The Spin Glass Paradigm

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I am very happy to be here (finally, my first scientific visit to Spain!).

An introduction to an interesting and debated subject.

The paradigm of Spin Glasses: from the analytic solution of the Mean Field theory, with its many new features, down to physics, biology, economics, optimization and more...

Mainly work with: Giorgio Parisi, Federico Ricci-Tersenghi, Felix Ritort, Juan J. Ruiz-Lorenzo and Francesco Zuliani.

Madrid and Zaragoza, May 1999

A walk through the main ideas and an illusory summary (appropriate to a many hour discussion, if any).

Paradigm. The Mean Field Theory and Replica Symmetry Breaking, RSB. How does it work, why does it work. Its dramatically new features.

The numerical methods. Smart numerical simulations (they better be!). Tempering.

The phase transition to the spin glass (RSB) phase. Characterization of the phase transition. Phase transition in field.

The dynamical behavior of the system. Memory, aging, and much more. Real spin glasses and memory experiments.

Real glasses. Complexity instead of disorder. Dynamical transition in REM like models.

Rigorous approach to disordered systems. Finite volume states.

Learning. Hopfield model. Neural networks.

Immunology.

Proteins, polymers.

Optimization.

Economics and game theory. [... more ...].

Spin Glasses? Why do we study spin glasses?

Systems with frustration and quenched disorder. Maybe frustration more crucial than disorder (real glasses).

Traps that do not change in time.

The study of Spin Glasses has led, in the last years, to a large amount of new physics, and created a new field, where things are indeed very difficult to understand.

Solution of Mean Field Theory

Replica Symmetry Breaking

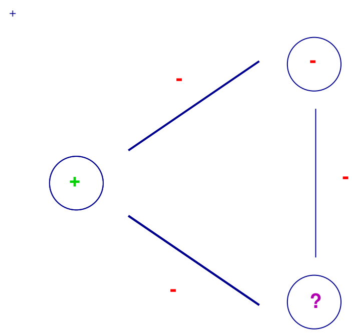
Many States

MF, infinite range $\longrightarrow$ short range (i.e. realistic)

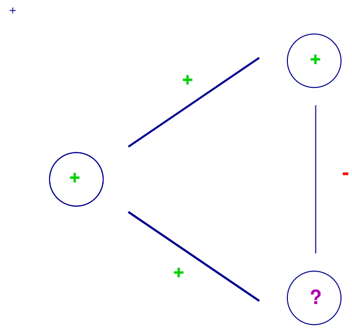
Concept of state

numerical results are a priori, but a clear picture is crucial for a systematic treatment

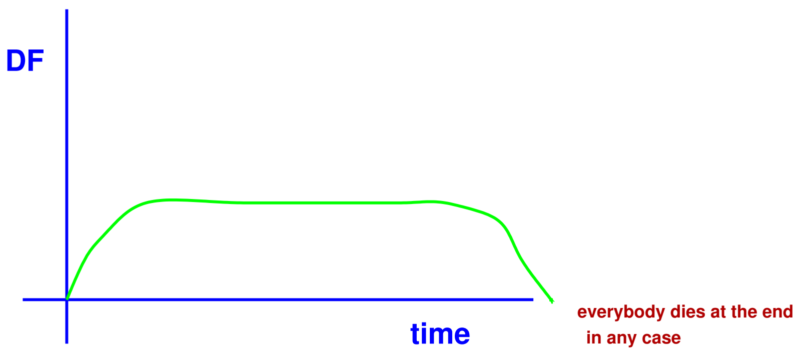
Frustration: antiferromagnet on triangular lattice.



One ground state in ferromagnet (but for Z_2 symmetry), many ground states here. Real life: A is friendly to B and C, but B and C are enemies.



Dramatic frustration. Consider a play. At each moment of the play, t, consider all triples of actors, and count the frustrated triples. In a Shakespeare typical play



(i.e. complexity is interesting).

Overlap among two replicas will play a crucial role (order parameter): it tells us about if typical configurations of the system are similar or not.

$$q^{(a,b)} \equiv \frac{1}{V} \sum_i \sigma_i^{(a)} \sigma_i^{(b)}$$

together with its distribution

$$P_J(q) \ , \quad P(q) \equiv \overline{P_J(q)}$$

N spins

$$H[\sigma] = H_{\{J\}}[\sigma]$$

$\{J\}$: quenched random couplings

$\langle \cdot \rangle$ thermal average, $\overline{\cdot}$ disorder average, $E\,(\,\cdot\,) \equiv \overline{\langle \cdot \rangle}$

Finite volume

$$P_{\{J\}}[\sigma] \propto e^{-\beta H_{\{J\}}[\sigma]}$$

Finite D: Edwards Anderson, $\sigma = \pm 1$, $\overline{J} = 0$, $\overline{J^2} = 1$.

$$H_{\{J\}}[\sigma] = {\sum_{i,j}}' \sigma_i J_{i,j} \sigma_j + \sum_i h_i \sigma_i$$

$\longrightarrow$ Sherrington Kirkpatrick mean field, $\overline{J^2} = \frac{1}{N}$.

$$H_{\{J\}}[\sigma] = \sum_{i,j} \sigma_i J_{i,j} \sigma_j + \sum_i h_i \sigma_i$$

Quenched disorder. Study:

$$\overline{\log Z_J} = \lim_{n \to 0} \frac{\overline{Z_J^n} - 1}{n}$$

Replicas

$$\mathcal{H}_J^{(n)} = \sum_{a=1}^{n} \mathcal{H}_J[\sigma^n]$$

Integrate over the quenched couplings $\{J\} \Longrightarrow$ replicas are coupled.

Now minimize the free energy F.

$Q_{a,b} \equiv \langle q_{a,b} \rangle$, is a new parameter that enters F and that we have to determine.

We will have to minimize F[Q], i.e. determine Q such that $\frac{\partial F}{\partial Q_{a,b}} = 0$, e.v. $\left[\frac{\partial^2 F}{\partial Q_{a,b} \partial Q_{c,d}} \right] \geq 0$.

Paramagnet: $q = 0$ (random state).

High T, one ground state, OK

But Low T, because of many ground states, there is symmetry breaking (RSB), and the solution with $Q_{a,b} = \mathit{constant}$ does not work (negative entropy etc.)

Here the broken symmetry is the permutation of different replicas.

$Q_{a,b}$ now depends on a and b.

Parisi scheme for RSB

$P(q)$ is trivial for normal magnets. It is a Gaussian centered at $q = 0$ in the high T phase and a couple of δ-functions at $q = \pm m^2$ in the broken phase.

