Exact theory of dense amorphous spheres in large dimensions

Giorgio Parisi

In this talk I will shortly discuss:

- Mean field theory for glasses.
- A new crucial phenomenon: the Gardner-(Gross-Kanter-Sompolisky) transition.
- The fractal picture arises.
- Conclusions

Mean field theory should be exact in some limit (e.g. infinite dimensions, long range....)

High temperature (or low density) the theory is trivial. The problems are at low temperature or high density. A phase transition lurks somewhere.

Two approaches

- Solve the model analytically by brute force or by ingenuity.
- Identify the correct order parameter and to prove later that nothing relevant is missing

Zeroth order approximation

neglect correlations in the liquid phase.

$g(x) = \exp(-\beta V(x))$

We can construct models of hard spheres (MK_x) with trivial correlations. (I skip the details: see Patrick's talk).

Frozen phase, where the particles are confined in a cage. The effects of the other particles forbid a given particle to move too much.

The local order parameter is the form of the cage $\psi_i(x - x_i)$.

Free energy functional (Wolynes '80') we can write a free energy that depends on the form and the positions of the cages (e.g. in 3 dimensions).

$$F[\psi_i(x - x_i)]$$

The global order parameter is the probability distribution of the probability of the cages:

$\mathcal{P}[\psi]$

We can trivialise the model, neglecting correlations in the liquid. We have a functional order parameter: a big mess for explicit exact computations (Mézard, GP, Tarzia, Zamponi).

Too many forms of the cages. Some approximation is needed.

The simplest approximation (Mézard and GP 1999). All cages are equal and Gaussian with radius A:

$$\psi_i(x_i) \propto \exp\left(-(x_i - x_i^{cage})^2/(2A)\right)$$

Systematic small A expansion. We can modify this add approximation correlations in the fluid case.

Good results. Hard spheres (GP and Francesco Zamponi).

- $\phi < \phi_d$ liquid
- $\phi > \phi_d$ the liquid breaks into states (lumps). The number of states is $\exp(N\Sigma(\phi, f)$ for $f_{min} < f < f_{max}$ f being the free energy in a state.
  f_{eq} minimise the total free energy.
  $\Phi = f - T\Sigma(\phi, f) \qquad (F = E - TS)$
  $\Sigma(\phi, f_{eq})$ is the equilibrium configurational entropy.
- At ϕ_K $\Sigma(\phi, P_{eq}) = 0$.
- At $\phi > \phi_K$ the partition function is dominated by a not large number of states $\Sigma(\phi, P_{eq}) = 0$

With replicas: one introduce m replicas.

$$X_i \equiv \{x_i^1 \cdots x_i^m\} \qquad \rho(X_i) \propto \int dx_i^{cage} \exp\left(- \sum_{a=1,m} (x_i^a - x_i^{cage})^2/(2A) \right)$$

Why m replicas?

The free energy of the different cages has a probability distribution that depends on m.

$$\frac{\partial \Sigma(f)}{\partial f} = \beta m$$

The introduction of replicas allows us to do probabilistic computations in a very fast and compact way!

We should be able to do all this without replicas (GP, Zamponi).

You can do the computation taking care of the correlations. You find reasonable results at $d = 3$ for the position of the transitions.

Infinity pressure states exist for $0.64 < \phi < .68$ in $d = 3$.

- We have the RFOT scenario.
- We can compute the critical line with good results (Infinity pressure states exist for $0.64 < \phi < .68$ in $d = 3$.)
- We predict generalised fluctuation dissipation relations.
- The pressure diverge as $(\phi_J - \phi)^{-1}$.
- Number of contacts at infinite pressure $6 - 6.1$. No isostaticity!!!
- The size of the cage is proportional to $(\phi_J - \phi)$
- The correlation function $g(r)$ is given by $Z\delta(r - 1)$ +smooth function

First reaction: happy. But critical exponents were missing.

No problem. We have mean field theory. Non-trivial critical exponents appear only at below the upper critical dimensions.

