A *new* dynamical transition in mean field disordered systems

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Structural glasses.

Mean field theory and the dynamical transition.

Cooling: quenching and annealing.

A new transition: its relations with the Gardner transition.

The mean field theory for hard spheres.

Surprises at infinite pressure.

Glasses



The specific heat depends on the cooling speed Speed-dependent entropy

Schematic view of the internal energy as function of the temperature:



The position of the dynamic line slightly depends on the cooling speed (on a logarithmic scale).

No precursor effects in static quantities (like in first order transitions).

Divergent correlation times (like in second order transitions). Large correlation length in the dynamics.

A systematic study of different mean fields models of spin glasses started in the '80. The aim was also to find the different universality classes.



Energy as function of the temperature. Dynamic line is the same for any non zero cooling rate. The limit $t \to \infty$ and $N \to \infty$ do not commute.

Correlation time is divergent at T_d .

Correlations function at equilibrium C(t) satisfies mode-coupling equations.

Mean field theory: \rightarrow Neglecting correlations.

Two branches:

- Infinite connectivity, e.g. Sherrington Kirkpatrick model, infinite dimensional models.
- Finite connectivity, e.g. diluted models, models on Bethe Lattices.

The homegenous *p*-spin model: p = 3

$$H = \sum_{i,k,l} J_{i,k,l} \sigma_i, \sigma_k, \sigma_l$$

$$J_{i,k,l} = 1/N$$
 random number $J_{i,k,l} = 3$ -J-symbols

First case random, second case is deterministic. Silvio Franz and John Hertz invented the second model and showed the equivalence with the first models. Important conceptual result.

TAP equations give equilibrium states, stable or metastable.

Two branches:

- The Ising case: $\sigma_i = \pm 1$
- The spherical case: $\sum_{i=1,N} \sigma_i^2 = N$



The dynamics transition that correspond to the breaking of the main valley in free energy into an exponentially large number of metastable states that are far away. The barrier for jumping is proportional to $N(T_d - T)^3$.

This is not a bifurcation: there are no premonitory signs in the statics (better, no signs whatsoever)..

Below the phase transitions the equilibrium states is the union of an exponential large number of metastable states.

The number of states that dominate equilibrium is the complexity $\Sigma(T)$. Who invented this namer for the *configurational entropy*???

There is a new *static* transition where the complexity becomes zero

 $\Sigma(T_s) = 0 \; .$

Below T_s only a few states dominate the equilibrium distribution. (Replica symmetry is broken at one step).

The spherical 3-spin model.

Metastable states are bona fide minima.

A metastable state can only disappear when increasing the temperature.

Any metastable state can be obtained by increasing the temperature starting from a low temperature states. State do preserve the ordering in free energy when temperature is changed (no temperature chaos). Isocomplexity

When you quench from infinite temperature go to the highest energy metastable states, that are the same you get by annealing from any temperature above the critical temperature.



The equilibrium dynamics has a divergent correlation time when we approach T_B from above.

The schematic mode coupling theory is valid. At T_c we have that the correlation decays as

 t^{-a}

where a satisfies the equation:

$$\Gamma(1-a)/\Gamma(1-2a) = X \equiv \lambda$$

This equation was found at short distance in time in different contexts by Sompolisky and Zippelius (spin glasses) and by Goetze (mode coupling equations for glasses).

The Ising p-spin model or p-spin non homogeneous spherical model, i.e. $H=H_{p=3}+H_{p=4}$

State do preserve the ordering in free energy when temperature is changed (i.e. temperature chaos).

Isocomplexity does not work.

The states do evolve in a continuous way with the temperature. We define

q(T,T')

as the overlap among two states at different temperature during cooling.

The overlap is a continuous function of the temperature q(T, T').

We can set up a state following procedure: Barrat, Franz and Parisi 1996.

Metastable state may become unstable by cooling the temperature. Biforcations: they breaks into states that are not very far one from the other.





The energies under cooling in the stable case.

Two possibilities:

These states may be equidistant one from the other (one step replica symmetry breaking).

They may be organised in a hierarchical structure (continuous symmetry breaking).