Here, in the mean field theory of spin glasses,

$$P(q) \equiv \overline{P_J(q)},$$

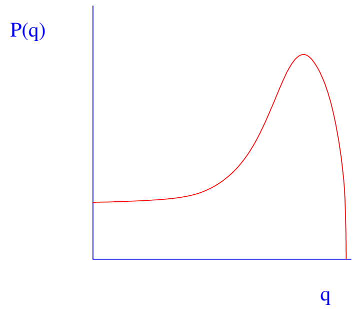
the equilibrium probability distribution of the overlap, is characterized by a function $q(x)$ or by its inverse $x(q)$ such that $\int \, dq \; P(q) \; q^s = \int \, dx \; q(x)^s$, i.e. $P(q) = \frac{dx}{dq}$.

(Iterative scheme: start by breaking the matrix Q in blocks, and iterate an infinite number of times.)

This is the solution of mean field. It contains many remarkable features.

Important questions related to finite D systems where new things have been learned recently are:

1. pattern of RSB, state structure. Potential problem: interfaces.



2. de Almeida Thouless line: there is a transition in a finite magnetic field (equilibrium + approach to equilibrium).

3. dynamical behavior, pattern of violation of FDT.

RSB looks more and more OK for MF (Guerra, Aizenman-Contucci)

Potential problems for finite D (Newman and Stein, heuristic + rigorous: we discuss here some of the findings that seem to imply that the RSB picture does indeed describe realistic models).

1. One finds a non-trivial $P(q)$ (as opposed to usual magnetic systems). In Mean Field, for $h \neq 0$, one finds that

$$P(q) = a\delta(q - q_m) + b\delta(q - q_M) + r(q)$$

2. If for large volumes $P(q)$ does not become a simple δ function correlation functions do not cluster.

3. Building of an ultrametric structure (also here there are numerical results). Sum rules.

$$\overline{P_J(q_{1,2})P_J(q_{3,4})} =$$
$$\frac{2}{3}P(q_{1,2})P(q_{3,4}) + \frac{1}{3}P(q_{1,2})\delta(q_{1,2} - q_{3,4})$$

$$\overline{P_J(q_{1,2})P_J(q_{2,3})P_J(q_{3,1})} =$$
$$\frac{1}{2}P(q_{1,2})x(q_{1,2})\delta(q_{1,2} - q_{2,3})\delta(q_{1,2} - q_{3,1}) +$$
$$\frac{1}{2}[P(q_{1,2})P(q_{2,3})\theta(q_{1,2} - q_{2,3})\delta(q_{2,3} - q_{3,1}) + \text{ two permutations}]$$

To study all that we will need numerical simulations. It is difficult, since we need to inspect a very complex phase space. Optimized Monte Carlo methods are mandatory. We use parallel tempering (in the family of density scaling, multi-canonical, tempering).

We consider S copies of the system (in the same realization of the quenched disordered couplings $\{J\}$)

$\sigma_1, \ldots \sigma_S$ (that together with the S τ_A copies we need for computing the overlap gives us $2S$ configurations of the system).

We enlarge the space of the degrees of freedom, by promoting β to be a dynamical variable. The configurations are allowed to exchange their value of β. Start with $\beta(\{\sigma_1\}) = \beta_1, \ \ldots, \ \beta(\{\sigma_n\}) = \beta_n$,

and after one full MC sweep of the spin variables propose to swap $\beta(\{\sigma_1\}) = \beta_2, \ \beta(\{\sigma_2\}) = \beta_1$, and so on for all adjacent β couples.

Use Metropolis weighting to accept the swap.

- Very effective.
- It does not need any normalization constant. No tuning, no fine tuning.
- Be careful to thermalization!

We start by discussing usual numerical results, proving the existence of a phase transition. We will try in the following to qualify it.

Here $4D$, clearer than $3D$, that is very close to the lower critical dimension (for example, very peculiar behavior of the Binder parameter).

Binary coupling, $J = \pm 1$ (allowing very effective multi-spin coding).

Many samples (from $3 \cdot 10^3$ at $V = 4^4$ down to $= .5 \cdot 10^3$ at $V = 10^4$).

Use the Binder cumulant to study the distribution probability of the order parameter

$$g_L = \frac{1}{2} \left(3 - \frac{\overline{\langle q^4 \rangle_L}(T)}{\left(\overline{\langle q^2 \rangle_L}\right)^2(T)} \right)$$

Shape of $P(q)$ at T_c is universal:

$$g_c \equiv \lim_{L \to \infty} g_L(T_c)$$

For ferromagnets:

$\lim_{L \to \infty} g_L(T > T_c) = 0$, $\lim_{L \to \infty} g_L(T < T_c) = 1$

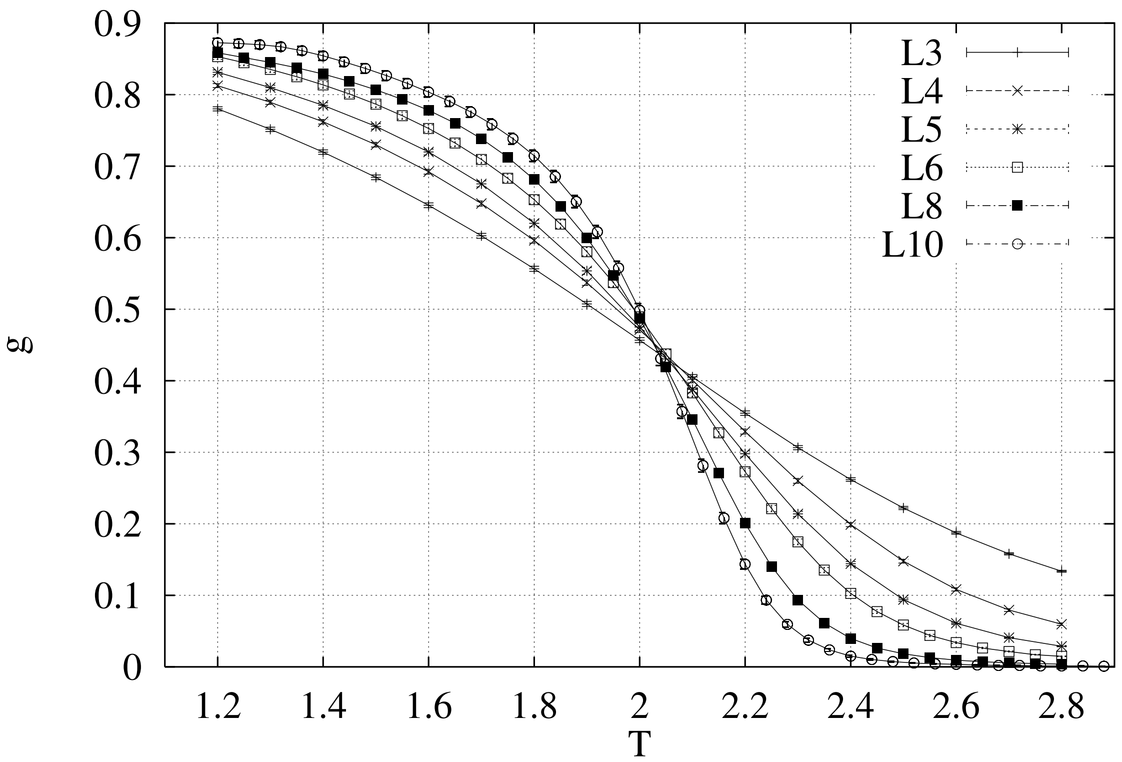
At T_c: crossing of different L curves of $g_L(T)$.