However: critical exponents are nearly independent from the dimensions.

Violations of isostaticity is worrying.

The troubles do not disappear with the dimension (nice computation in the infinite dimension limit $\hat{\phi} \equiv 2^d/d\phi$)

No problem: the distribution of the cage is far from being Gaussian. It may contains a power law tail.

However.....

Idea: Kurchan, GP, Zamponi

All cats are grey in the dark and all functions are Gaussian in infinite dimensions d.

$$\delta(|x| - d) \approx \exp(-x^2/2) \approx \exp(-d^{1/2}|x|)$$

(microcanonical and canonical ensamble)

$$\delta(H - NE) \approx \exp(-\beta H)$$

So we can dream to take $P_i(x_i)$ to be a Gaussian.

We have esplicitly check that Gaussian is OK when $d \to \infty$

Final approximation

$$\phi_i(x_i) \propto \exp\left(-(x_i - x_i^{cage})^2/(2A)\right)$$

The number of particle interacting at a given time with a given particle is of order d, a Gaussian distribution is natural.

Conclusions: we should have the the results of GP and Zamponi are correct unless....

unless something new happens: an instability, i.e. divergence of a susceptibility.

Replica Symmetry Breaking (Kurchan, GP, Urbani, Zamponi) instability.

Check stability: for each particle we define the squared radius of cage (the mean squared displacement).

$$\Delta_{TOT} = \sum_{i=1,N} \Delta_i \qquad \langle \Delta_{TOT}^2 \rangle - \langle \Delta_{TOT} \rangle^2 \equiv N\chi$$

The susceptibility χ can be computed and its given by

$$\chi^{-1} \propto \phi_G - \phi$$

Theory does not work for $\phi > \phi_G$.

$$G_{i,k} = \langle \Delta_i \Delta_k \rangle_c \qquad G^2(x) = \overline{G^2_{i,k} \delta(x_i - x_k - x)}$$

What happens for $\phi > \phi_G$??

Biforcations: each solutions for the cage's is surround by many solutions

$\psi_i^\alpha(x) = \psi_i^*(x) + (\phi - \phi_G)^{1/2}\psi_i^\alpha(x) \qquad \alpha = 1.....$

