Learning About Spin Glasses

Enzo Marinari

(Cagliari, Italy)

I thank the organizers...

I am thrilled since...

(Realistic) Spin Glasses: a debated, interesting issue.

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

Connected work, among other, by Berg and Janke, Kawashima and Young.

SCRI, Tallahassee, March 1999

A schematic summary of this talk: 3 parts.

1. Mean Field Theory of spin glasses, and its dramatically new features.

2. *Standard* evidence about the nature of the phase transition and of the broken phase.

3. Sensitive issues and numerical evidences about them (interfaces, Gibbs states, droplet or non-droplet).

I will not try to enter in all details of the open debate (there is too much to say) but only try to signal the ones that look like the crucial questions.

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

Overlap among two replicas will play a crucial role (order parameter):

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

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.

$Q_{a,b} \equiv \langle q_{a,b} \rangle$, F[Q], Q such that $\frac{\partial F}{\partial Q_{a,b}} = 0$, e.v. $\left[\frac{\partial^2 F}{\partial Q_{a,b} \partial Q_{c,d}} \right] \geq 0$.

High T, one ground state, OK ($Q_{a,b} =$ constant).

Low T, many ground states, symmetry breaking (RSB).

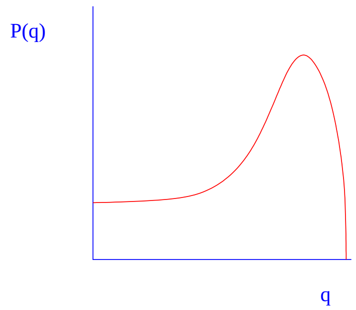
Here symmetry is permutation of different replicas.

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

Parisi scheme for RSB

$P(q) \equiv \overline{P_J(q)}$ is the equilibrium probability distribution of the overlap, 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. $P(q) = \frac{dx}{dq}$. 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:

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

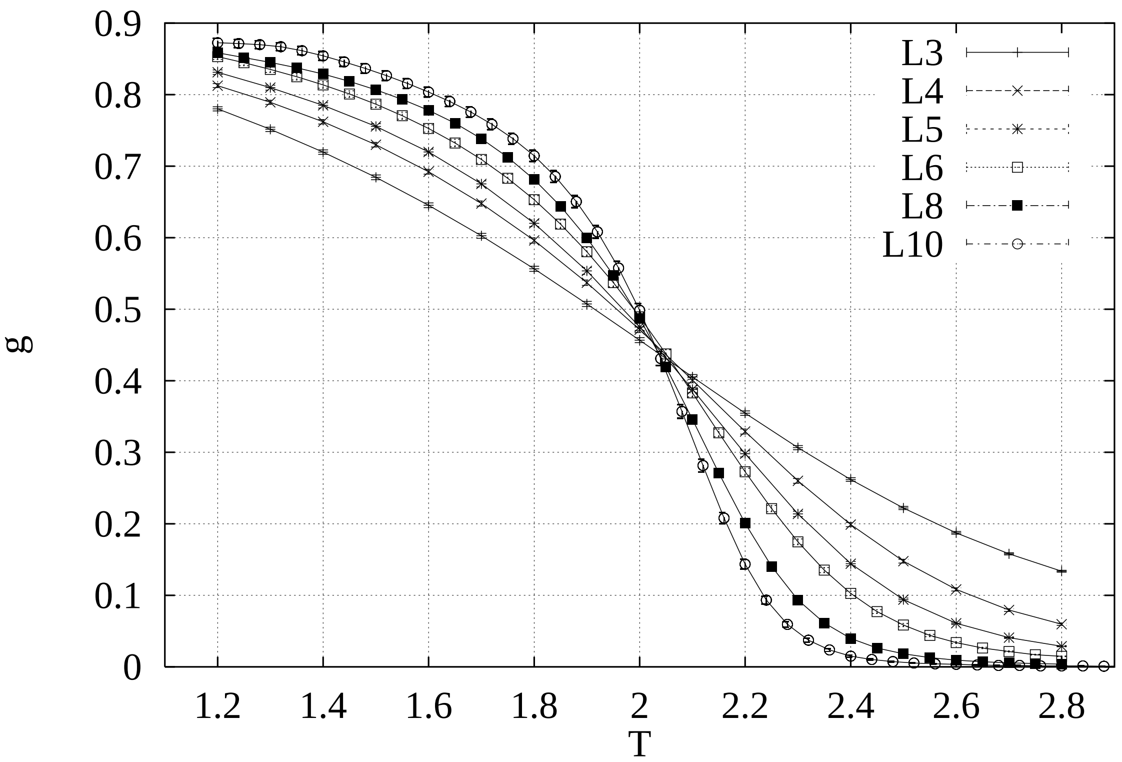
At T_c: crossing of different L curves of $g_L(T)$.

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, ...).