In the RSB solution of MF spin glasses the infinite volume limit of g is not 1 in the broken phase.

P(q) non-trivial $\Longrightarrow$

$$g(T < T_c) = \frac{3}{2} - \frac{1}{2}\frac{\int \ dP(q) \ q^4}{\left(\int \ dP(q) \ q^2\right)^2}$$

It is difficult to be sure that at fixed $T < T_c$ the different curves tend to a limit different from 1. We will gather the same evidence with other methods (see later).



Different kind of analysis (linearization, derivatives, ...).

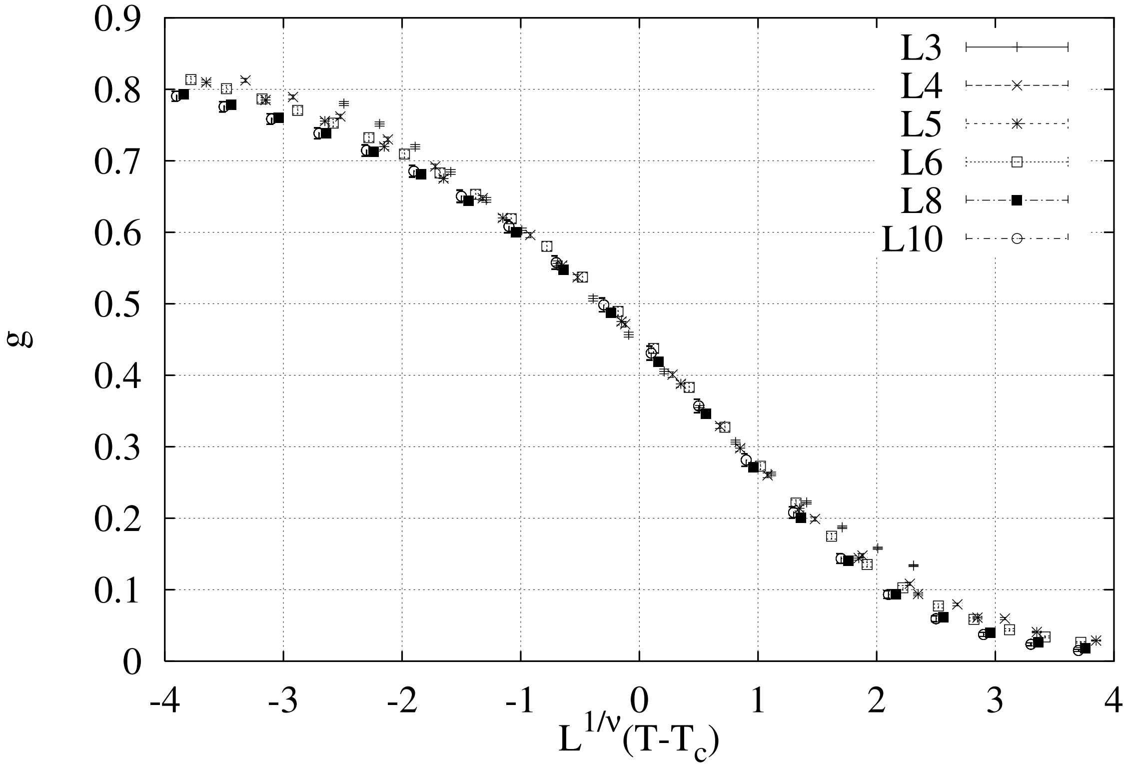
Error by jack-knife and binning.

Close to T_c: $g(L,T) \simeq \overline{g}\left(L^{\frac{1}{\nu}}(T-T_c)\right)$

$$T_c = 2.03 \pm 0.03$$

$$\nu = 1.00 \pm 0.10$$

Scaling is good.



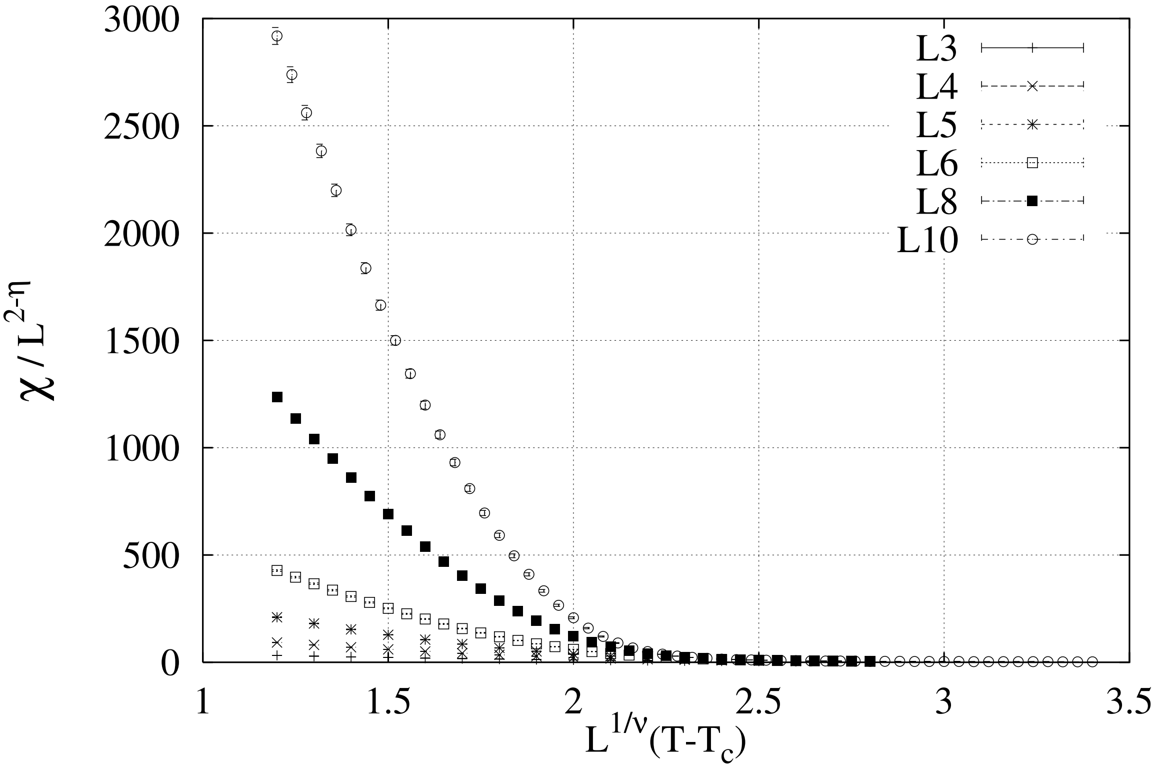
The overlap susceptibility.

