The Phase Space of

Spin Glasses at Low T

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In this lecture I will present a basic introduction to some of the work done in collaboration with:

- Carlo Amoruso, Alain Billoire
- Stefano Ciliberti, Cirano de Dominicis
- Irene Giardina, Florent Krzakala
- Jovanka Lukic, Olivier Martin
- Andrea Pagnani, Giorgio Parisi
- Federico Ricci-Tersenghi, Juan Ruiz-Lorenzo
- Francesco Zuliani

Les Houches, March 2003

My dream summary (forget half of it).

- $T = 0$, $T \neq 0$. Low T equilibrium valleys in Spin Glasses: EM, Martin and Zuliani, PRB 64 (2001) 184413. See Olivier Martin for ground states and spongy picture/s.
  1. Removal of ± 1 Degeneracy.
  2. Parallel Tempering.
- Ultrametricity. It is difficult according to 1997 work Cacciuto, EM and Parisi, JPA 30 (1997)L263. I will also use work by Franz and Ricci-Tersenghi and byParisi and Ricci-Tersenghi.
  1. Stochastic Stability (Parisi, Guerra, Aizenman-Contucci).
  2. Sum Rules. (EM, Parisi, Ricci-Tersenghi and Zuliani, J Stat Phys 98 (2000) 973; de Dominicis, Giardina, EM, Martin, Zuliani tbp)
  3. Clustering. (Domany, Hed, Palassini and Young, cond-mat 0104264; Ciliberti-EM tbp)
- Dynamics and Time Scales. Billoire+EM JPA 34(2001)2.)
- Exact Partition Functions in $2D$ SG. Lukic, EM, Martin tbp.

Supposedly ideas and techniques useful in different contexts (maybe all the new adventures in optimization could use some of that too).

Low T Equilibrium valleys of $3D$ Spin Glasses

EM, Martin, Zuliani. A first few details.

$3D$ Edwards Anderson Spin Glass. $L \nearrow 12$.

Low T.

First conclusion: $T > 0$ similar to $T = 0$.

Remove Z_2 symmetry ± 1. Define valleys. They turn out to have a free energy distance of order one, but an internal energy distance growing with L: interplay of energy and entropy.

Valleys $\longrightarrow$ space filling clusters...

Overlap $q_i \equiv \sigma_i \tau_i$.
Link overlap $q_{i,\mu}^{\text{link}} \equiv q_i q_{i+\mu}$.

Two spin configurations differing by a global minus sign have $q_i = -1$, $\forall i$ but $q_{i,\mu}^{\text{link}} = +1$, $\forall i$.

Consider two typical spin configurations (or two ground states). Consider the interface (IF) among equal and inverted regions: it is done from regions such that

$$q_{i,\mu}^{\text{link}} = -1 \ .$$

Probability of finding an IF on a random link:

$$\rho \equiv \frac{1}{2}\left(1 - q^{\text{link}}\right)$$

1. Ferromagnet. IF is confined in a region of width L^z $(z < 1)$. IF density $\longrightarrow 0$ as $L^{-\alpha}$, with $\alpha \geq (1 - z)$. For ferromagnets $\alpha = 0$.
2. $z = 1$, density $\longrightarrow 0$ as $L^{-\alpha}$. For $L \to \infty$: $D_F(IF) = D - \alpha$. IF is here a fractal (not multi-fractal) object.
3. $\alpha = 0$, density $\longrightarrow K \neq 0$, $q^{\text{link}} \longrightarrow \tilde{K} \neq 1$. IF is space filling.

Understanding Spin Glasses at low T: not easy.

Numerical methods (Monte Carlo): severe critical slowing down.

“in all the cold phase”

Optimized numerical methods (see later in this lecture).

Ground state computations (see Olivier martin lecture). Here advantage is that you are sure you are studying “the correct $T = 0$ physics” (no trapping from severe critical slowing down).