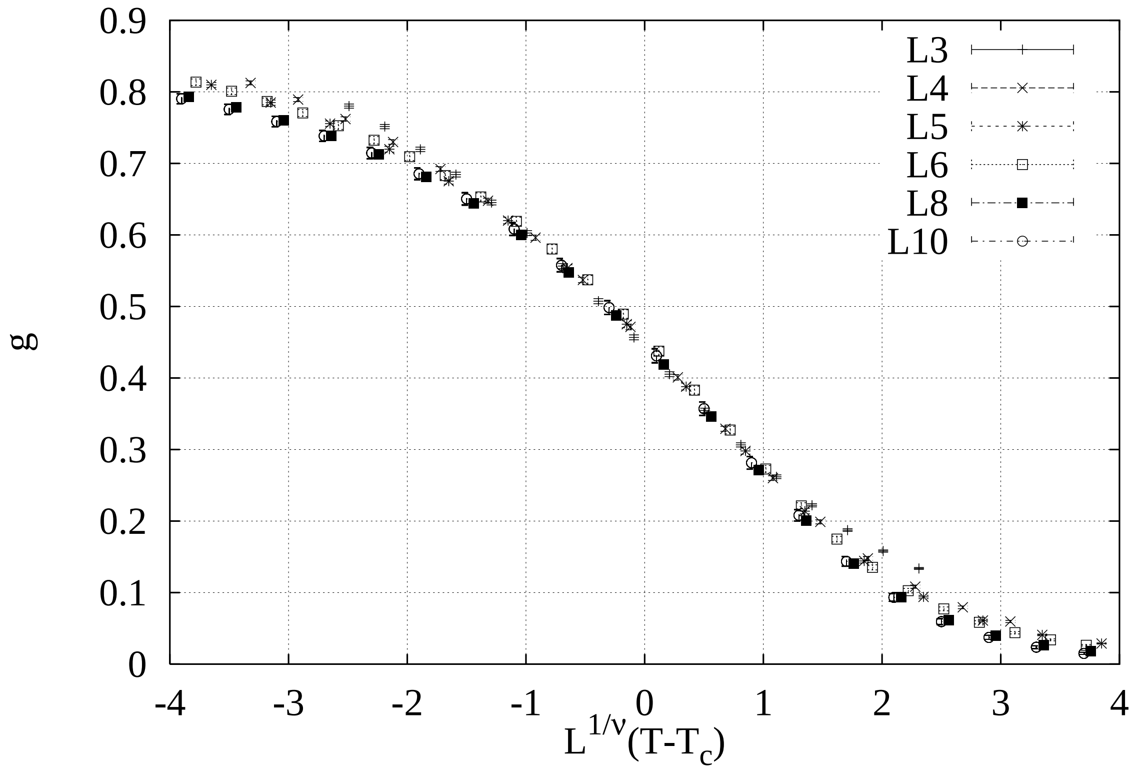
Error by jack-knife and binning.

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.



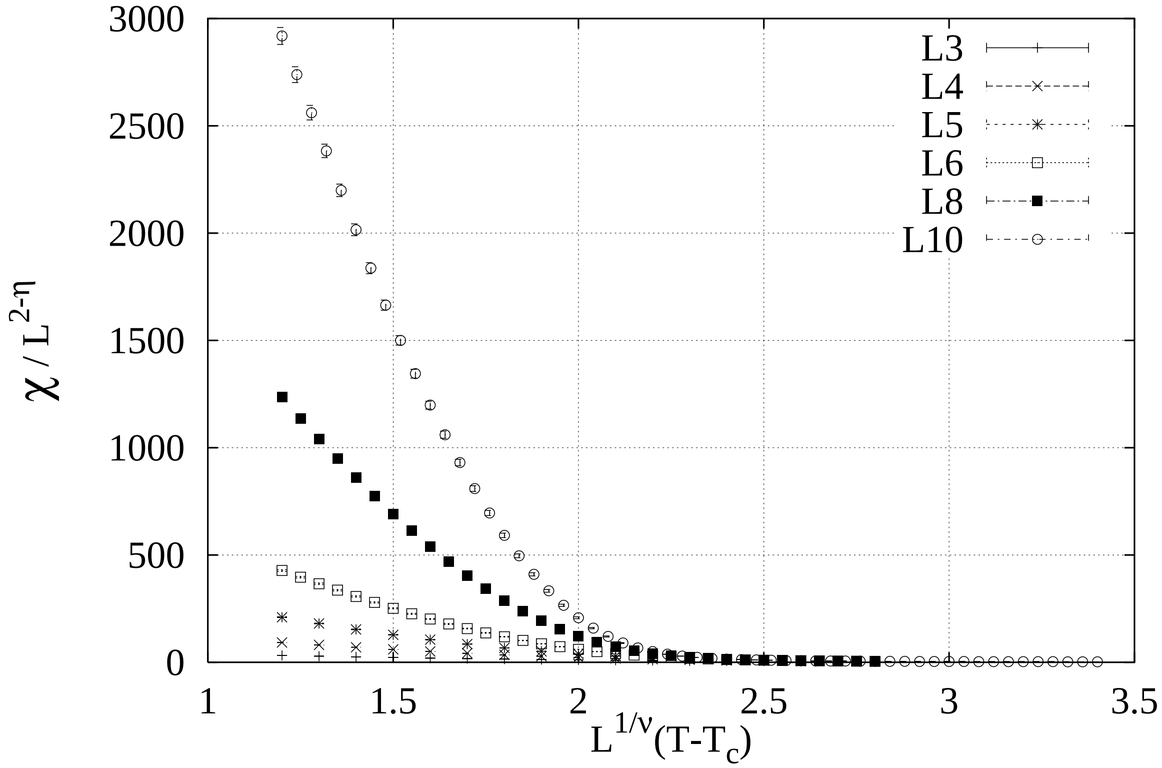
The overlap susceptibility.

