Classical and quantum landscape in glasses

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Let me summarize the standard approach to the low temperature behaviour of glasses in the quantum regime.

The approach is semiclassical: one derives the quantum behaviour from the basic properties of the classical landscape. Of course the final results will crucially depend on the supposed classical properties.

We known (e.g. from numerical simulations) that in a glassy system there are many different local minima of the classical energy that have similar energy.

It is assumed that:

- In a first approximation each classical local minimum corresponds to a different quantum state.
- While classical tunnel among these states is exponentially forbidden at $T \approx 0$, quantum tunnel events are possible within the experimental time scale and they play a crucial role.

In the simplest picture the classical landscape is composed by a collection of bistable systems (Two Level Systems). Each TLS weakly interacts with the others TLS's. For example one (or few atoms) may stay in two different classical minima.

Each TLS is characterized by the energy difference (ΔE) and by the quantum tunnelling time.

We define the density (per unit volume) of TLS at given ΔE: $\rho(\Delta E)$.

We assume a random distribution of these parameters. Very nice result for the specific heat $C(T)$:

$$\rho(0) > 0 \quad \longrightarrow \qquad C(T) \propto T \, .$$

More detailed arguments tell us that the thermal conductivity is proportional to T^2.

Experiments do agree on these predictions, but there are some discrepancies with more detailed predictions.

For example friction does go to zero when $T \to 0$ much slower than predicted.

Is the classical picture correct?

I think not. In the last years a different picture has been put forward.

The new analysis is based on a careful study of mean field theory (Charbonneaux, Kurchan, G.P., Urbani, Zamponi; Franz, G.P., Urbani, Zamponi).

Mean field theory should be valid in two limits:

- When the space dimensions go to infinity.
- In the Mari-Kurchan model.

Mean field theory had recently a spectacular success for hard spheres at high pressure.

The Mari-Kurchan model

$$H = \frac{1}{2} \sum_{i,k=1,N} V(x_i - x_k - \Lambda_{i,k}) \qquad \Lambda_{ik} = -\Lambda_{k,i} \qquad \langle \Lambda^2 \rangle \to \infty$$

In the liquid phase

$$g(x_i - x_k - \Lambda_{i,k}) \propto \exp\left(-\beta V(x_i - x_k - \Lambda_{i,k})\right)$$

The first term of the virial expansion becomes exact in the limit $\langle \Lambda^2 \rangle \to \infty$.

No acustic phonons are present in the Mari-Kurchan model.

¿What is a glass and how do we characterize the glass transition?

At low temperature the particles becomes jammed. They cannot move because the other particles cannot move. The diffusion is very small and the viscosity is very large

At low temperatures the characteristic time becomes very large: it firstly increases of a factor 10^{18} and then it becomes too large to be measured.

¿ Does the characteristic time diverges at a finite temperature or does it remain finite at all temperature?

The phase space of the system breaks down into many ergodic regions (valleys) and each particle is confined in a cage.

The number of valleys is exponentially large with the size of the system.

¿What happens when we cool a system?

When we cross the glass transition the system becomes frozen in one valley of the landscape.