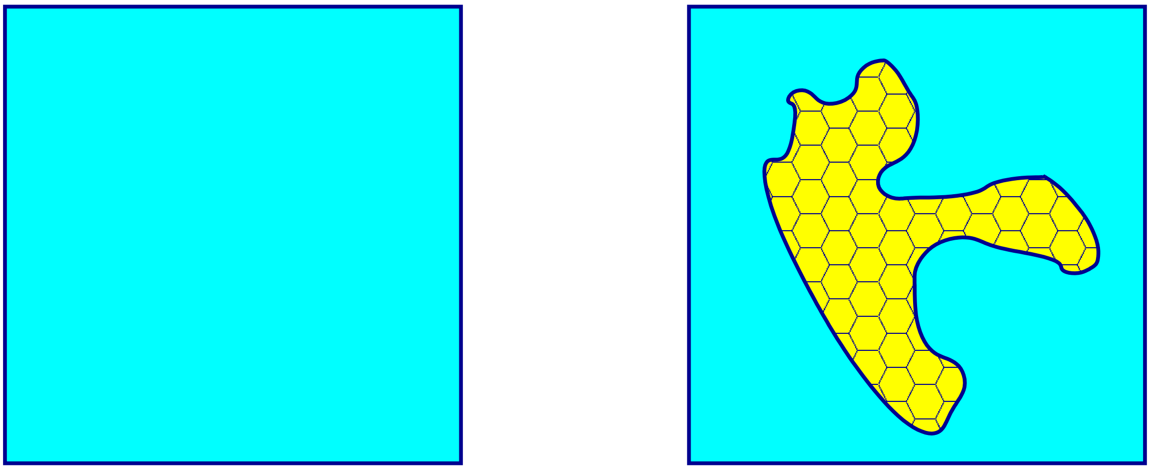
But: is that connected with finite T physics? (note that the question is very relevant also for landscape of optimization problems).

?? MF $\Longrightarrow$ Finite D systems $\Longleftarrow$ Droplet ??

Finite (but low) T.

Clustering to determine valleys $\longrightarrow$ “states”.

Find typical clusters (differences among two valleys).



Space filling and topologically highly non trivial.

This analysis is natural for ground states (compare ground states under different boundary conditions or after some perturbation or additional constraint).

Here: we have generalized these ideas for finite T: learn how to deal with thermal fluctuations.

- Generation of equilibrium configurations.
- Comparison of these configurations.

Making a long story short:

1. build and classify clusters of configuration differences;
2. "large" clusters have finite probability as $L \to \infty$;
3. definition of valleys by (simple) clustering;
4. different valleys turn out to be "very" different";
5. associate states to valleys.

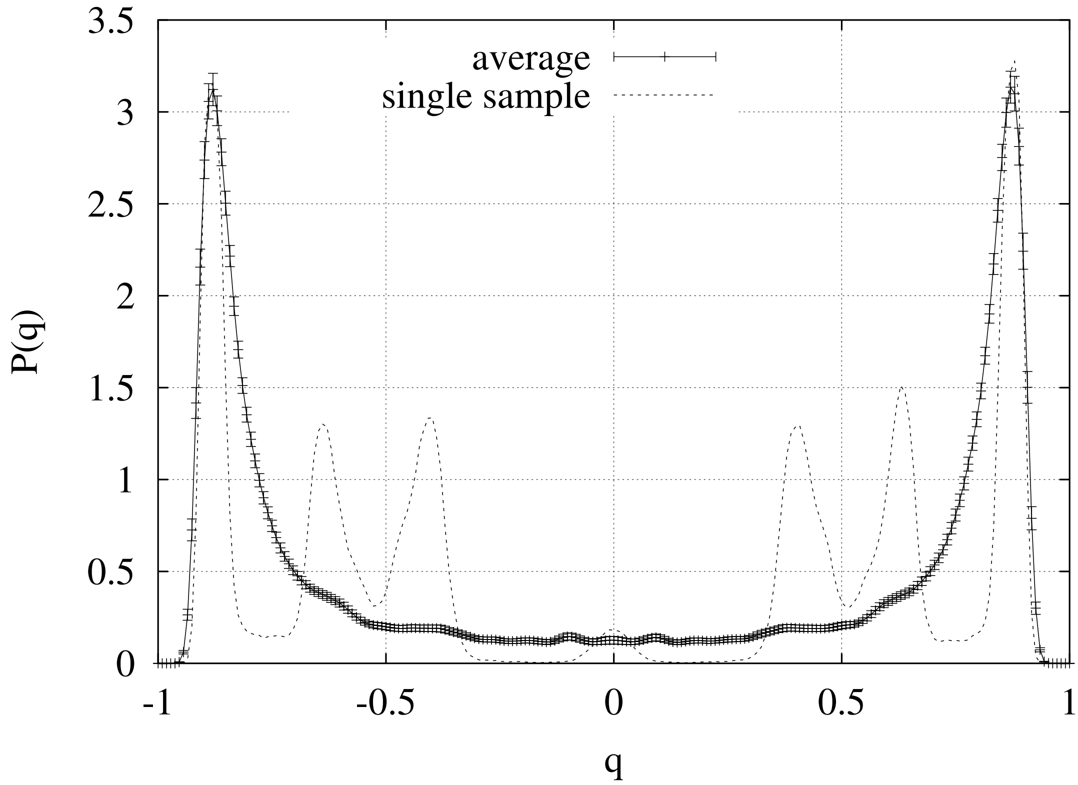
$3D$ Edwards-Anderson Spin Glass.