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

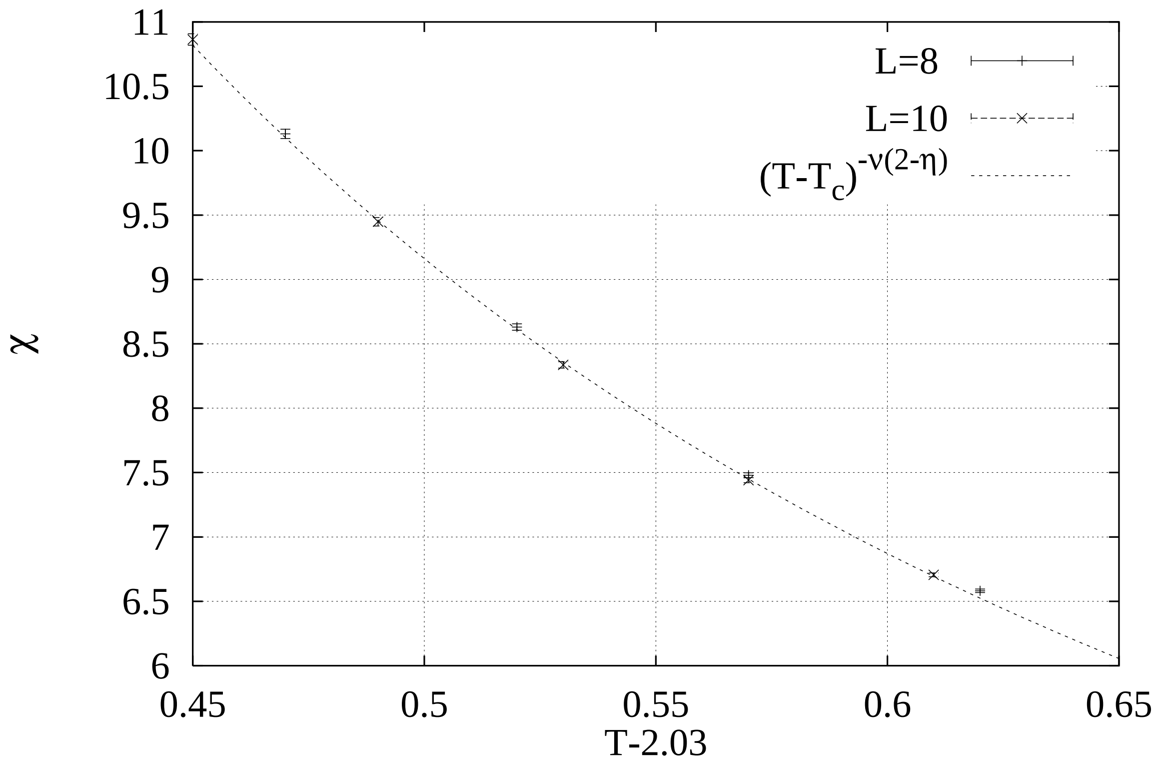
$$\chi_q(L, T = T_c) \simeq L^{2-\eta}$$



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

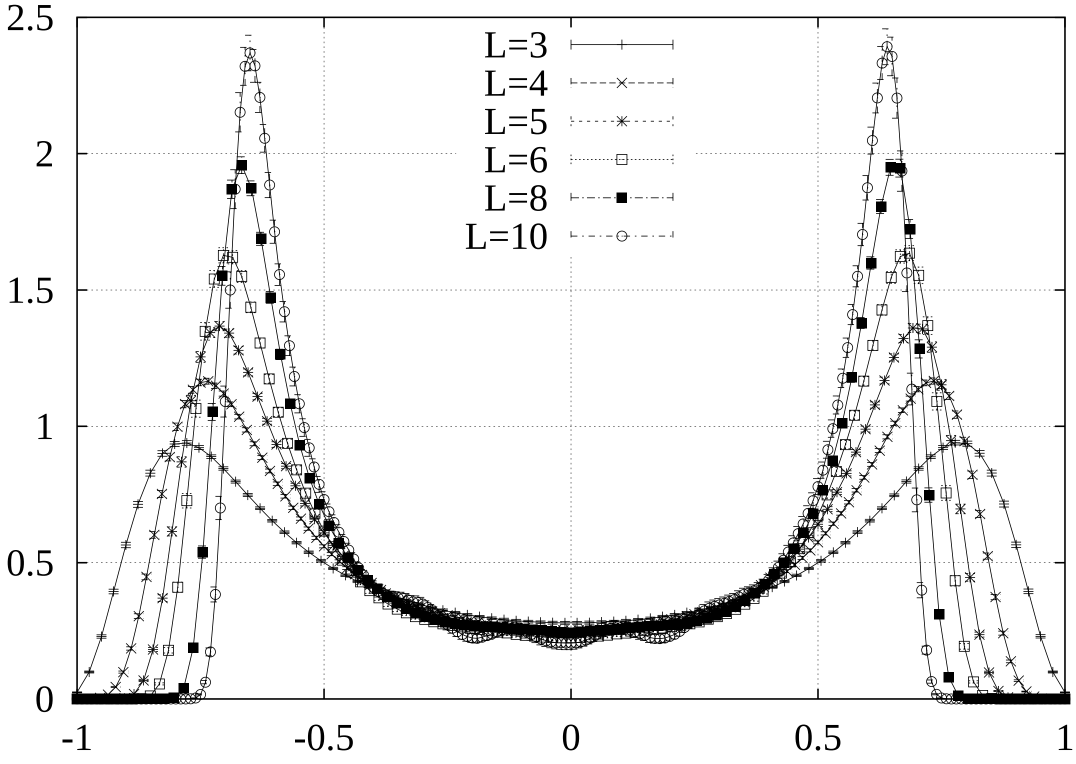
$$\eta = -0.30 \pm 0.05$$

$P(q)$, $T < T_c$ (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.