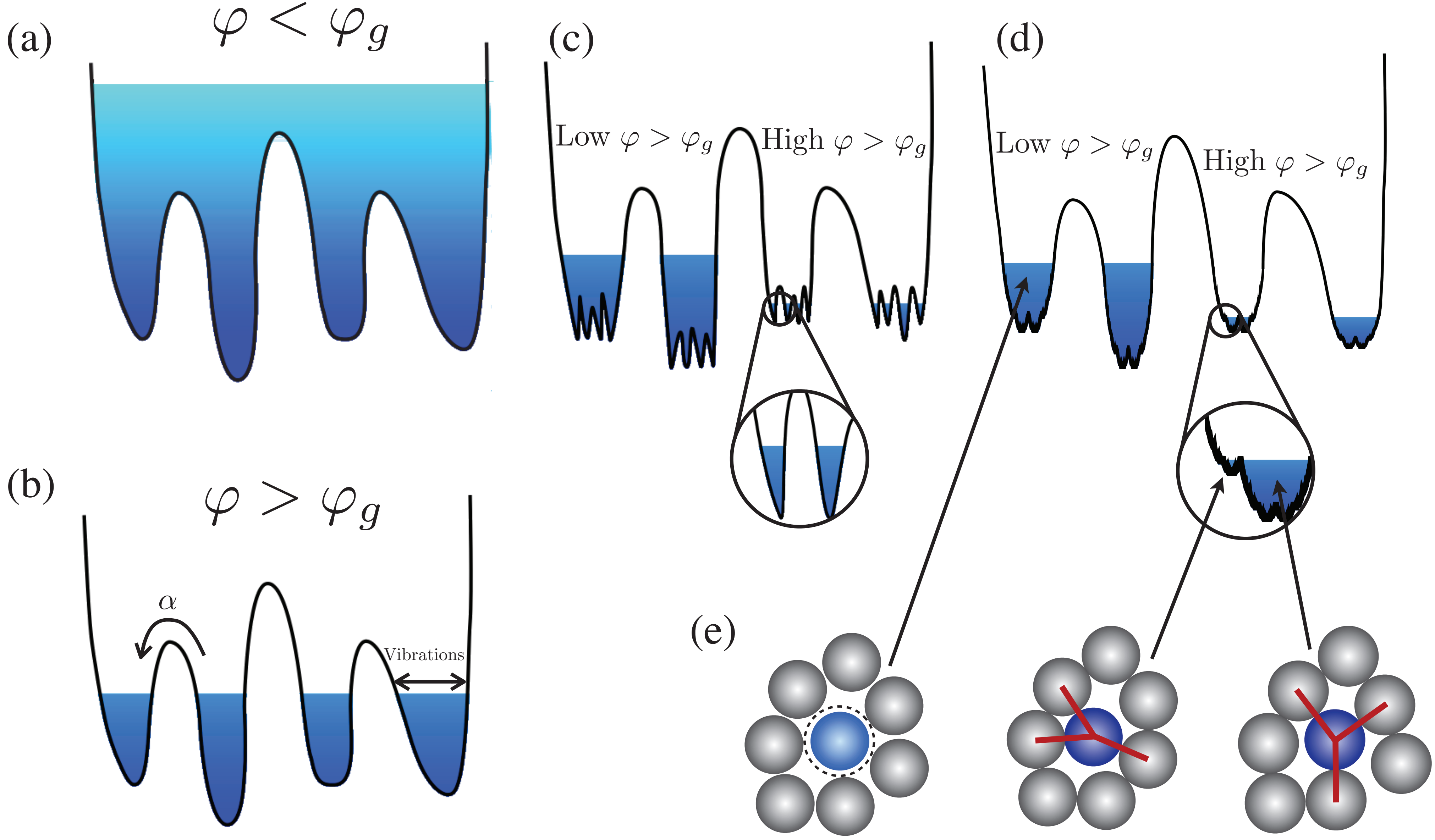
$\psi_i^\alpha(x) = \psi_{state}(x - x_i^\alpha) \qquad P(x_i^\alpha)$ is Gaussian centered around x_i.