$$H = -\sum_{\langle i,j \rangle} \sigma_i J_{i,j} \sigma_j \ ,$$

$J = \pm 1$ with probability one half (multi-spin coding).

$T_c \sim 1.1$: here we use $T = 0.5$ and $L = 6$, 8, 12. Parallel tempering (see later): "good convergence". Here Z_2 symmetry helps.

512 samples per lattice size and T value.



From MMZ. Well thermalized.

$P_J(q) \neq P(q)$ is not it?

Define overlap among two spin configurations selected independently according to their a priori probability.

$$q(C_1, C_2) \equiv \frac{1}{N} \sum_{I=1}^{N} \sigma(i)\tau(i)$$

Let $|G|$ be the cardinality of the set of sites where the two configurations differ, G. Then

$$q = 1 - \frac{2|G|}{N} \; .$$

Peaks of $P_J \longrightarrow$ configurations classified in valleys (states).

We classify follow Houdayer, Krzakala and Martin.
Define categories:

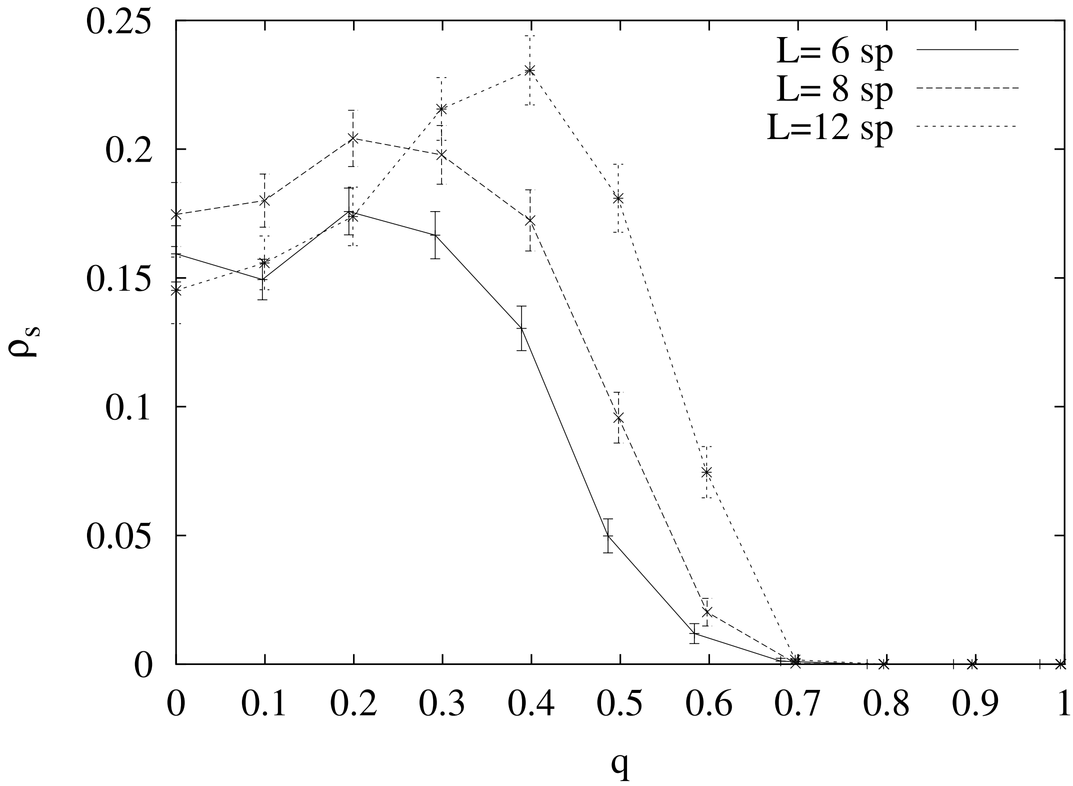
1. G is sponge-like if it and its complement both wind around the lattice in all three spatial directions;
2. G is droplet-like if it does not wrap the lattice, in no directions;
3. G is intermediate in all other cases.

