Can a Gardner transition explain the marginal stability of jammed packings?

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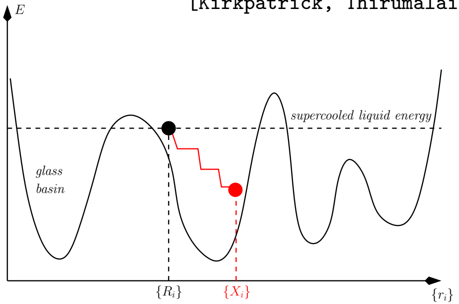
Outline

The RFOT/energy landscape picture

[Goldstein, Stillinger, Weber et al. 1969 - ...]
[Kirkpatrick, Thirumalai, Wolynes 1987-1989]



The supercooled liquid is a collection of glasses

Each equilibrium liquid configuration R belongs to a metastable glass state

Consider a second copy of the system, X. At time $t = 0$ we have $X = R$. Time evolution can be such that $X \sim R$ at all times (in the glass), or that X diffuses away from R at long enough times (in the supercooled liquid). The dynamics of X is the equilibrium dynamics of the liquid.

Relaxation in the supercooled liquid is like escaping from a metastable state – except that the process is repeated over and over [Krzakala and Zdeborova, JCP (2011)]

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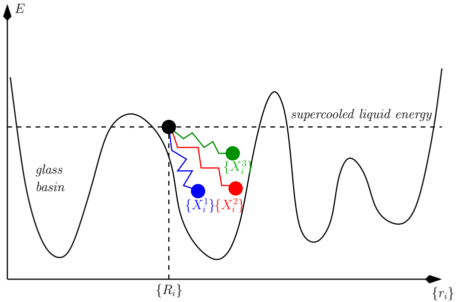


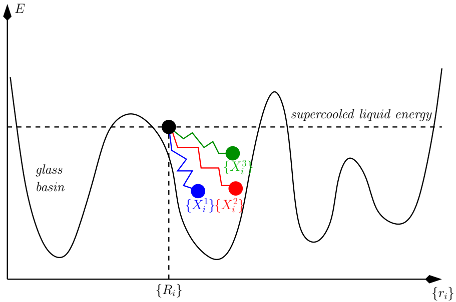
$F_g = -k_B T \int dR \frac{e^{-\beta H[R]}}{Z} \log Z[X|R] \qquad Z[X|R] = \int dX e^{-\beta' H[X] + \beta' \varepsilon \sum_i (X_i - R_i)^2}$

Need replicas: $F_g = -k_B T \lim_{n \to 0} \log \left[\int dR e^{-\beta H[R]} Z[X|R]^n \right] - F_{\rm liq}$

The replicated system is a homogeneous and isotropic "molecular liquid" and can be treated by using standard liquid theory

This is called the "state following" replica computation: we select a state at temperature β and follow it at β'

The RFOT/energy landscape picture



Another related computation consists in taking *m* coupled replicas at temperature β and let them choose their state [Monasson, 1995]

In this case, by tuning β and *m* we can select, for each energy, the typical states at that temperature and energy

In jargon, this is called the 1RSB scenario

Outline

Marginal stability - a puzzle

In the 1RSB picture, the states at $T = 0$ ("inherent structures") are well defined minima
The vibrational spectrum has no zero modes

This picture can be transposed to hard spheres (with $\beta \to p$ and $-E \to \varphi$)
Jammed packings correspond to the inherent structures [Krzakala, Kurchan 2007]
The 1RSB picture leads to many good predictions for thermodynamics and structure of hard sphere glasses [Parisi, FZ 2005-2010]

However, jammed packings have many zero modes! [O'Hern, Langer, Liu, Nagel 2002]
These zero modes leads to criticality at jamming, with many associated critical exponents
Very successful scaling theories can be constructed, based on a marginal stability principle [Wyart, Silbert, Nagel, Witten 2005]

Marginal stability is based on the empirical observation that packings are *isostatic*
Question: where is marginal stability in the replica picture? Can we derive marginal stability from first principles?