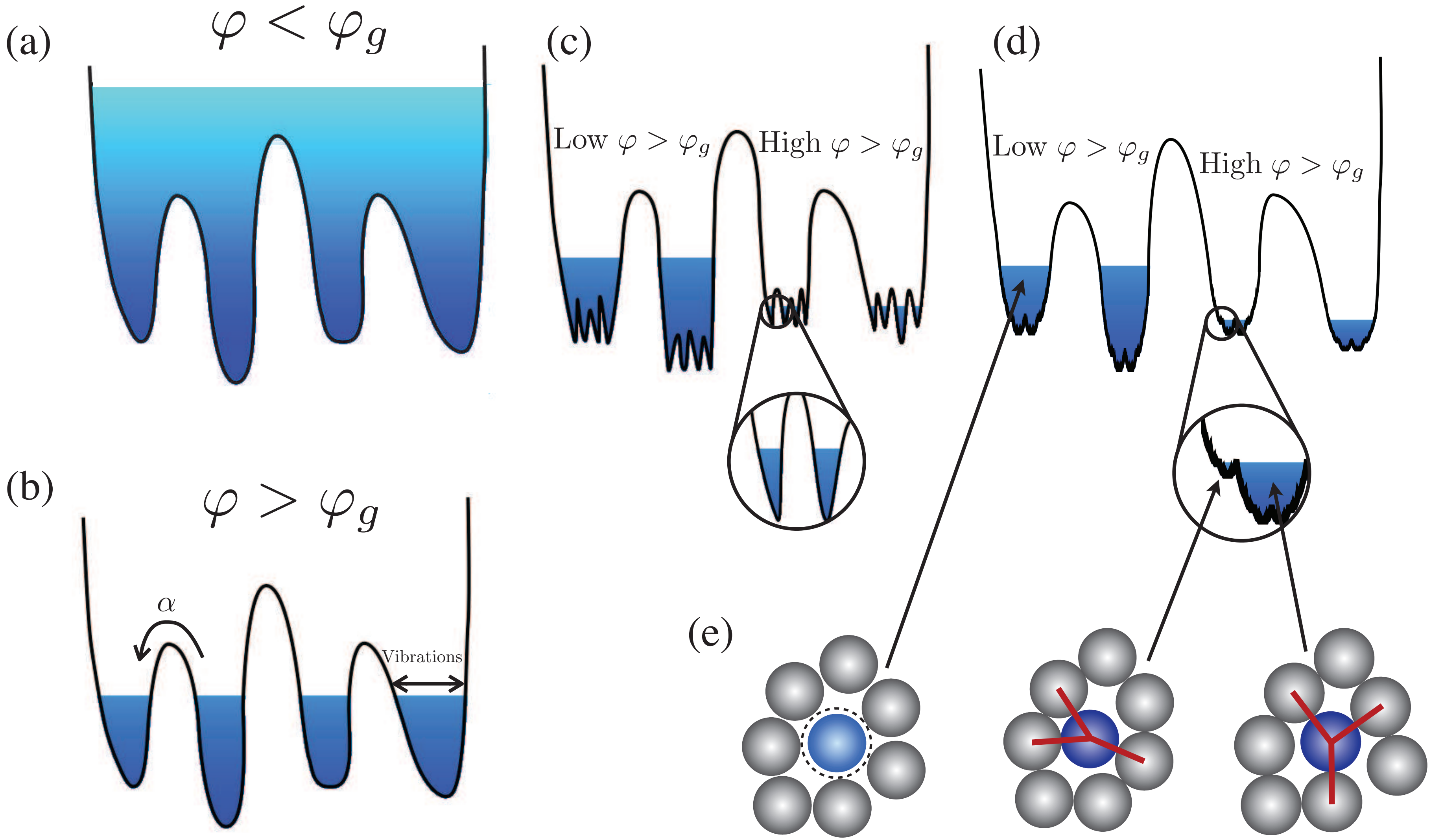
Naively we expect that nothing happens by further decreasing the temperature.

In mean field theory we cross a new transition: the Gardner-(Gross-Kanter-Sompolisky) transition.

Each valley splits into smaller valleys that spit in smaller valleys.