here no "clustering" is needed.

We find that density of sponge-like increase for $L \nearrow$.

Decompose:

$$P(q) = P_{\text{sponge}}(q) + P_{\text{droplet}}(q) + P_{?}(q)$$



Density of sponges. Do we have sponges in infinite volume limit?

Support increases with size.

$$P_{\text{sponge}}(q \simeq 0) \simeq \ \text{constant}$$

Now we build valleys. Clustering.

Hierarchical tree is built in in the mean field solution. Does it naturally appears also in $3D$?

this is the leading question of this lecture...

Valley $\rightarrow$ state.

So: save in a thermalized Monte Carlo time series a number of (independent) configurations: try and cluster them.

If valleys are really well separated (we are in finite volume + maybe at the end there are no real valleys) the clusterization turns out to be meaningful.

Clustering method for defining a valley. Set a cutoff value $q^* \sim d^*$ (distance is derived from overlap). If $d_{AB} < d^*$ the two configurations A and B are in the same valley.

It works.

- some stability under variation of q^* (i.e. of d^*);
- corresponds to the $P_J(q)$ structure.

d^* too small: fraction it too much. d^* too large: merge by brute force all configurations in a single valley.

After that we have valleys, and we can analyze them. Check how do they differ. In this analysis $q^* = 0.5$, and we select disorder realizations that generate more than one valley.

Free energy of a valley α:

$$e^{-\beta F_\alpha} = \sum_{A \in \alpha} e^{-\beta H(C_A)}$$

that equals the number of times that MC visited this valley.

This is the weight of the valley. Monte Carlo gives that to us “for free”.

Order the valleys by increasing free energy:

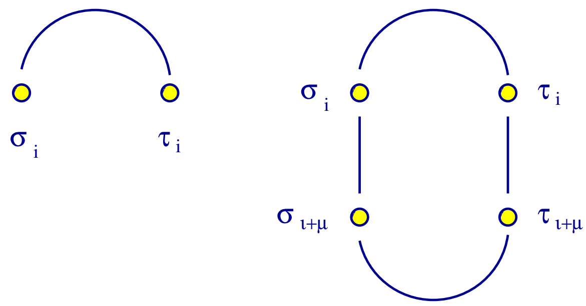
$$\Delta F \equiv F_2 - F_1 \geq 0 \; ; \quad e^{-\beta \Delta F} = \frac{\mathcal{N}_2}{\mathcal{N}_1}$$

ratio of number of configurations in each valley. ΔF is order one in mean field. It is also of order one in our numerical data in $3D$ (meaning that the fraction of configurations that pass our tests is sizable).

Now the internal energy of a valley.
$E_\alpha = \langle E_A \rangle_{A \in \alpha}$.
We measure $P(\Delta E \equiv E_2 - E_1)$, where E_1 is the internal energy of the valley with smaller free energy, and E_2 of the second one. We find