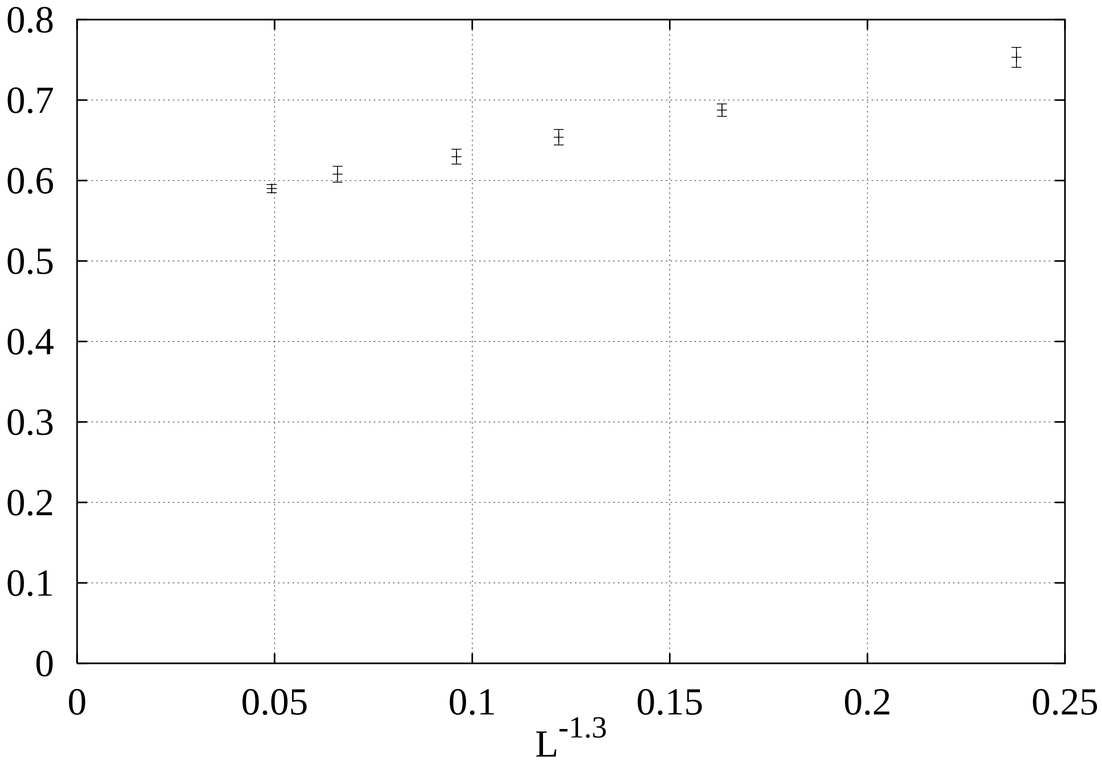


q_{MAX} such that $P(q = q_{MAX}) = \max$ versus $L^{-1.3}$.

The exponent (-1.3) is from the best fit.

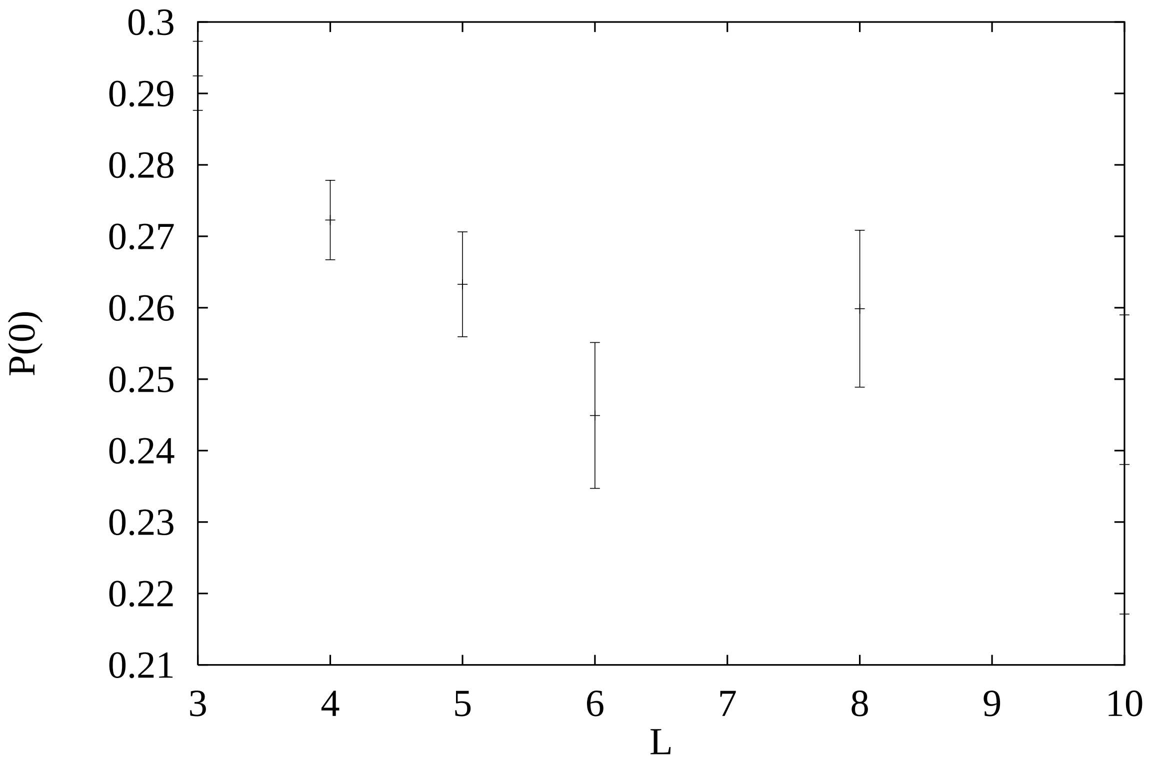
$$q_{MAX}(L) = q_{MAX}(L = \infty) + \frac{c}{L^{\alpha}}$$