Type II instability

Therefore the qualitative phase structure is the following: Energy in the stable phase.



Generic feature: for T near T_d (a detailed study has been done by Franz, Parisi and Ricci-Tersenghi)

$$T_D - T_B \propto (T_D - T_I)^{1/2}$$

Why this transition is important?

After thermalise in the low temperature phase, when you cool you find a glass transition inside the glass phase, with a value of a given by

$$C(t, T_B) \propto t^{-a} \qquad \tau \propto (T - T_B)^{1/a}$$

$$\Gamma(1 - a) / \Gamma(1 - 2a) = X(T_B) \qquad X(T_d) = X$$

Below T_B we aspect generalised fluctuation dissipation (Cugliandolo Kurchan) with a parameter $X_{CK} \approx X(T_B)$.

The situation is similar to the Sherrington Kirkpatrick model in a field (De Almeida Thouless transition).



The energies under cooling in the stable case.

Why the two models have a different behaviour at low temperature?

The answer is the Gardner transition. Let us consider what happens at equilibrium. In some systems it is possible that the various equilibrium states biforcate into many other equilibrium states.

This fact was unexpected and it was discovered by Elizabeth Gardner in the p spin Ising system in the 'eighties. It happens in many systems.

This transition is likely to be connected to Johari-Goldstein relaxation (but I have to study the phenomenology).



The energies under cooling in the stable regions.

The lines end at the instability point.

What happens at lower temperatures?

Two formalisms:

- Quasi dynamical formalism (Franz and Parisi)
- Simple state following with Replica Symmetry breaking .

Are they equivalent?????

Hard Spheres of diameter 1 at high pressure: glass transition and jamming

Large dimension D limit. (Series of papers: last one, Charbonneau, Kurchan, Parisi, Zamponi, Urbani on Nature Communication.

Trivial liquid phase. Reduced density $\phi = \rho V_D$. For $\phi < \exp(DA)$ A = .07338 there are no corretions to the first order of the virial expansion.

Increasing the pressure there is a glass transition and there is a jammed phase at infinite pressure. No crystallisation for a reasonable time scale (e.g. 10^7 natural time units) if D > 3 or D = 3 and with a binary mixture.

Glass transition happens at large dimension at $\phi = O(D) << \exp(DA)$. Crystallisation become strongly suppressed in high dimensions.

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 $P_i(x - x_i)$.

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

 $\mathcal{P}(P)$

We have a functional order parameter: a big mess (Mézard, Parisi, Tarzia, Zamponi).

Idea All cats are grey in the dark and all functions are Gaussian in infinite dimensions. So we can take $P_i(x_i)$ to be a Gaussian.

Final approximation

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

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

With replicas: one introduce m replicas.

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



Replica Symmetry Breaking Many subcages distributed in a similar faction, organised in an hierarchical way:

With replicas:

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

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 apparently non-rational exponents.

Only if we use 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:

$$g(r) = 2D\delta(r-1) + C(D)(r-1)^{-\alpha}$$
 $\alpha = 0.41269$

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.



Hard spheres at D = 4.

Conclusions

The dynamical transition is not an isolated point but it is the end point of a line of second order transitions that are present during cooling.

These transitions correspond to a divergence of the correlation time in the low temperature phase (Johari-Goldstein relaxation?).

The transition point depend on the amount of thermalisation.

Below the transition point replica symmetry is broken in a continuous way: hierarchical organised states.

The breaking of replica symmetry is crucial to get qualitatively correct predictions in the jammed state (infinite pressure) of hard spheres.

A panoplia of of non-trivial critical exponents describe the behaviour of jammed hard spheres. The exponents seems to be independent from the dimension. They can be computed analytic using sophisticated replica symmetry arguments.

To do list:

- Fully understand the behaviour in the low temperature phase.
- Finite D phenomenology (the dynamical transition become a crossover point finite D).
- Renormalization group around the transition point.
- Why exponents for jamming do not depend on the dimension?
- Do we get all the exponents in an accurate way?
- Clearly identify the transition in numerical experiment and in the real world.