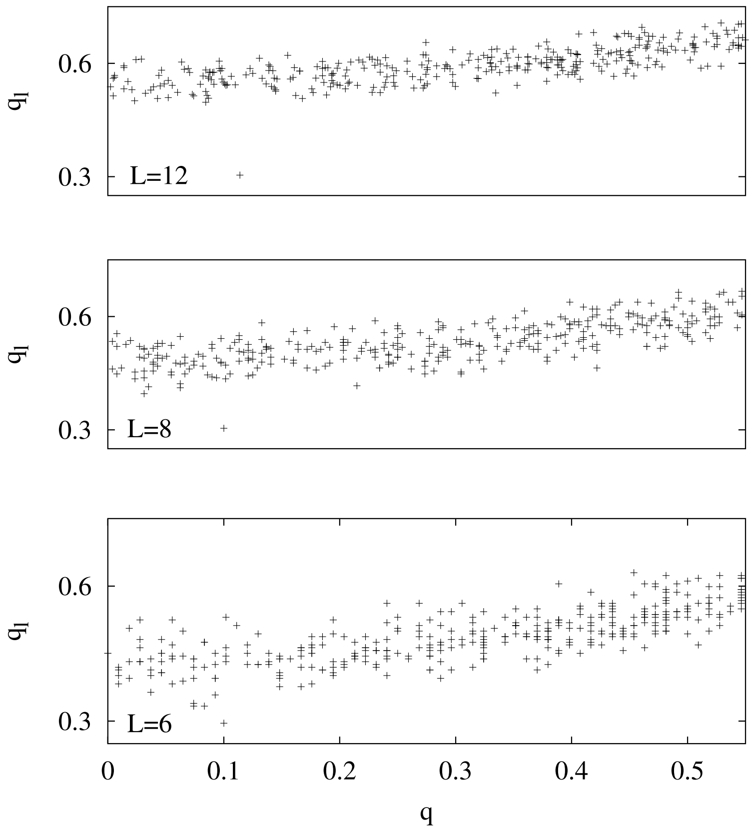
1. $\langle E \rangle > 0$ (this is not completely trivial: $F_2 > F_1 \Longrightarrow E_2 > E_1$)
2. The width of $P(\Delta E)$ grows with L (as opposed to the case of the free energy). Entropy must be balancing it.
3. Correlation $(\Delta E, \Delta F)$ is small.

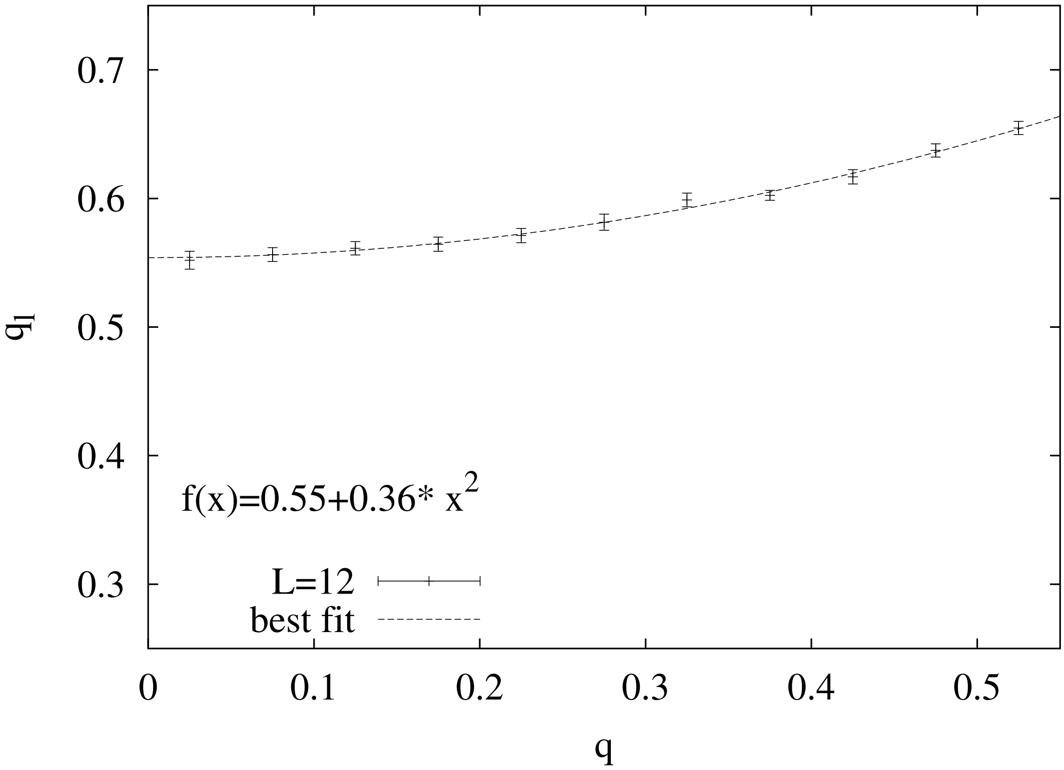
Spin and link overlap.



q_{link} is becoming, as L increases, a deterministic function of q.