In the Replica Symmetry Broken phase of a spin glass

$$\chi_q \equiv V\langle q^2\rangle$$

At $T = T_c$ (determined by Binder cumulant) scaling is like

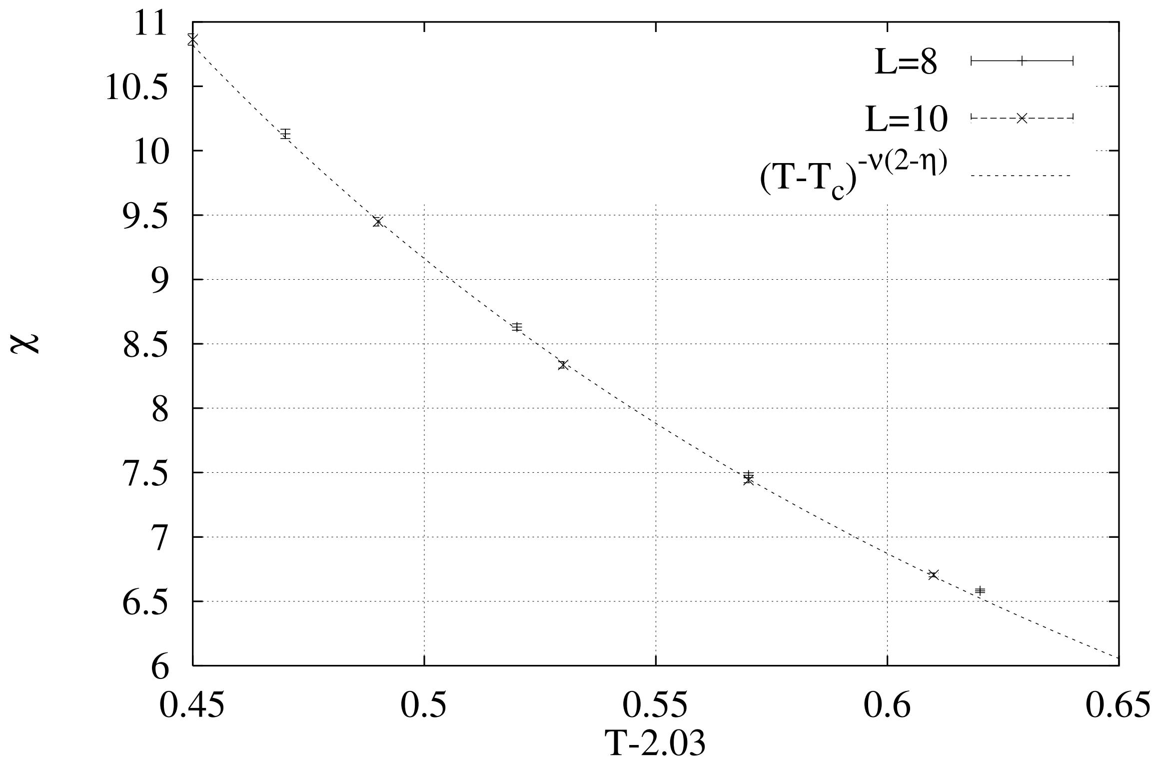
$$\chi_q(L, T = T_c) \simeq L^{2-\eta}$$



There are at least two more ways to determine η.

One is based on using off-critical data, with $L \gg \xi$. Here

$$\chi_q(T) \simeq (T - T_c)^{-(2-\eta)\nu}$$



The second method is based on the scaling $P(q \simeq 0, T = T_c) \simeq L^{\frac{D-2+\eta}{2}}$ (see later). They all give consistent results. We find

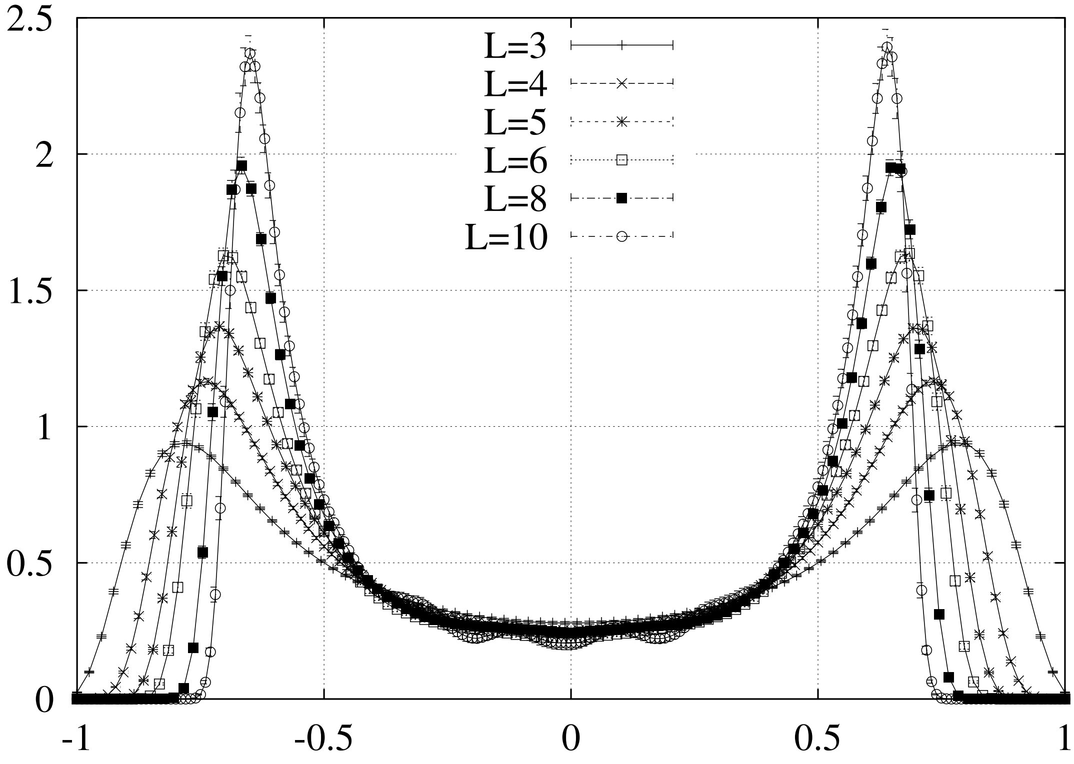
$$\eta = -0.30 \pm 0.05$$

$P(q)$, $T < T_c$ (here $T \simeq 0.6 T_c$).

It is non trivial (for a ferromagnet in the broken phase, two δ-functions center in $\pm m^2$).