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



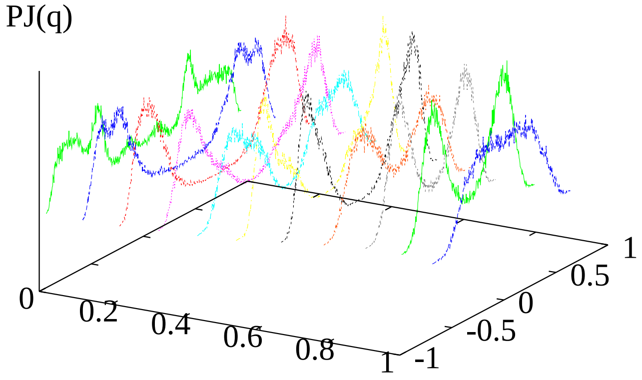
$P(q \simeq 0)$ versus L.

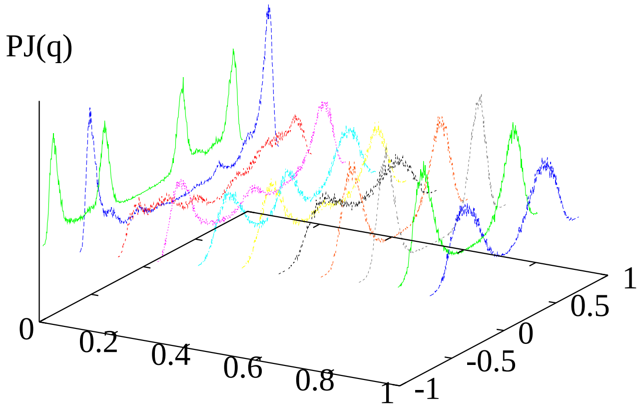
No decrease.



Smoothness SK $\to$ 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).

(With this transparency we are entering the third and last phase of this talk, concerning debated issues).

Interfaces and Local Overlaps

$$V = L^3,\ 1 \ll B \ll L$$

Region of size B^3: $q_B \equiv \frac{1}{B^3} \sum_{i \in B} q_i$.

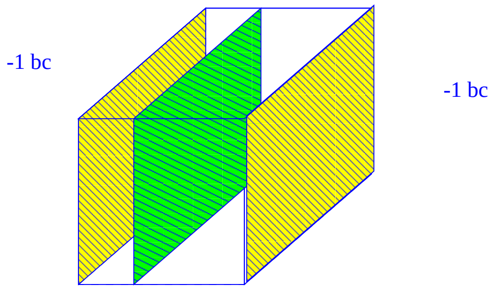
$$P_B(q) = \lim_{L \to \infty} P_B^L(q)$$

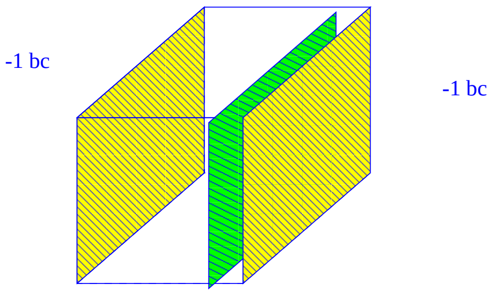
In the Replica Symmetry Breaking Ansatz one finds that $\lim_{B \to \infty} P_B(q) = P(q)$

The presence of interfaces can make $P_{B=\infty}(q)$ peculiar. Let us discuss about interfaces.

A non-trivial $P(q)$ can be obtained without the need of a non-trivial Symmetry Breaking (Fisher-Huse, van Enter). 3D ferromagnet.

yz: periodic bc, x: antiperiodic bc, $T < T_c$: domain wall.





$m(i_x) = \frac{1}{N_y N_z} \sum_{i_y, i_z} \sigma(i_x, i_y, i_z) = f\,(i_x - I)$

where I is the position of the interface in the x direction.

I can be everywhere, and f can tend to $-m$ for large negative argument and to $+m$ for large positive argument, or it can tend to $+m$ for large negative argument and to $-m$ for large positive argument.

In these conditions $P(q) = \frac{1}{2m^2}$ for $-m^2 \leq q \leq m^2$.

The RSB approach can tell the difference between true RSB and such a trivially non-trivial P(q). Both local overlaps and correlation functions do so.

In the situation that we have described, where RS is not broken:

$$\lim_{B\to\infty} P_B(q) = \frac{1}{2}\left(\delta\left(q - m^2\right) + \delta\left(q + m^2\right)\right)$$

since the probability of hitting an interface is negligible when $B \ll L$. Local measurements can show when RSB predictions are valid and when they are not.