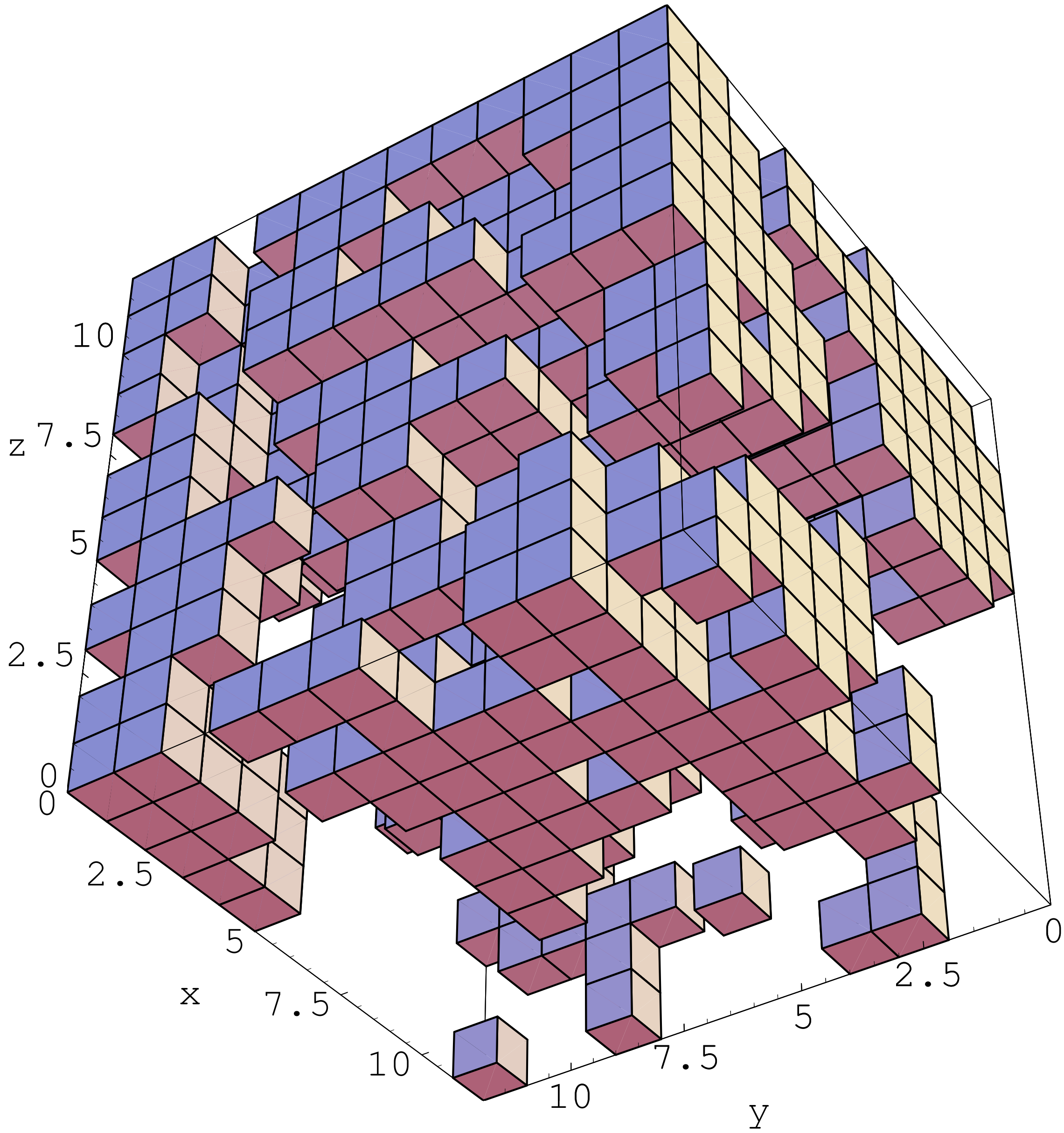
This agrees with ground state computations EM and Parisi, PRL 86 (2001) 3887.