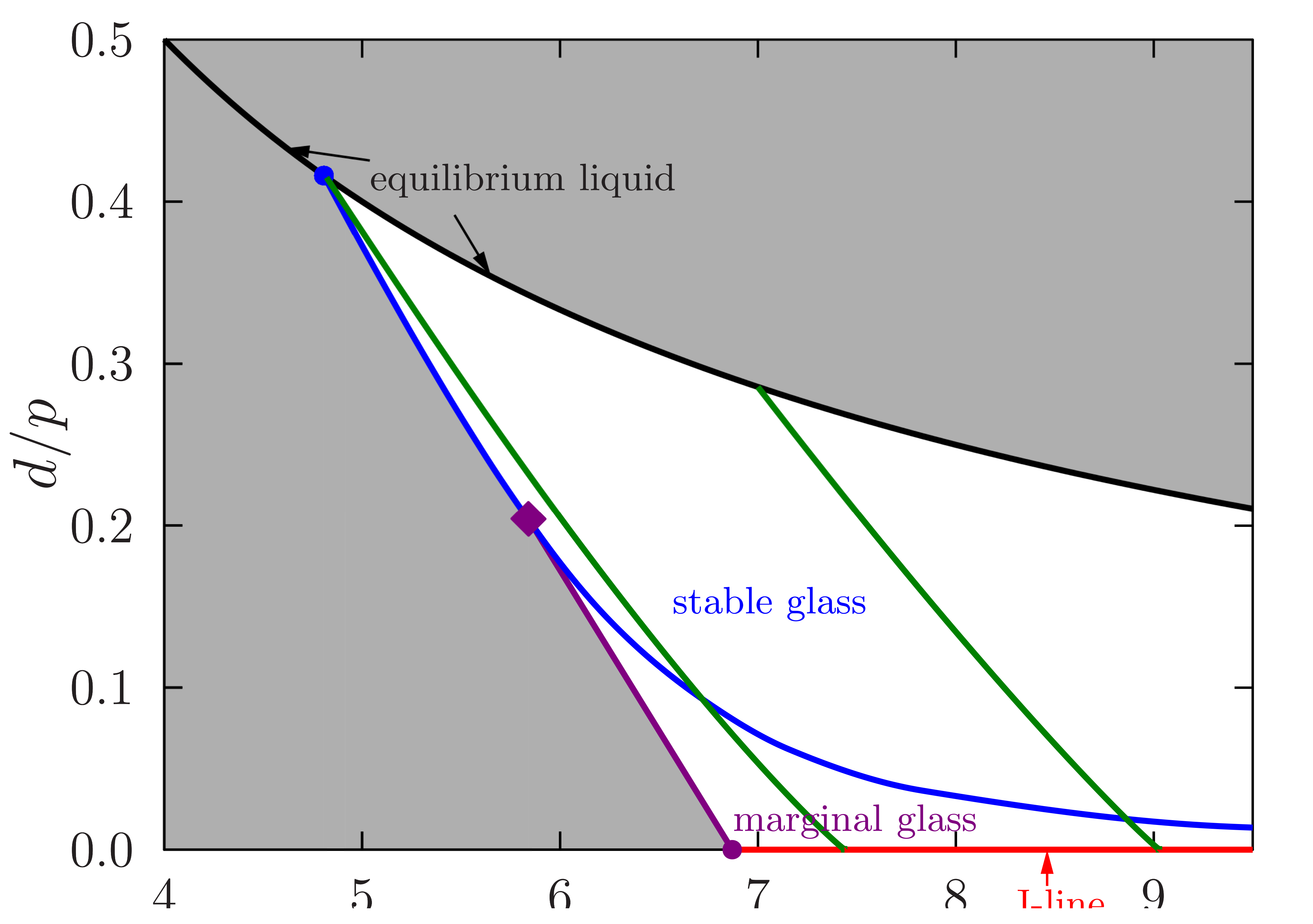
Each state breaks into a family of states that are nearby one to the other.

We can define a complexity for the states and a complexity for families:

$$\frac{\partial\Sigma_{states}(f)}{\partial f} = \beta m_{states} \qquad \frac{\partial\Sigma_{families}(f)}{\partial f} = \beta m_{families}$$

$$m_{states} = m_{families} + A(\phi - \phi_G)$$


(a)
$\varphi < \varphi_g$
(b)
$\varphi > \varphi_g$
α
Vibrations
(c)
Low $\varphi > \varphi_g$
High $\varphi > \varphi_g$
(d)
Low $\varphi > \varphi_g$
High $\varphi > \varphi_g$
(e)



0.5
0.4
0.3
0.2
0.1
0.0
d/p
4
5
6
7
8
9
equilibrium liquid
stable glass
marginal glass
J-line

We have seen two levels RSB.

Three levels: states are grouped into families, that are grouped into orders....

Continuous Replica Symmetry Breaking

Many subcages distributed in a similar faction, organised in an hierarchical way:.

We consider K levels: The distribution of the center of masses of the $(k+1)^{th}$ level are at distance squared of order $1/K$ from the one of the $(k)^{th}$ level. We can write explicit formulae for the various distributions.

At the end of the day we have to do the limit $K \to \infty$. One finds states that are organised in a hierarchical way.

The probability distribution is rather complex. It needs a certain amount of heavy mathematics to prove that the construction has some sense and the the $K \to \infty$ limit has a probabilistic limit.

It took 30 years of works to prove (with many decisive contribution of Francesco Guerra) that this structure of states is correct in the Sherrington Kirkpatrick model of spin glasses. 20 years to prove that the computation of the free energy based on these ideas was correct and 10 additional years to prove the structure of the states is correct.