Idea: in spin glasses, marginal stability is seen in the Sherrington-Kirkpatrick model
It is associated to what is called in jargon "full RSB"
Do hard spheres show full RSB at jamming?

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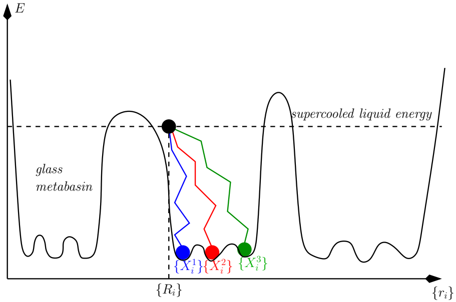
Metabasins and full RSB



Idea: the bottom of the basins is not a well defined minimum
It is very "rugged" with a huge number of sub-minima separated by small barriers
For $N \to \infty$ the number of minima diverges and the size of the small barriers vanishes
This leads to zero modes and marginal stability

In jargon, this is called the full RSB scenario

In the SK model, this happens at any temperature in the glass phase
(no separation of scales of the barriers)
Generically, this happens only at low enough temperature: there are two transitions

[Gardner, 1985]

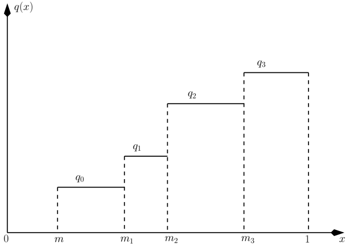
Full RSB in the Ising p-spin model

Full RSB equations for the free energy of the Ising p-spin:

$Q_{ab} = \frac{1}{N} \sum_i S_i^a S_i^b \qquad \Lambda_{ab} = \frac{p}{2} Q_{ab}^{p-1}$

The structure of states can be encoded by "hierarchical matrices"
A closed algebra, blocks of size $1 > m_{k-1} > m_{k-2} > \cdots > m_1 > m > 0$

$$Q = \begin{pmatrix} 1 & q_2 & q_1 & q_1 & q_0 & q_0 & q_0 & q_0 \\ q_2 & 1 & q_1 & q_1 & q_0 & q_0 & q_0 & q_0 \\ q_1 & q_1 & 1 & q_2 & q_0 & q_0 & q_0 & q_0 \\ q_1 & q_1 & q_2 & 1 & q_0 & q_0 & q_0 & q_0 \\ q_0 & q_0 & q_0 & q_0 & 1 & q_2 & q_1 & q_1 \\ q_0 & q_0 & q_0 & q_0 & q_2 & 1 & q_1 & q_1 \\ q_0 & q_0 & q_0 & q_0 & q_1 & q_1 & 1 & q_2 \\ q_0 & q_0 & q_0 & q_0 & q_1 & q_1 & q_2 & 1 \end{pmatrix}$$



$$-\beta f_{\infty \mathrm{RSB}} = \frac{\beta^2}{4}\left[1 - \int_m^1 dx q(x)^p + 2\int_m^1 dx \lambda(x) q(x) - 2\lambda(1)\right] + \frac{1}{m} \log\left[\int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi\lambda(m)}} e^{-\frac{z^2}{2\lambda(m)}} e^{\beta m f(m,z)}\right]$$

$$f(1,h) = T \log\cosh(\beta h)$$

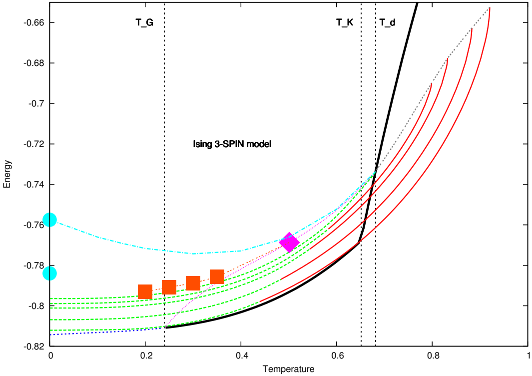
$$\frac{\partial f}{\partial x} = -\frac{1}{2}\frac{d\lambda}{dx}\left[\frac{\partial^2 f}{\partial h^2} + \beta x \left(\frac{\partial f}{\partial h}\right)^2\right]$$