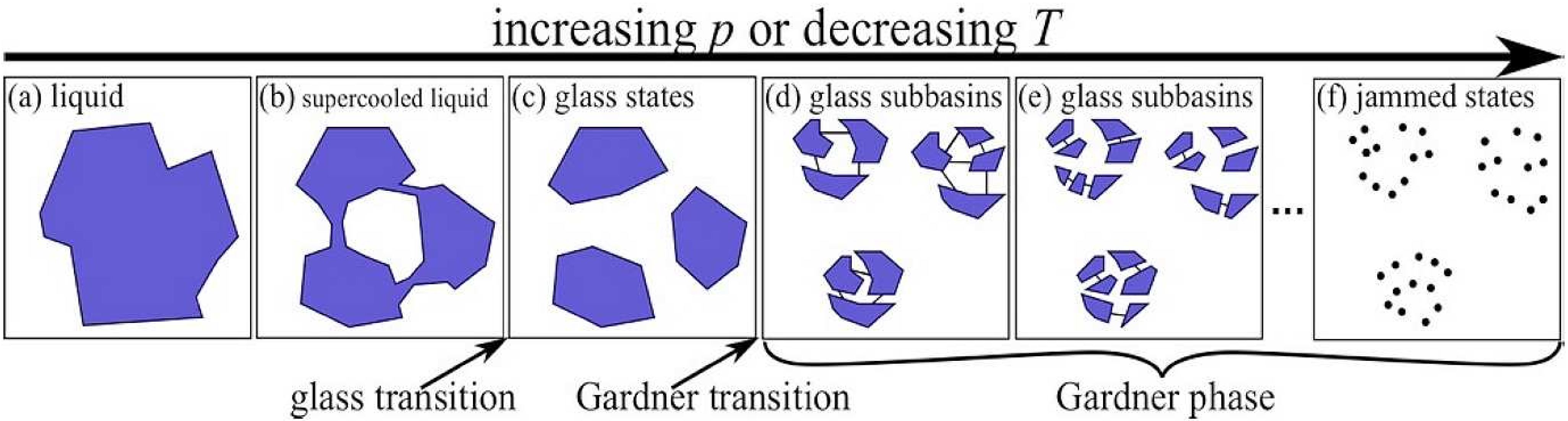
You end up with an infinite number of valleys organized in an hierarchical way.

Tha same picture happens (rigorously) in the Sherrington-Kirkpatrick model for spin glasses and it is called spontaneous replica symmetry breaking.



Increasing the density $\longrightarrow$ Lowering the temperature for soft spheres.

The Garner transition



At finite high pressure cages break up in smaller cages that are not too far one form the others (Kurchan, GP, Urbani, Zamponi)

At infinite process each jammed state is surrounded by other jammed states that form a fractal in configuration space (Charbonneau, Kurchan, GP, Urbani, Zamponi)

This cage breaking process is described by a functional order parameter $y(\Delta)$.

Hard spheres

Infinite pressure $\longrightarrow$ zero temperature.

At infinite pressure many spheres are at contact, i.e. at distances exactly equal to the diameter D of the spheres.

Long range correlations appears in this limit. We can define some critical exponents for local quantities:

$$g(r) \propto (r-D)^{-\gamma}\,, \text{ for } r > D\,; \quad P_{forces}(f) \propto f^{\theta}\,; \qquad \overline{\Delta^2} \propto p^{-\kappa}\,.$$

- $\Delta_i^2 \equiv \lim_{t\to\infty} t^{-2} \int_0^t dt' dt'' (x_i(t') - x_i(t''))^2$ is the size of the cage of the i^{th} particle
- p is the pressure
- f is the force on a sphere.

A naive theory gives $\theta = \gamma = 0 \qquad \kappa = 2$.

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A phenomenological analysis (Wyart), similar in spirit to the one done 50 years ago for the standard phase transitions, gives the following relations for the exponents:

$$\gamma = 1/(2+\theta) \qquad \kappa = (1+\theta)/(3+\theta)\,.$$

Large scale numerical simulations give:

$$\gamma \approx \theta \approx .4 \qquad \kappa \approx 1.4\,.$$

A naive theory gives $\theta = \gamma = 0 \qquad \kappa = 2$.