Numerical simulations show, as we have seen, a clear, non-trivial $P(q)$. $P(q \simeq 0) \neq 0$, and the maximum at q_{MAX} becomes sharper with increasing L.

Maybe this is an effect faked by interfaces? From the work by Newman and Stein:

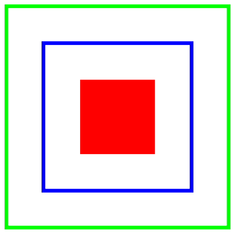
Essentially all the simulations of which we are aware compute the overlap distribution in the entire box. [...]

We suspect that the overlaps computed over the entire box are observing domain wall effects arising solely from the imposed boundary conditions rather than revealing spin glass ordering [...]

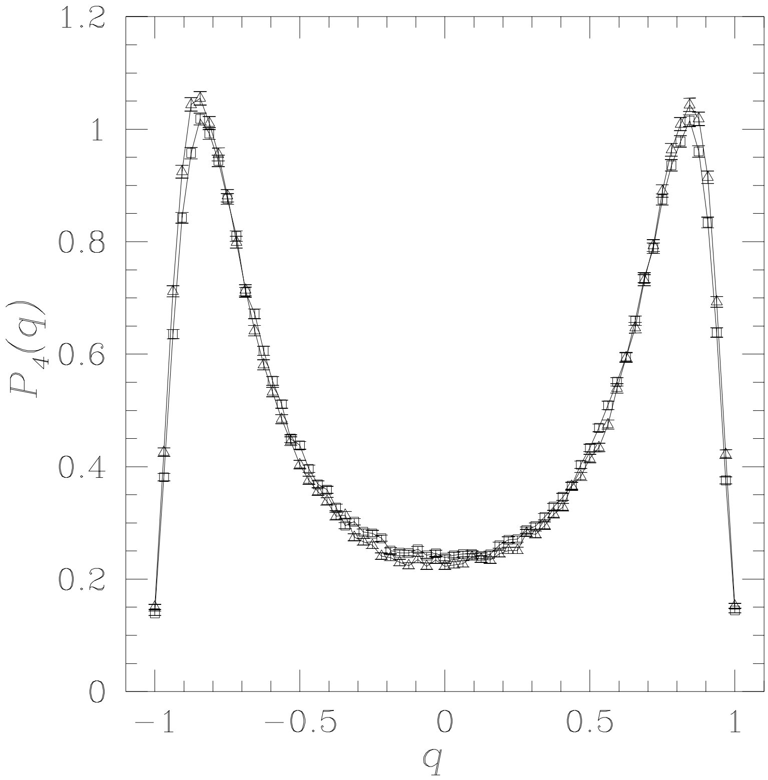
In other words if overlap computations were measured in *small* windows far from any boundary, one should find only a pair of δ–functions [...]

This is a very interesting issue, worth to check.

Block size $B = 4$. Triangles $L = 8$. Squares $L = 12$.
$T \simeq 0.7\ T_c$, $3D$.



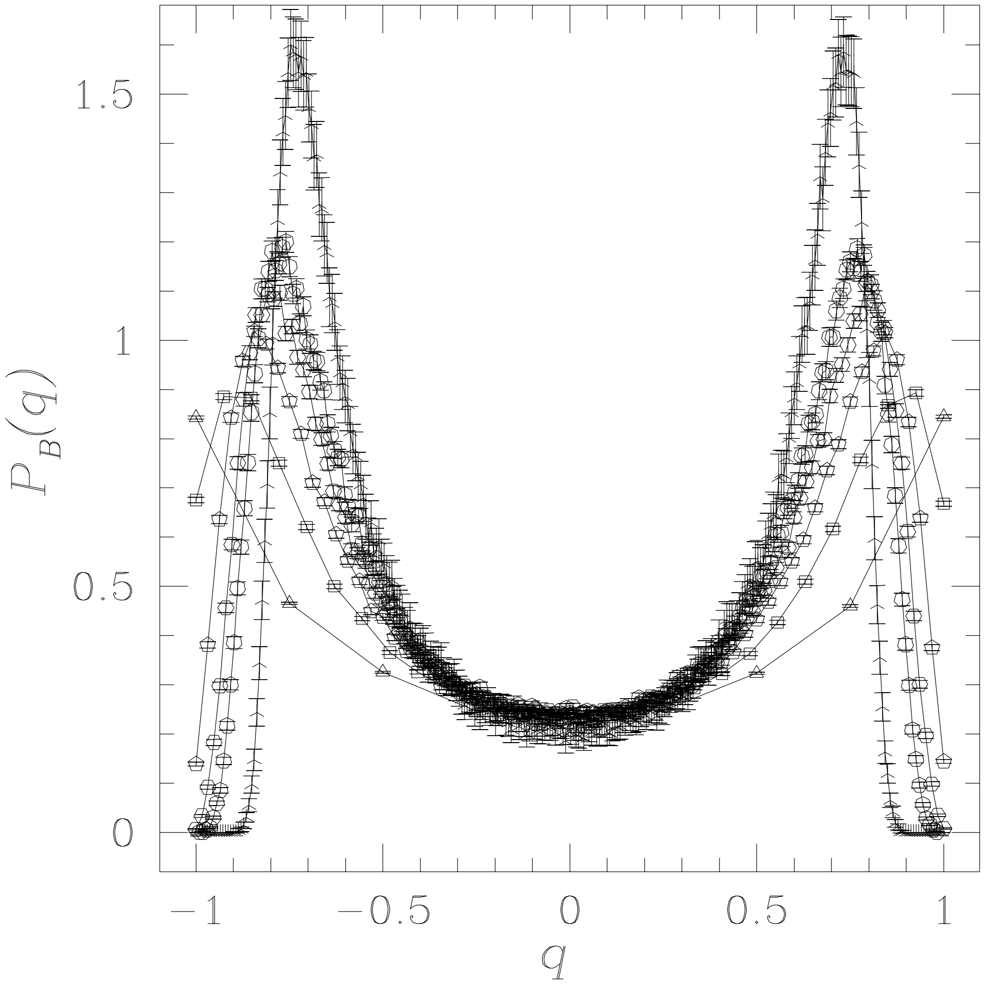
Parallel Tempering $\Longrightarrow$ equilibrium ok.