With replicas:

$$\rho(X_i) \propto \exp\left(-\sum_{a=1,m;b=1,m}\left(x_i^a - x_i^b\right)^2/(2A_{a,b})\right)$$

where A is a matrix that encodes the probability distribution of the states.

The model can be solved and we arrive to non linear differential equations very similar to those of the Sherringon-Kirkpatrick model.

The low temperature behaviour of SK correspond to infinite pressure in hard spheres.

Highly non trivial scaling limit with non-rational exponents.

We can apply the same ideas to glasses (CKPUZ)

After long long algebraic manipulations we get the final expression of the non trivial part of entropy in the full RSB case in the $d \to \infty$

We introduce a function $\Delta(x)$ in the interval $[m:1]$

$$S_{\infty\mathrm{RSB}} = -m \int_m^1 \frac{\delta y}{y^2} \log\left[\frac{y\Delta(y)}{m} + \int_y^1 \delta z \frac{\Delta(z)}{m}\right] - \widehat{\varphi}\, e^{-\Delta(m)/2} \int_{-\infty}^{\infty} \delta h\, e^h [1 - e^{m f(m,h)}] \,,$$

$$\frac{\partial f(x,h)}{\partial x} = \frac{1}{2}\dot{\Delta}(x) \left[\frac{\partial^2 f(x,h)}{\partial h^2} + x\left(\frac{\partial f(x,h)}{\partial h}\right)^2\right] \,,$$

$$f(1,h) = \log \Theta\left[\frac{h}{\sqrt{2\Delta(1)}}\right] \qquad\qquad f_{SK}(1,h) = \log(\tanh(\beta h))$$

$\Theta(x)$ is the error function. The function $\Delta(x)$ parametrise the distribution of the size of the cages.

One step RSB formulae can be obtained as a limit of the full RSB formulae. Three regimes

- Low pressure: Liquid phase
- Intermediate pressure: one step RSB phase: i.e. glassy systems with well separated cages
- High pressure: full RSB phase with cages organised in an hierarchical way.

A Gardner type transition separates the one step RSB phase from the full RSB phase.

A detailed analysis

$y = 1/m$

We introduce $k(y)$ simply related to $\Delta(y)$

$\frac{1}{\gamma(y)} = y\kappa(y) - \int_1^y \delta z \kappa(z) \qquad \gamma(y) = y\Delta(y) + \int_y^{1/m} \delta z \Delta(z)$

In the same way as in the SK model, the stationarity condition can be simplified. We introduce a function $\widehat{P}(y,h)$ that satisfies a simple differential equation

$$\frac{\partial \hat{P}(x,h)}{\partial x} = \frac{1}{2}\dot{\Delta}(x)\left[\frac{\partial^2 \hat{P}(x,h)}{\partial h^2} + 2x \frac{\partial f(x,h)}{\partial h}\frac{\partial \hat{P}(x,h)}{\partial h}\right] ,$$

$\kappa(y) = \frac{\widehat{\varphi}}{2\gamma^2(y)} \int_{-\infty}^{\infty} \delta h \, e^h \widehat{P}(y,h) \widetilde{f}'(y,h)^2 \qquad q(y) = \int dh P(y,h) m(y,h)^2.$

One can prove marginal stability $\chi = \infty$ and

$1 = \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} \delta h \, e^h \widehat{P}(y,h) \widetilde{f}''(y,h)^2 \ . \qquad 1 = \int dh P(y,h) \left(\frac{dm(y,h)}{dh}\right)^2$

Cavity interpretation with Zamponi is in progress.

Interesting limit: pressure going to infinity, $m \to 0$. This is the jamming limit!

The marginal stability condition

$1 = \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} \delta h \, e^h \widehat{P}(y,h) \widetilde{f}''(y,h)^2$

implies isostaticity.

Scaling limit when the pressure goes to infinity. The following scaling form reproduces itself in the equations.

$$\widehat{P}(y,h) \approx y^a p(hy^b)$$

How to determine the exponents a and b?