Peaks are moving (for $L \to \infty$ $\delta(q \pm q_{EA})$). We should check they do not go to zero.

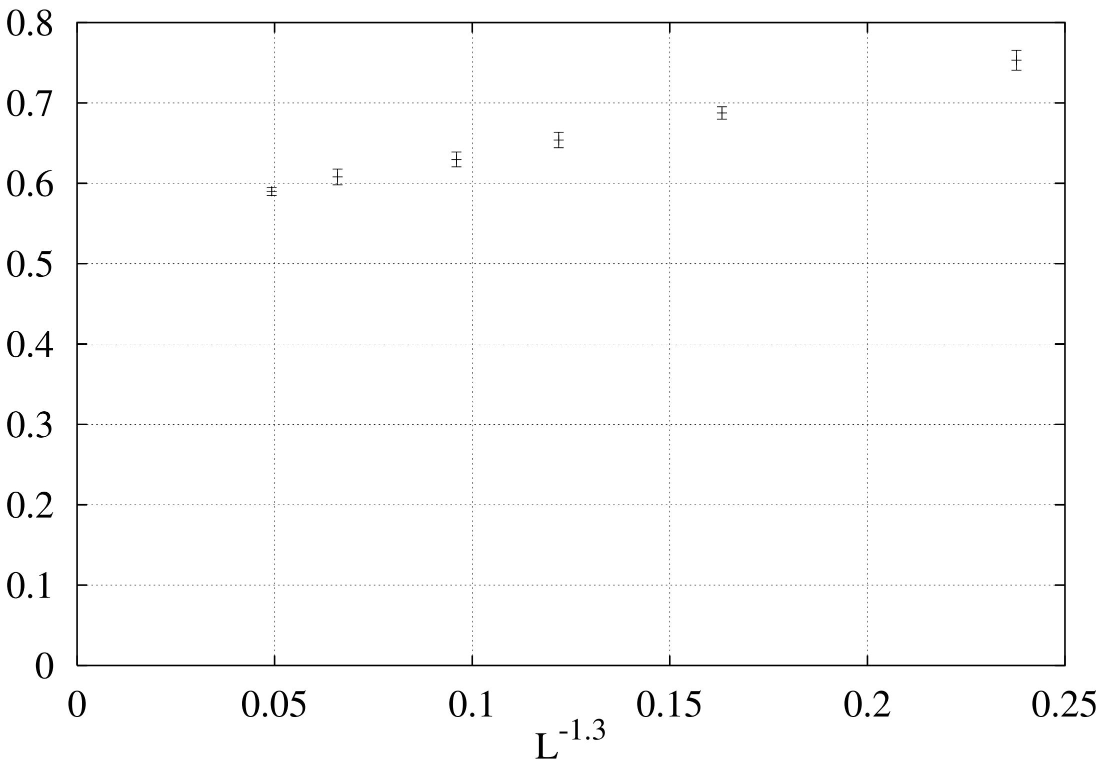
We should show that $P(q \simeq 0)$ does not change with L.



q_{MAX} such that $P(q = q_{MAX}) = \max$ versus $L^{-1.3}$.
The exponent (-1.3) is from the best fit.

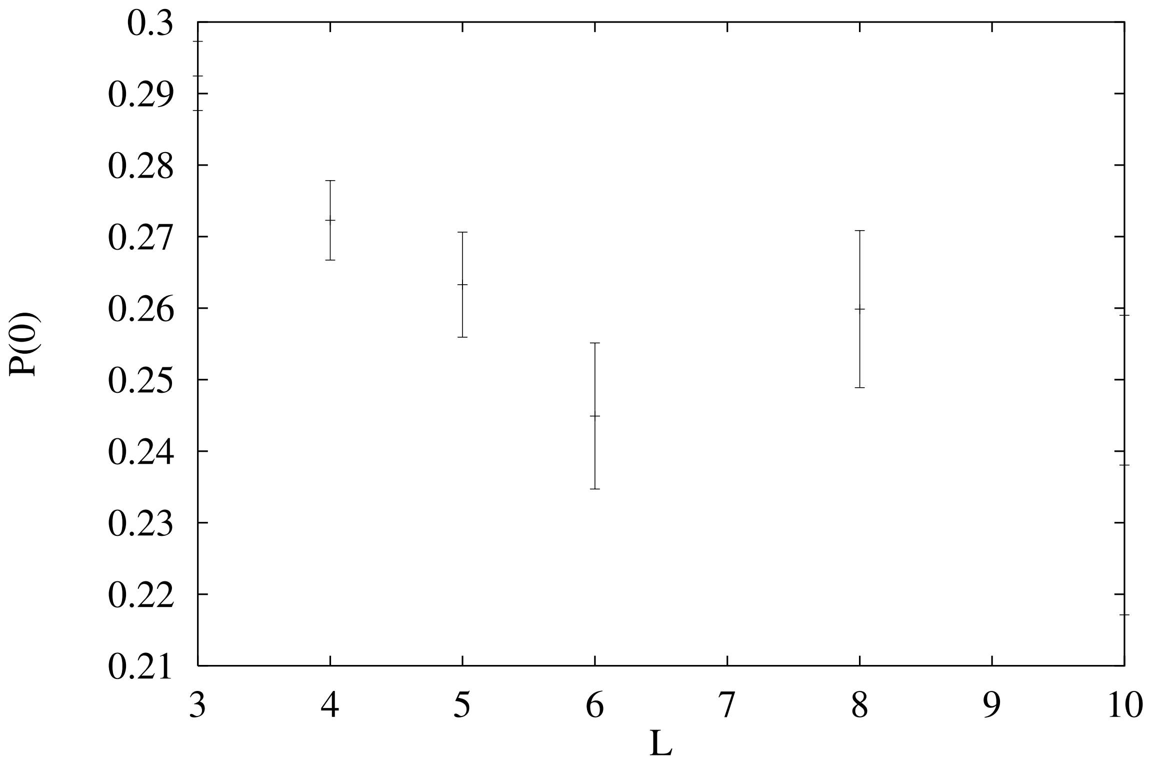
$$q_{MAX}\,(L) = q_{MAX}\,(L = \infty) + \frac{c}{L^{\alpha}}$$

$\alpha \simeq 1.3$ is consistent with MF analytic computations.



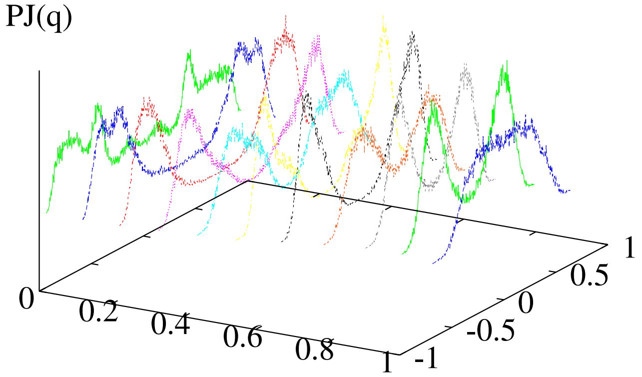
$P(q \simeq 0)$ versus L.