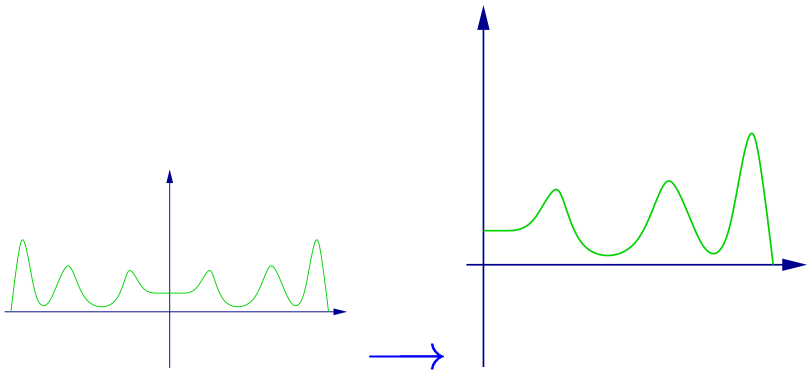
There are different procedures for analyzing these fluctuations at finite T: they give a consistent picture.

Quadratic dependence: mean field like. Good best fit.



A typical sponge (difference of local magnetizations after projection to ± 1). Looks "space filling".

Slicing Configuration Space Start from a set of configurations such that $\{C\} \Longrightarrow P(q)$, that we plot on the left, and generate, by inverting part of them, a new set of configurations such that $\{C'\} \Longrightarrow P^{(+)}(q)$, that we plot on the right:



This is needed in many situations (we will discuss testing of clustering and sum rules). We could apply a small magnetic field, but this is cumbersome.

So transform your configuration set. In the limit $V \to \infty$ one could use the fact that $V m_A = O(\sqrt{V})$ to select the right sign. This is not (at all) good enough on our typical volumes: it will leave you with a large tail of $P(q)$ with the wrong sign.

We do the separation using q.

Fix C_1.

- Flip C_2 if $q_{12} < 0$;
- Flip C_3 if $q_{13} + q_{23} < 0$;
- Flip C_4 if $q_{14} + q_{24} + q_{34} < 0$; ...
- $\ddots$

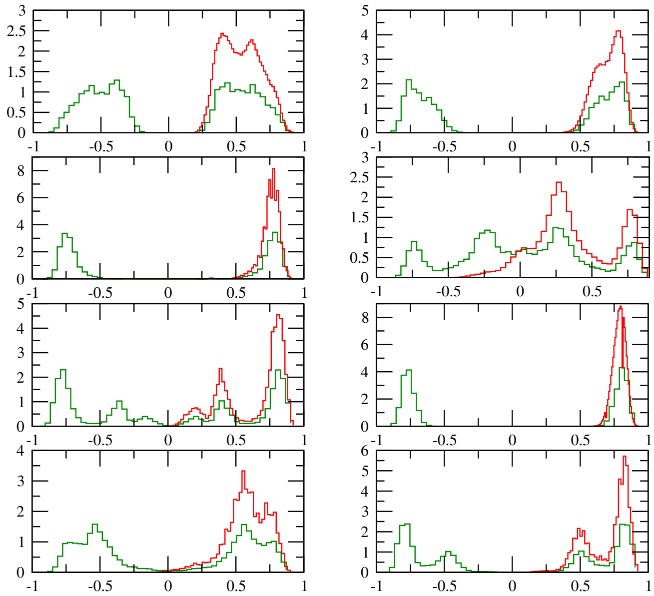
Now you can apply some mutations: select B and flip it if it has negative overlap with the rest. Do it in random order and in sequential order (can help a bit, never much).

Normally the process reaches very good results.

(in very complex samples a tail of $P(q)$ for $q < 0$ can still survive).

Other possible approach: use hierarchical cluster itself, see later.

Here results of selection of the phase space with two methods.