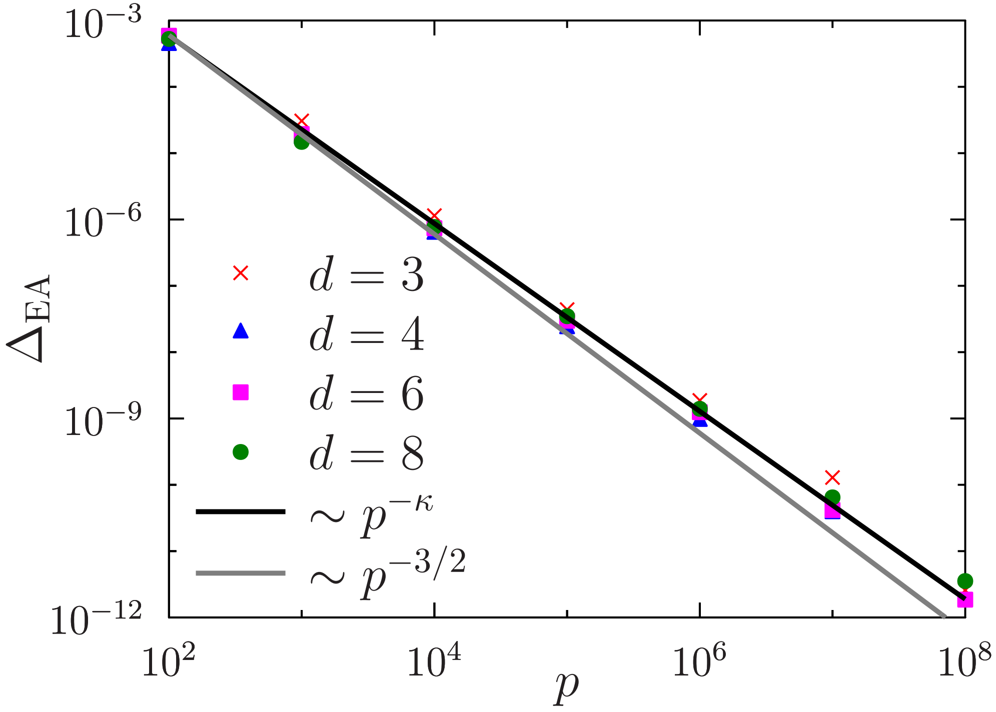
Surprising Results

After a long computations one finds (Charbonneau, Kurchan, GP, Urbani, Zamponi) the exact values of the exponent that are apparently irrational:

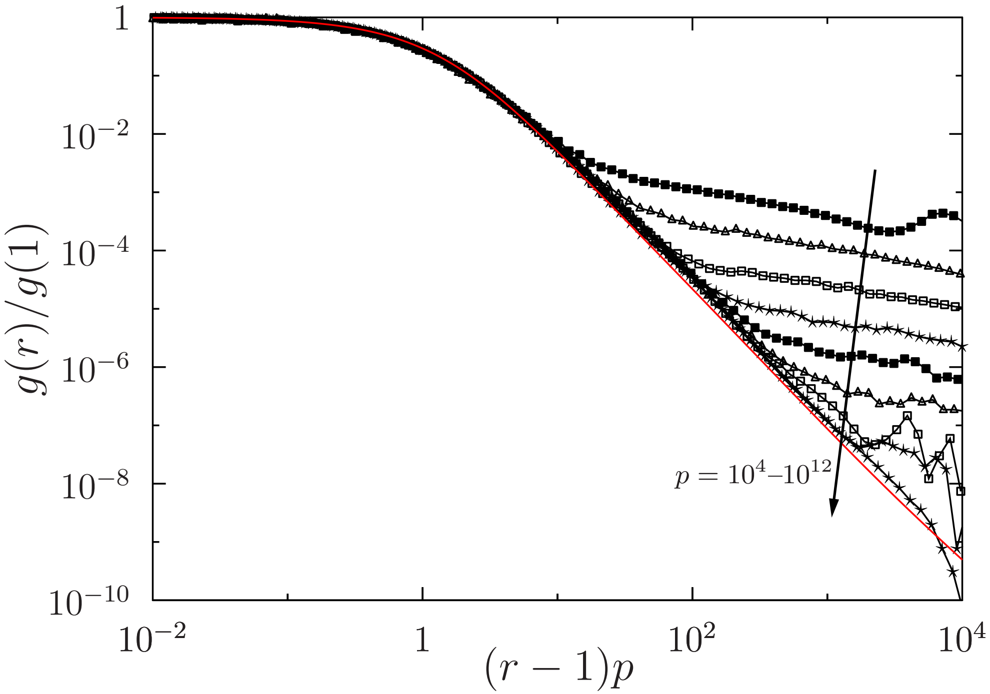
$\gamma = 0.41269\ldots \qquad \theta = 0.42311\ldots \qquad \kappa = 1.41574\ldots.$

The computations uses heavily the very compact replica symmetry breaking formalism that was developed for spin glasses.