1. Small finite size effects: better than full $P(q)$
2. non-trivial
3. no substantial dependence on L
4. no approach to δ-function

$T \simeq 0.7\,T_c$, $3D$. Fixed lattice size $L = 12$. From $B = 2$ (lower curve, triangles). To $B = 12$ (sharper peaks, arrows.

The major changes in $P_B(q)$ are for increasing B. They are related to the usual (strong) L-dependence of the full $P(q)$.



These data are from cond-mat/9804017, published in J. Phys. A.

Overlap Sum Rules

In Mean Field (Mézard, Parisi, Sourlas, Toulouse and Virasoro) we have seen already some of the relations that relate expectations of $P_J(q)$.

Consider 4 or 3 real replicas. One finds that

(*) $E(q_{12}^2 q_{34}^2) = \frac{2}{3} E(q_{12}^2)^2 + \frac{1}{3} E(q_{12}^4)$, $E(\,\cdot\,) \equiv \overline{\langle\,\cdot\,\rangle}$

(**) $E(q_{12}^2 q_{23}^2) = \frac{1}{2} E(q_{12}^2)^2 + \frac{1}{2} E(q_{12}^4)$ with one replica in common

(Building blocks of ultrametricity). q_{12} and q_{34} are not independent.

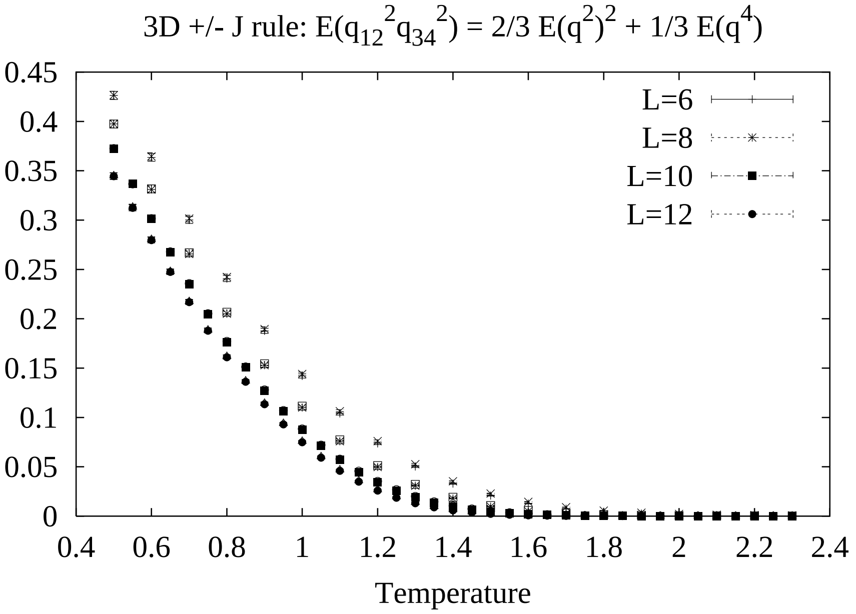
Parisi, Ritort, Ruiz, EM (*) holds with good accuracy for $3D$ spin glasses.

Guerra, Aizenman Contucci and Parisi: rigorous proof and more relations. Proof is also valid for finite D EA model if some continuity hypothesis holds (Guerra).

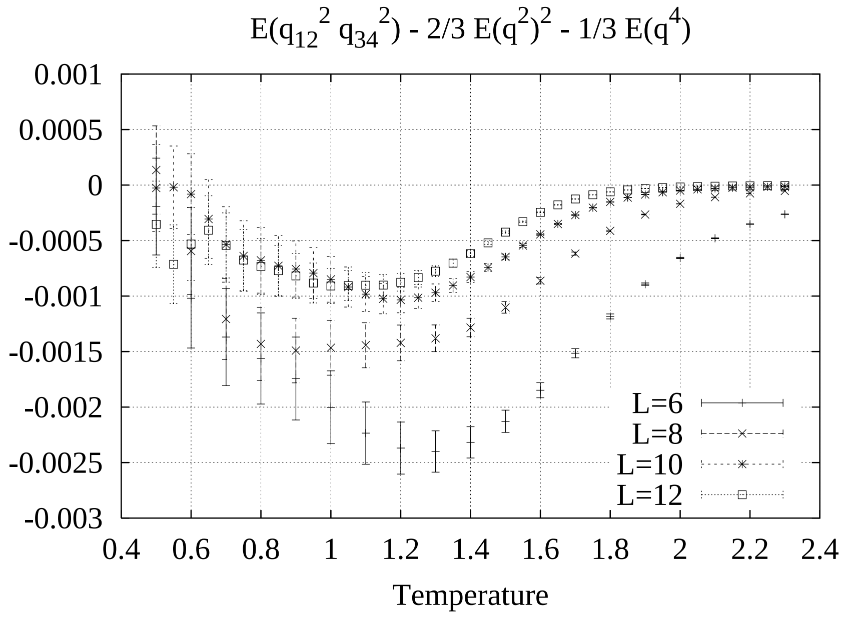
This is the main point of the discussion that emerges again: are typical equilibrium configurations of the, say, $3D$ model, similar to the ones of the SK model?

