations with Spin Glasses

Vector Spin-Glass models: the vector p-spin

$$H[\mathbf{S}] = -\sum_{(\boldsymbol{i}),\boldsymbol{\alpha}} J_{i_1\ldots i_p}^{\alpha_{i_1}\ldots\alpha_{i_p}} S_{i_1}^{\alpha_{i_1}} \ldots S_{i_p}^{\alpha_{i_p}}$$

- $i = 1, \ldots, N$
- $\vec{S}_i = (S_i^1, \ldots, S_i^m), \qquad |\vec{S}_i| = 1, \qquad \forall\, i$
- $P(J_{i_1\ldots i_p}^{\alpha_{i_1}\ldots\alpha_{i_p}}) = \mathcal{N}(0, \frac{p!}{2\,N^{p-1}}), \qquad i_1 \neq i_2 \neq \ldots \neq i_p$
- $m > 2$ and $p > 2$.

The p-spin is the simplest model of the glass transition.

Phenomenology

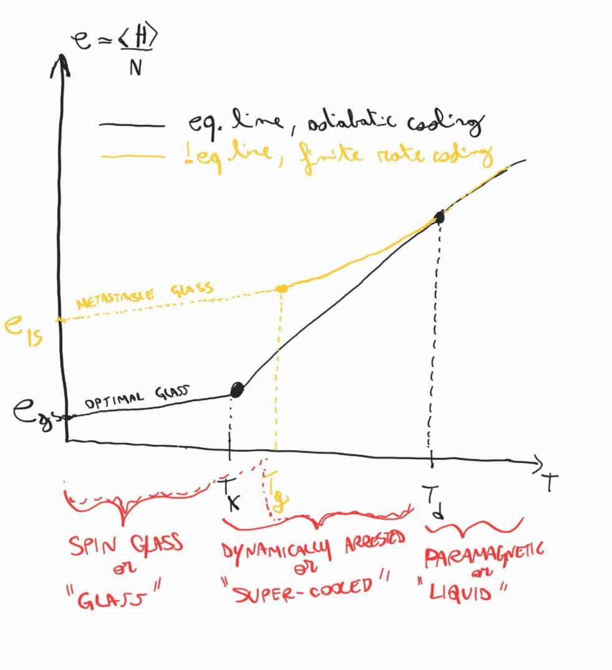
The phenomenology of the p-spin is very reach:

- For $T > T_d$ we are in a **paramagnetic phase**: there is only one equilibrium state, *relaxation in equilibrium dynamics is exponentially fast* after $t \gg \tau$.
- At $T = T_d$ there is a **dynamical transition**, $\tau \sim |T - T_d|^{-\gamma}$: relaxation becomes very slow and *the system remains correlated to the initial configuration* $C(t) \sim q$. The equilibrium free-energy is regular, so there is no thermodynamical transition.
- For $T_K < T < T_d$ there is a **complexity** Σ of the equilibrium states: $\mathcal{N} \sim e^{N\Sigma}$ *states with fixed free-energy contribute equally to equilibrium*

  $$Z \sim \sum_\alpha Z_\alpha = \int_{f_{min}}^{f_{max}} df\, \Omega(f) e^{-N\beta f} \sim e^{-N[\beta f_* - \Sigma(f_*)]}$$

  where $\Omega \sim e^{N\Sigma}$ and $Z_\alpha \sim e^{-N\beta f_a}$.
- At $T = T_K$ the **equilibrium complexity vanishes**, and *equilibrium is determined by a finite number of states with minimal free-energy*. Here, the specific heat has a jump, so there is a thermodynamical phase transition.

A model for glass formation



Energy landscape at $T = 0$: Stable Minima

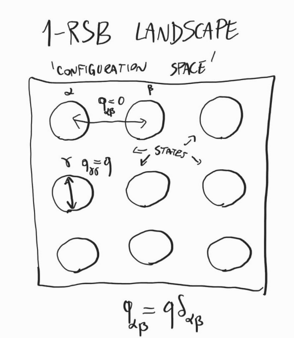
There is a One-Step Replica Symmetry Broken (1RSB) energy landscape with exponential many minima:

$$\mathcal{N}(E) \sim e^{-N\Sigma(E)}, \quad E_{gs} \leq E \leq E_{mg}$$
$$\Sigma(E) \neq 0, \quad E > E_{gs}$$

- A level E *represents a class of glasses* formed with a certain protocol of cooling, the optimal glass is the one at $E = E_{gs}$.
- A given state at a level E represents a particular glass.