We can resort to the indignity of solving numerical the equations and to extract the exponents by fitting the solution.

Non linear velocity selection An example

$$\dot{\phi}(x,t) = -\frac{\partial^2 \phi(x,t)}{\partial x^2} + \phi(x,t) - \phi^2(x,t)$$

Propagating front: at large time

$$\phi(x,t) \approx f(x - vt) \qquad -vf(z) = \frac{d^2 f(z)}{dz^2} + f(z) - f^2(z)$$

The equation for f has a solution for any v.

Theorem: if $\phi(x,0) = 1$ for $x < 0$ and $\phi(x,0)$ goes fast to zero sufficiently fast.

$$\phi(x,t) \approx f(x - v^* t)$$

The velocity v^* is fixed by a marginal stability condition.

The a and b can be computed analytically form the previous equations in the scaling regime.

For example a can be computed as function of b by solving an eigenvalue equation.

We can find b by imposing the marginality condition.

$1 = \frac{\widehat{\varphi}}{2} \int_{-\infty}^{\infty} \delta h \, e^h \widehat{P}(y,h) \widetilde{f}''(y,h)^2$

At the end we find

$$a = 0.29213 \qquad b = 0.70787 \qquad a + b = 1$$

Only if we use continuous replica symmetry breaking we find at infinite pressure:

Isostaticity: the number of contacts of spheres Z is equal o ND: each sphere has in the average $2D$ contacts.

The correlation function $g(r)$ has a singularity at $r = 1$:

$$g(r) = 2D\delta(r-1) + C(D)(r-1)^{-\alpha} \qquad \alpha = 0.41269 \equiv a/b$$

The quasi-contact exponent α has been measured by several groups in dimension D ranging from 2 to 13, all obtaining roughly $\alpha \approx 0.4$.

The most precise estimates being $\alpha = 0.41(3)$ for $D = 3$.

Without continuous replica symmetry we have

$$g(r) = Z\delta(r-1) + O(1) \qquad Z > 2D \qquad \text{WRONG!!!}$$

Why fractal?

If we sum over all the sub-cages we can define a function $\rho_i(x)$.

We can define a correlation function

$$C(r) = \overline{\int dx dy \rho_i(x) \rho_i(y) \delta(|x-y| - r)}$$

$C(r)$ has a power like behaviour corresponding to a fractal dimension

$$\mathcal{D} = \frac{2}{\kappa}$$

Open problems.

- Can you explain all this in a simpler way, e.g. without replicas? Likely yes (GP and Zamponi in preparation).
- Can you prove that gives the exact result in one of MK_x models? I hope so, but it is not clear when (2 years or 20 years?)
- What happens in finite dimensions at jamming? Everything seems ok, but why?
- What happens to the Gardner transition in finite transition? It is still there or not?
- If yes, can we pinpoint the Gardner transition numerical simulations and in experiments?

We must:

- Many other quantities have to be computed. In particular the spectrum of small oscillations.
- We should be able to do precise computation in the dynamics. (MCT like equations, but not MCT).
- We need to complete the extension of the results to finite dimensional models.
- Compare the prediction for the dynamical correlations with numerical simulations and with experiments.
- Compute systematically $1/d$ corrections.
- Understand the renormalization group approach in finite dimensions.

The MKK model

We consider a random regular lattice of coordination number z. On each site i we have a variable x_i that is a d-dimensional vector in box of side L and volume L^d. For each link we have a random shift s_{ik}.

We are interested the configurations such that for each link i, k

$$|x_i - x_k - s_{i,k}| > 1$$

In a first approximation forget the shifts s. In each box we have spheres of diameter 1.

Each sphere see the sphere on the nearby box. The density is

$\rho = zL^{-d}$

The SK limit is obtained when $z \to \infty$ at fixed ρ.

We are interested to compute the entropy as function of ρ. i.e. the volume in configuration space where all the bounds are satisfied.

$S(\rho) \to \infty$ when $\rho \to \rho_j$. The pressure $(-dS/d\rho)$ goes to infinity at ρ_j.