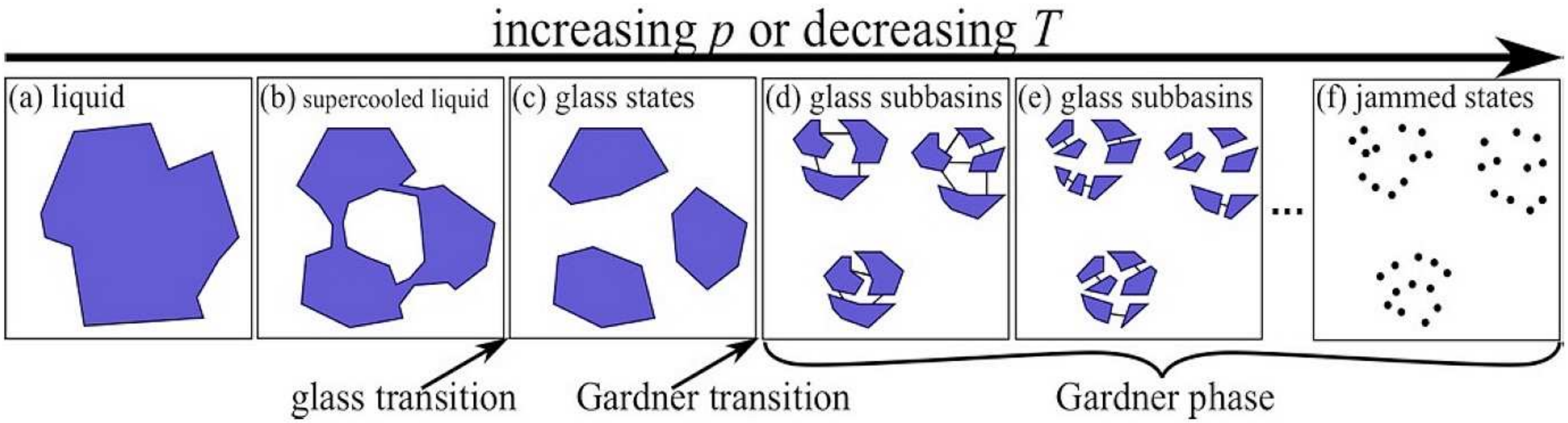
Numerical simulations tell us that the corrections to mean field theory exponents from 2 dimensions up to ∞ are absent (or very small).



Cage size Δ versus pressure.



The correlation $g(r)$ near $r = D = 1$.



New predictions form mean field theory for *classical* soft spheres.

- There are minima that differ from the ground state by a small simultaneous movement of a large number of particles.
- The spectrum of harmonic excitations around a minimum has an excess of low energy modes that are quite distinct from the phonons.
- The effects of a local perturbation extend at very large distances.
- Long range correlations are present.
- Slow approach to equilibrium is expected (e.g. ageing phenomena).

The existence of these new states should have deep consequences in the *quantum* case.

We can conjecture that:

- These states will give contributions to the correlations and response functions with a peculiar behaviour in the low momentum region. The corresponding excitations are rather extended. This should be relevant for the behaviour of small momentum quantities.
- The tunnelling amplitudes could be quite large.
- These states strongly overlap and they cannot be considered as the superposition of independent two level systems. This is very interesting because there is an experimental evidence for the failure of the predictions coming from independent two level systems.

First consistency checks

- We must solve the quantum soft sphere model in the infinite dimensions limit and find the low temperature behaviour.
- We must study the quantum Mari-Kurchan model in finite dimensions. We can look to quantum numerical simulations for the static quantities and study the dependence on the dimension.

Further questions

- In the previous model we could find all the classical minima and quantum barriers and check if the semiclassical approximation gives the correct results for the statics.
- ¿Can we use the same approximation for the dynamics?
- The tunneling states are strongly interacting. ¿Does this explain the experimental data? ¿Can we construct a phenomenological theory?
- ¿Can the strong interaction of the tunnelling state induce some kind of phase transition?
- There is a glassy material where a mysterious quantum transition has been observed at very low temperatures, i.e. at 5.84 mK. ¿How to explain the experimental data?