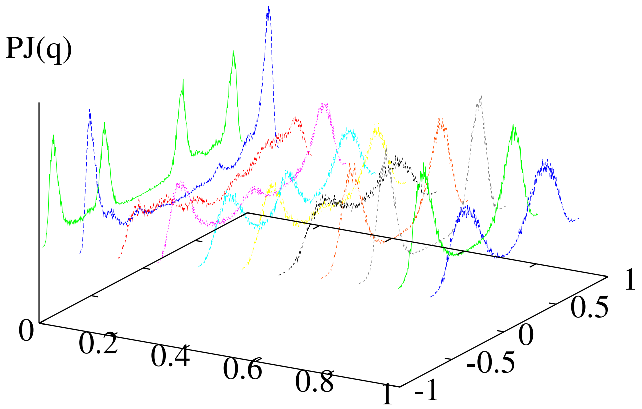
No decrease.



Smoothness SK $\rightarrow$ EA? $H_\epsilon = (1-\epsilon)H_{3D} + \epsilon H_{SK}$

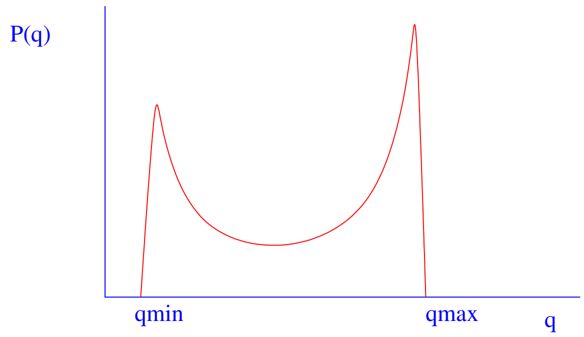
$3D$, 8^3 spin, $T = \beta^{-1} = 0.7$. $P(q)$ smooth, $P_J(q)$ no.





No *modified droplets* (with one couple of δ function for each sample, but support depending on the sample).

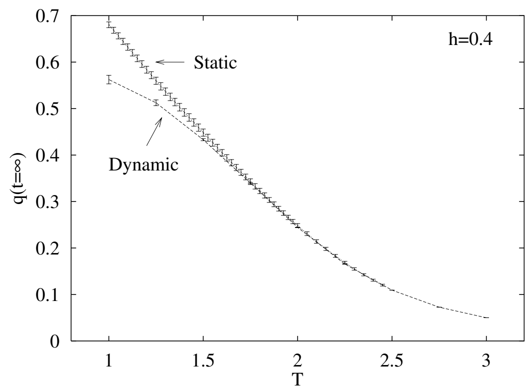
Existence of a transition in field. A very important issue (so different from usual ferromagnets).



Use a quasi-equilibrium technique. Start with two different $T = \infty$ configurations (random different spins, some couplings $\{J\}$).

$q(t=0) = 0$

Then annealing (with slower and slower scheduling). Extrapolate to infinite time with power law convergence: $E(t) \to E_{true}$, like all one replica quantities, $q(t) \to q_{min} \neq q_{ave}$



Compute q_{ave} from equilibrium simulations. Be careful in fitting.

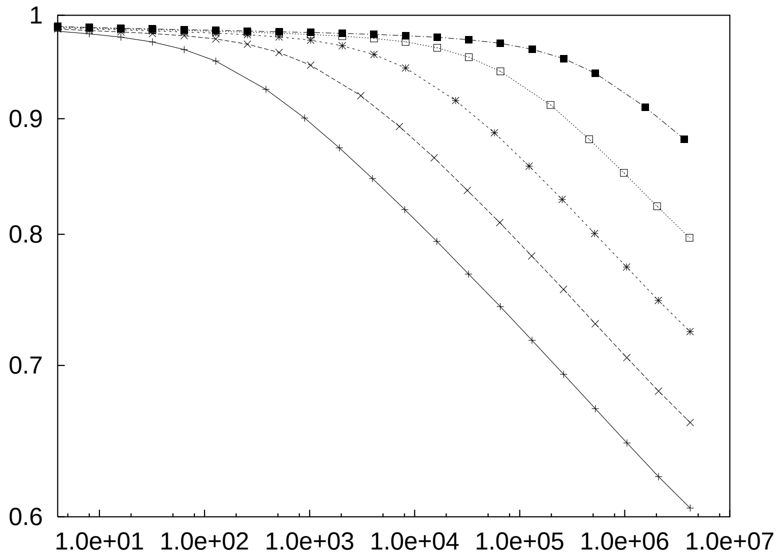
The dynamical properties of spin glasses are very interesting (both from experiments and from theory). First very interesting phenomena are aging phenomena.

$C(t,t_w) \equiv \frac{1}{N}\sum_i \overline{\langle \sigma_i(t_w)\sigma_i(t+t_w)\rangle}$ depends both on t and on t_w.

$C(t,t_w) \simeq (q_{EA} + a t^{-x})\, \frac{f(\frac{t}{t_w})}{f(0)}$, RSB.

$C(t,t_w) \simeq (\log(t))^{-y}\, \tilde{f}\left(\frac{\log(\frac{t}{\tau})}{\log(\frac{t_w}{\tau})}\right)$, droplet.

RSB is OK with experiments.



(from Parisi, Ricci-Tersenghi and Ruiz).

Violations of the Fluctuation Dissipation Theorem, FDT.

$$C(t,t') \equiv \langle A(t)A(t') \rangle$$

$$R(t,t') \equiv \frac{\delta \langle A(t) \rangle}{\delta \epsilon(t')}\Big|_{\epsilon=0}$$

with

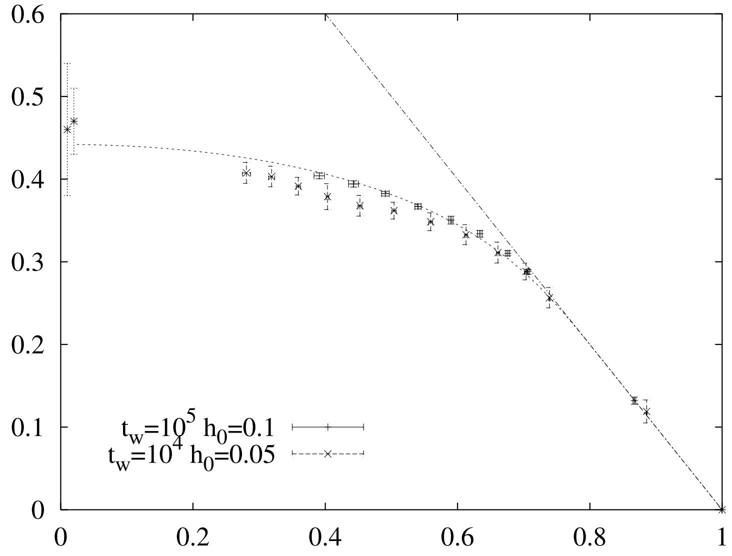
$$H' = H + \int \epsilon(t) A(t) dt$$

$$\text{FDT: } R(t,t') = \beta\theta(t-t')\frac{\partial C(t,t')}{\partial t'}$$

In spin glasses:

$$R(t,t') = \beta X\,(C\,(t,t'))\theta(t-t')\frac{\partial C(t,t')}{\partial t'}$$

X is connected to Parisi static $x(q)$.