[Parisi, 1979-1980] [Gardner, 1985]

Full RSB in the Ising p-spin model

A prototypical example: the Ising p-spin model $H = -\sum_{ijk} J_{ijk} S_i S_j S_k$
Exactly solvable model, using replicas – but still work in progress

[Montanari, Ricci-Tersenghi, 2003-2005]
[Tonosaki, Takeda, Kabashima, 2007]
[Krzakala, Zdeborova, 2010]
[Rizzo, 2013]



A complete understanding the consequences for dynamics is in progress, need to generalize the work of [Cugliandolo-Kurchan, 1993]

Outline

Dimensional (in)dependence of jamming

All the physics of jamming, and in particular marginal stability, does not depend on dimension (numerical simulations in $d = 2 \cdots 13$)

[Goodrich, Liu, Nagel, PRL 2012]
[Charbonneau, Corwin, Parisi, FZ, PRL 2012]

Hard spheres in $d \to \infty$ can be solved exactly [Kurchan, Parisi, FZ JSTAT 2012]
A theory of hard spheres in $d \to \infty$ is also (with minor modifications) a theory of hard spheres in $d = 3$ (we need to include more terms of the virial series, under suitable approximations)

Δ plateau of mean square displacement in the glass, p pressure
In the scaling theory, all non-trivial exponents controlled by $\Delta \sim p^{-3/2}$...

[Ikeda, Berthier, Biroli, JCP 2013]

...which is a direct consequence of marginal stability [Wyart, Silbert, Nagel, Witten 2005]

1RSB gives $\Delta \sim 1/p$. What about full RSB?

Note: in the p-spin, at 1RSB level $1 - q \sim T$, while at full RSB level $1 - q \sim T^2$!
Marginal states are "stiffer", pseudo-gap in the distribution of local fields
$\chi_{\rm LR} \sim \beta(1 - q_{\rm EA}) \sim T \ll \chi_{\rm jump} \sim \beta(1 - q) \sim 1$
$E_{\rm LR} = h^2/\chi_{\rm LR} \gg E_{\rm jump} \sim h^2/\chi_{\rm jump}$

For spheres,
$\mu_{\rm LR} \sim T/A_{\rm LR} \sim Tp^{3/2} \gg \mu_{\rm jump} \sim T/A_{\rm jump} \sim Tp_{\rm jump}$
$E_{\rm LR} = \mu_{\rm LR}\gamma^2 \gg E_{\rm jump} = \mu_{\rm jump}\gamma^2$

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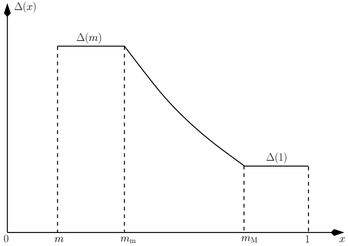
Infinite dimensional hard spheres

Exact solution of replicated hard spheres in $d \to \infty$.
Parametrization in terms of a mean square displacement matrix
$\alpha_{ab} = d \langle u_a \cdot u_b \rangle \qquad \Delta_{ab} = d \left\langle (u_a - u_b)^2 \right\rangle = 2\alpha_{aa} - 2\alpha_{ab}$

Replicated free energy: $s[\hat{\alpha}] = \text{const.} + \frac{d}{2} \log \det(\hat{\alpha}^{m,m}) - \frac{d}{2} \widehat{\varphi} \mathcal{F}(2\hat{\alpha})$