Two data points (LHS and RHS) on each plot point.

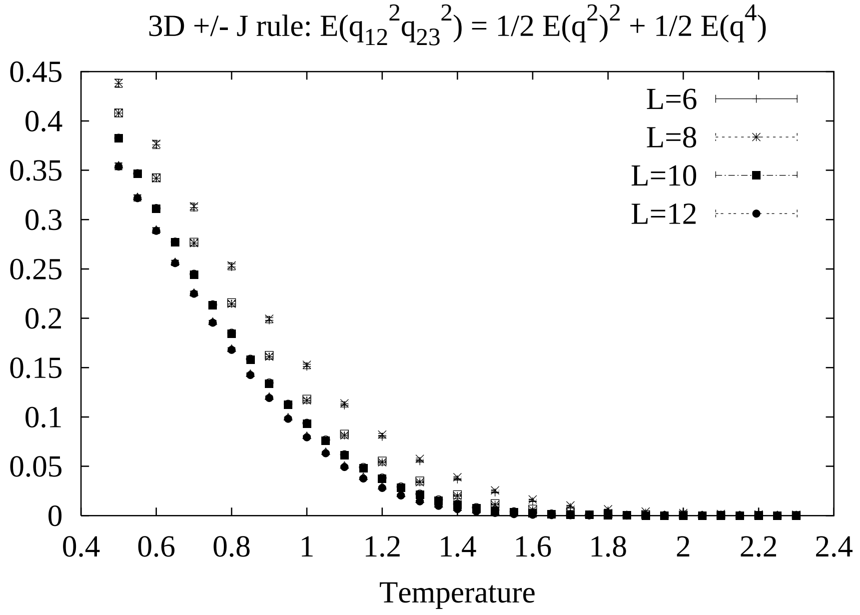
The difference cannot be appreciated on this graph. But shows the non-trivial q^2 in the broken phase.

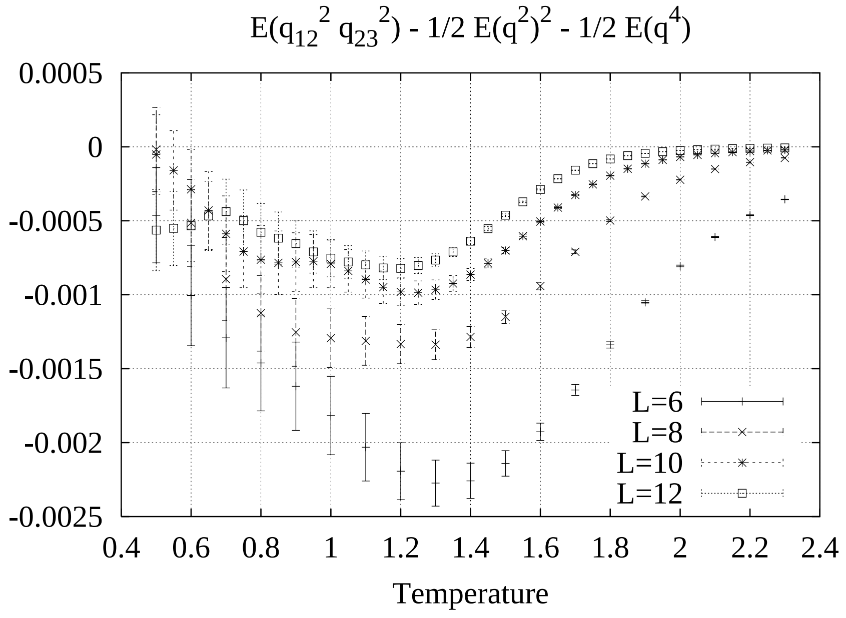


Satisfied with very good accuracy. Stronger effects close to T_c. Converges to zero with a power law.



It works perfectly also for the 3 replica case. This is a strong step toward ultrametricity.





Coupling Replicas

Couple two copies of the system. You can use

$$H_q[\sigma,\tau] = H_0[\sigma] + H_0[\tau] + \frac{\epsilon}{V}\sum_i \sigma_i \tau_i$$

or for example

$$H_{q_E}[\sigma,\tau] = H_0[\sigma] + H_0[\tau] + \frac{\tilde{\epsilon}}{V}\sum_{i,\mu} \sigma_i \sigma_{i+\mu} \tau_i \tau_{i+\mu}$$

Compute $\lim_{\epsilon\to 0^+} q(\epsilon)$ and $\lim_{\epsilon\to 0^-} q(\epsilon)$ or do it for $\tilde{\epsilon}$ (avoid possible troubles due to interfaces).

$$\text{RSB:} \quad \lim_{\epsilon\to 0^+} q(\epsilon) = q_+ + A_+ \epsilon^\lambda$$
$$\lim_{\epsilon\to 0^-} q(\epsilon) = q_- + A_- |\epsilon|^\lambda$$