On the need of a careful analysis of numerical data, and on the danger of scaling plots.

$G(r,t) = \langle q_0(t) q_r(t) \rangle$, at equal times.

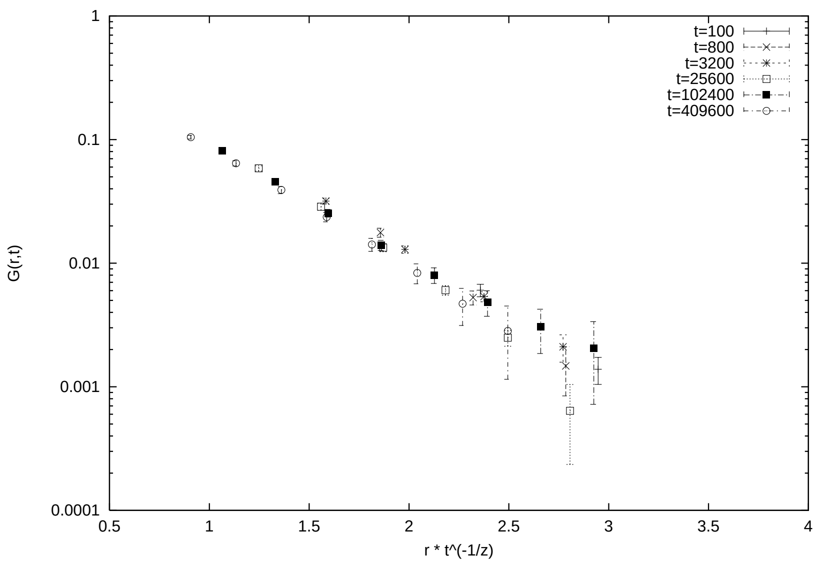
A simple droplet growth would imply $G(r,t) \simeq \overline{q} + Ae^{-\frac{r}{\xi(t)}}$, $\xi(t) \simeq t^{\frac{1}{z}}$, $z \simeq 10$.

RSB implies a more complex behavior. $q \simeq 0$ sector: $G(r) \simeq r^{-\mu}$, $\lim_{r\to\infty} G(r) = 0$.

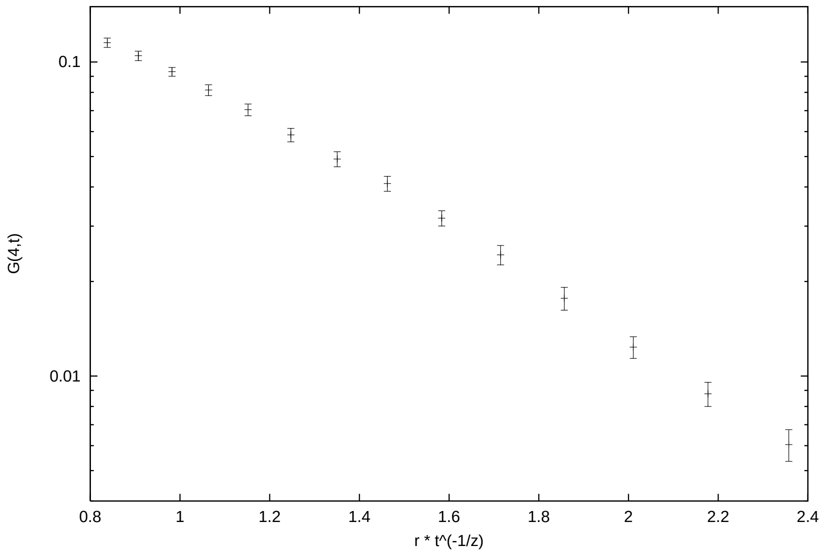
We had verified the Ansatz

$$G(r,t) = \frac{g}{r} e^{-\left(\frac{r}{\xi(t)}\right)^{\frac{3}{2}}}.$$

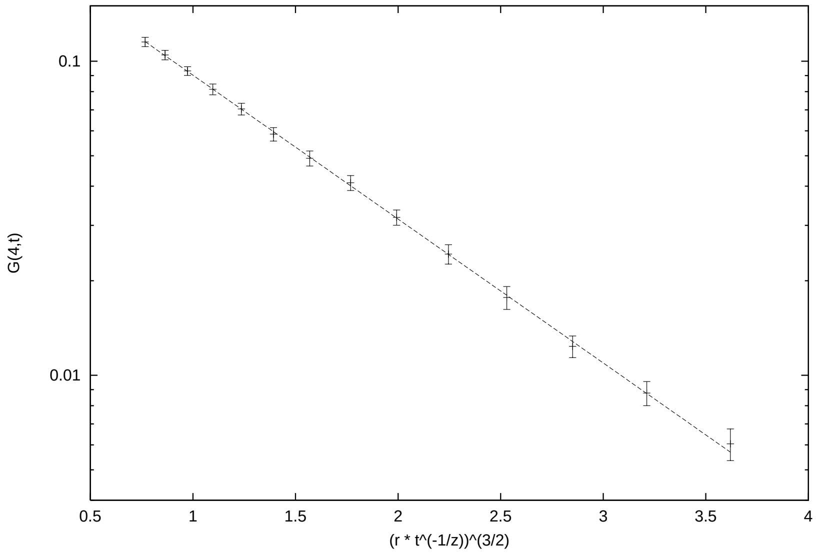
But scaling plot seems linear (T. Konori et al.):



Let us look more carefully. This can still look linear:



but it is not:

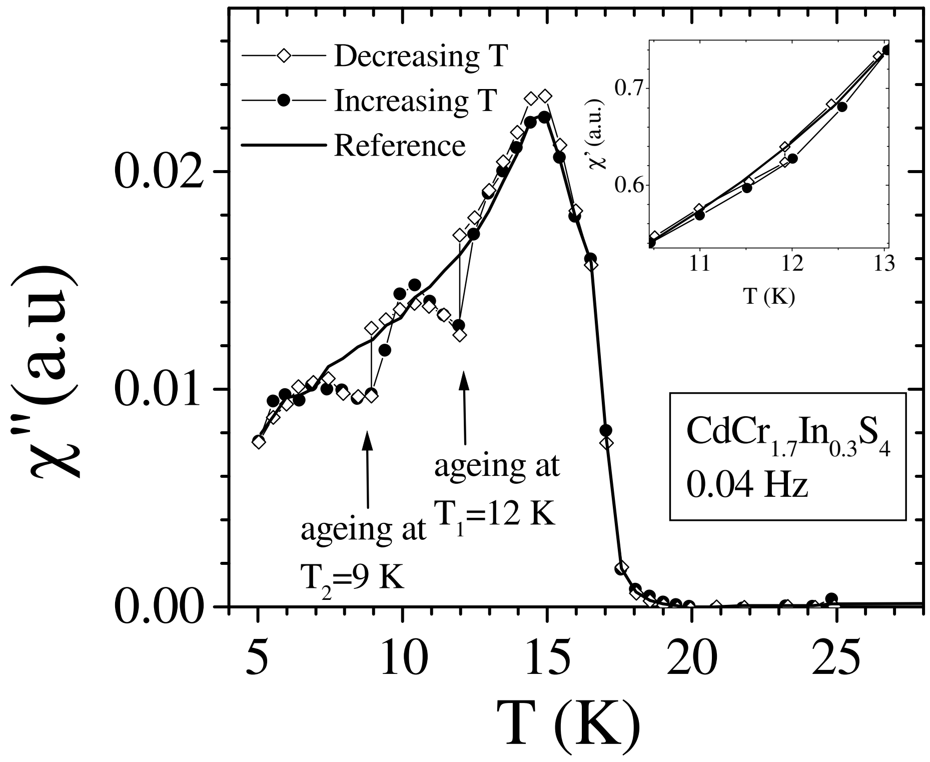


All the detailed analysis completely confirms our scaling Ansatz, not compatible with simple domain growth (and other evidences point toward the same direction).

Real experiments on spin glass materials also show a very high degree of complexity: let us discuss for example a recent double memory experiment (Jonason et al., `cond-mat / 9904410`).

Insulating spin glass. Very low frequency ac field. Measure relaxation of susceptibility (time scale: $10 \to 10^5 s$).

Cooling from $T_0 > T_{SG}$ at constant rate, but for two stops at $T_1 < T_2 < T_{SG}$. Heating at constant rate.



Is RSB theory useful to describe real glasses? Understanding real glasses is an interesting goal.

Answer is probably and hopefully yes. Let us discuss why.

First point is about the Random Energy Model (REM) class of models. (SK is described by continuous Parisi function $x(q)$, here different, but generic...): here values E_k are random, with probability

$$P(E) \propto e^{-\frac{E^2}{2N}}$$

$$Z = \sum_{k=1,M} e^{-\beta E_k}$$

There is a low T phase. Transition is different than in SK. In some respects like for second order. p-spin model:

$$H_J^{(p)}(\{\sigma\}) = \sum_{i_1,i_2,\ldots,i_p}' J_{i_1,i_2,\ldots,i_p} \sigma_{i_1} \sigma_{i_2} \ldots \sigma_{i_p}$$

SK like transition: only for $p = 2$. REM-like transition is generic: $p \geq 3$. $p \to \infty$: get exactly REM.

SK: $q_{EA} - q_{min}$ is small for $T \simeq T^-$. REM: in the broken phase q can only take two values. q_{min} and q_{EA}. Here $q_{EA} - q_{min} = O(1)$ as soon as $T < T_c$.

The dynamic behavior

REM: $T_d > T_c$.

2-time correlators are singular at T_d.

This property is shared by structural glasses.

SK: $T_d = T_c$.

Systems without disorder.

Replica theory allows to describe them.

One gets a RSB cold phase like in the REM universality class.

A complex coupling can produce the same effect of quenched disorder. For example:

$$H = \frac{1}{\sqrt{N}} \sum_{j,k=1}^{N} \sin\left(\frac{2\pi jk}{N}\right)(\sigma_i - \sigma_j)^2 \,, \quad \sigma = \pm 1$$

In some situations: an ordered state exists, but it has very low entropy and the system does not find it (improbable crystallization).

Effective quenched disorder is induced by slow dynamics.

Memory of Neural Networks.

Storage capacity.

(Brain is quite mean field: cortex is not fully connected but very connected: 10^7 elementary nets each done of 10^4 fully connected neurons).

Use analitic techniques of replica theory.

$$J_{ij} = \frac{1}{N} \sum_{\mu=1}^{p} \xi_i^\mu \xi_j^\mu$$

$$E = -\frac{1}{2} \sum_{i,j} S_i J_{ij} S_j$$

Memorized pattern: $S_i = \xi_i^\mu$ for $i = 1, ..., N$.

$p < p_c = \alpha_c N$: remember.

$p > p_c$: no memory.

α_c with RSB is 0.145.

Random Manifolds

Sometimes it is difficult to apply Replica Theory: the variational approach.

Fluctuating Random Manifolds with Quenched Disorder.

$\longrightarrow$ crucial practical problems. Proteins, for example.

x: D dimensional vector

ω: N component interface

$$h[\omega] = \frac{1}{2} \int d^D x \sum_{\mu=1}^{D} \left(\frac{\partial \omega}{\partial x_\mu} \right)^2$$

$$+ \int d^D x \; V(x, \omega(x))$$

i.e. rigidity term plus external random potential.

$$\overline{V(x,\omega)\,V(x',\omega')}$$

$$= -\delta^{(D)}\left(x-x'\right) N f\left(\frac{(\omega-\omega')^2}{N}\right)$$

$$f\left(\frac{\omega^2}{N}\right) \sim \left(\frac{\omega^2}{N}\right)^{(1-\gamma)}$$

One typically measures

$$\overline{\langle(\omega(x+l)-\omega(x))^2\rangle} \simeq_{l \gg x} l^{2\zeta}$$

There are many metastable states: complex problem.
Use Replica's and find the replicated Hamiltonian

$$H^{(n)} = \frac{1}{2}\int d^D x \sum_{a=1}^{n}\sum_{\mu=1}^{D}\left(\frac{\partial\omega_a}{\partial x_\mu}\right)^2$$

$$+\frac{\mu}{2}\int d^D x \sum_{a=1}^{n} \omega_a(x)^2$$

$$+\frac{\beta}{2}\int d^D x \sum_{a,b=1}^{n} N f\left(\frac{(\omega_a(x)-\omega_b(x))^2}{N}\right)$$

This is a typical case where perturbation theory is not enough.

Variational approach: select best quadratic Hamiltonian

$$H_V = \frac{1}{2} \int dk \; \omega_a(k) \; G^{-1}_{a,b}(k) \; \omega_b(k)$$

Replica symmetric and RSB solution $\longrightarrow$ hierarchical symmetry breaking.