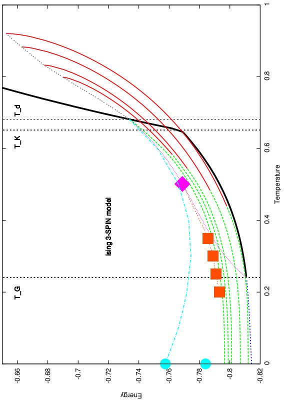
After some long calculations:

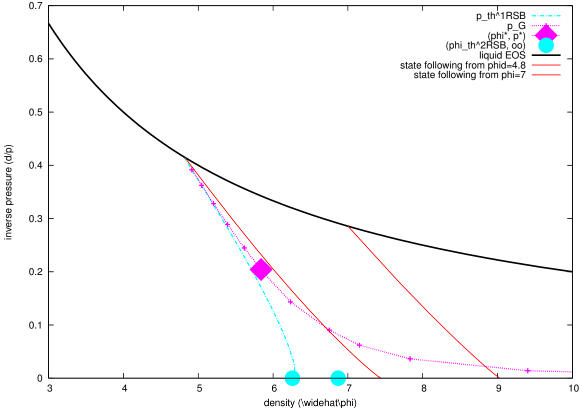
$$
\begin{aligned}
s_{\infty \mathrm{RSB}} &= -\frac{d}{2} m \int_m^1 \frac{dy}{y^2} \log \left[y\Delta(y) + \int_y^1 dz \Delta(z) \right] \\
&\quad - \frac{d}{2} \widehat{\varphi}\, e^{-\Delta(m)/2} \int_{-\infty}^{\infty} dh\, e^h [1 - e^{mf(m,h)}] \\
f(1,h) &= \log \Theta \left[\frac{h}{\sqrt{2\Delta(1)}} \right] \qquad \Theta(x) = (1 + \mathrm{erf}(x))/2 \\
\frac{\partial f(x,h)}{\partial x} &= \frac{1}{2} \dot{\Delta}(x) \left[\frac{\partial^2 f(x,h)}{\partial h^2} + x \left(\frac{\partial f(x,h)}{\partial h} \right)^2 \right]
\end{aligned}
$$



Note the strong similarity with the p-spin model!
[Kirkpatrick-Thirumalai-Wolynes, 1987-1989]

Infinite dimensional hard spheres - results





See also [Krzakala-Kurchan, 2007]

Outline

Summary

- The replica equations for hard spheres in $d = \infty$ are extremely similar to the ones of the Ising p-spin
- Technically, however, there are many important and subtle differences (this is way this work is progressing slowly!)
- The phase diagram is identical, with $T \to 1/p$ and $-E \to \varphi$
- At high pressure (low temperature) there is a Gardner phase where full RSB occurs
- In the Gardner phase, meta-states are split into sub-states
- Full RSB states are *marginally stable*

Perspectives

Work in progress:

- Solve the full RSB equations and obtain the scaling of $\Delta(1)$ versus p
- Complete the state following calculations and estimate the location of the Gardner transition for the different glasses
- Dynamics and the threshold?
- Extension to $d = 3$ is relatively straightforward (with approximations)

Produce predictions and test them:

- Direct investigation of the potential energy landscape? (cfr. de Souza's talk, and Heuer)
- χ_4 is divergent in the whole Gardner phase (but pay attention to phonons), compare with Ikeda-Berthier-Biroli
- Off-equilibrium dynamics in the Gardner phase, FDT violations
- A complex rheology with multiple time scales (as in the SK model)? (cfr. Yoshino's talk)

Dreams:

- What happens to a full RSB solution in finite dimensions? How is it modified by nucleation? Can we justify marginality beyond mean field?
- Is there any interaction between the soft modes of the full RSB solutions and the ones associated to the dynamical transition? (in mean field no, but what happens beyond mean field?)
- A connection with tunnelling "two-level" systems at low T? [Kuhn, EPL 2003]

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