$E_{gs} \leq E < E_{mg}$:
We call such a glass a **Stable Glass**: the system in this state is *stable against small perturbations*. This is due to the structure of the energy landscapes: indeed, states are far from each other

$$\frac{1}{N}|\boldsymbol{S}_\alpha - \boldsymbol{S}_\beta|^2 = 2(1 - q_{\alpha\beta})$$
$$q_{\alpha\beta} = q_m < 1 \quad \text{if } \alpha \neq \beta$$

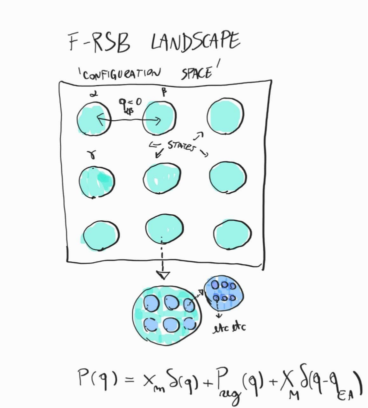


Energy landscape at $T = 0$: Marginal Minima

At $E = E_{mg}$, the landscape changes and becomes as the Parisi or Full RSB landscape:

We talk about **Marginal Glasses**: in this context

- ***Minima are arbitrary close and have flat directions***, a continuous variety of overlap is populated until the q_{max}.
- Thus ***an infinitesimal perturbation induces a change of energy minimum***: 'if I move a bit, I can change valley'.



For $E > E_{mg}$ there are other marginal energy minima: however, I did not study this region 😬.

Mean field stable glasses have localised low-energy excitations

In order to study fluctuations around an energy minimum

- Compute the Hessian matrix of H and diagonalise it, in order to get the distribution of the eigenvalues, $\rho(\lambda)$.
- The connection between the eigenvalues and the normal modes of vibration is : $\lambda = \omega^2$ and $D(\omega) = 2\omega\rho(\omega^2)$.

Result ($N \to \infty$):

$$\rho(\lambda) \propto \begin{cases} \lambda^{m-1}, & E_{gs} \leq E < E_{mg} \quad \overbrace{\textbf{Stable Glasses}}^{\text{'few small frequencies'}} \\ \sqrt{\lambda} & E = E_{mg} \quad \overbrace{\textbf{Marginal Glasses}}^{\text{'a lot of small frequencies'}} \end{cases}$$

$$\boldsymbol{v}(\lambda) = (\vec{v}_1(\lambda), \ldots, \vec{v}_N(\lambda))$$

$$|\vec{v}_i(\lambda)|^2 \underset{\lambda \to 0}{\overset{N \to \infty}{\propto}} \begin{cases} E_{mg} - E, & i = M \\ o(1), & i \neq M \end{cases}$$

Stable glassy minima display localisation in their softest eigenvectors!

Mean field models of Spin Glasses can exhibit localised eigenvectors!

- Physical Problem: low energy excitations of glasses.
- Glasses: disordered system, use spin glasses to model them.
- Vector p-spin: used to model localised soft normal modes.

	Glasses	**Mean-Field Vector p-spin**
$D(\omega)$	ω^4	ω^{2m-1}
Localisation	Yes	Yes

Perspectives

- In a recent work it was shown that in sparse graphs (an approximately tree-like structure where each node-i.e. spin- is linked -i.e. interacts- with a finite number of other nodes) the $m = 2$ Spin Glass can exhibit localised excitations with $D(\omega) \sim \omega^4$: I would like to check it this holds for any m.
- In a marginal Spin Glass one can study non-linear excitations, jumps in energy related to the fall in a new energy minimum: the statistics of this jumps can provide information on the $T = 0$ distribution of the overlaps between states.

Thank you!