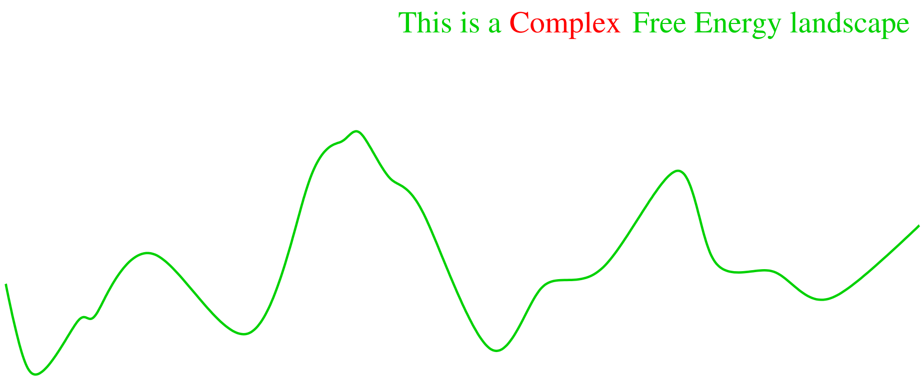


The two methods give the same result, quite satisfactory.

Optimized Monte Carlo Methods: Parallel Tempering

For Tempering and Parallel Tempering see: EM and Parisi 1992, Tesi et al. 1995; Geuer and Thompson 1994; Hukushima et al. 1995.

Free Energy Barriers



Difficult to cross. Crucial to cross.

If we change T free energy barriers change. When T increases barriers become smoother and smoother. When T reaches T_c the landscape has been flattened.

Idea:let the system walk in temperature space, going down to the low, interesting T value, and up all the way, through a chain of intermediate T values up to some $T \gg T_c$.

(A bit like annealing, but needs to be always at thermal equilibrium: tempering is annealing for free energy).

Generic class of methods where you modify the probability distribution π:

$$\int \pi O \sim \int \nu O' \ , \quad \text{where } \nu = \frac{\pi}{\rho} \ , \quad O' = \rho O$$

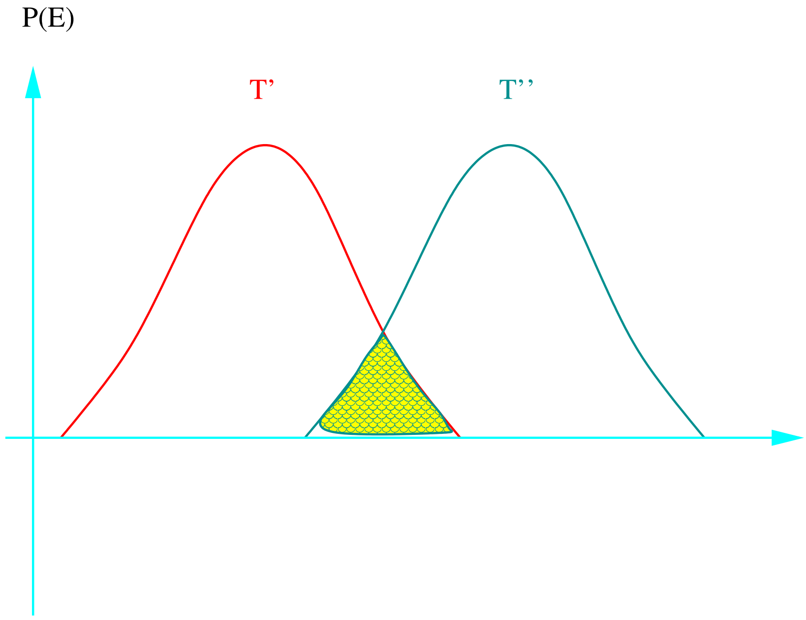
density scaling or umbrella sampling

Here the method is very simple since you have exactly the Boltzmann distribution at each T value (no reconstruction is needed: just select data at the correct T value). The method:

- select a discrete set of T values, $T_{(\alpha)}$: $\alpha = 0, 1, 2, \ldots, M$. Here $T_0 = T_{\text{min}}$ (typically smaller than T_c) and $T_M = T_{\text{max}}$ (typically larger than T_c).
- Clone your system M times, i.e. consider M configurations C_α of your system.
- start by assigning $T(C_0) = T_0$, $T(C_1) = T_1$, $\ldots$, $T(C_M) = T_M$.
- go ahead with Monte Carlo sweeps.

Two parts of Monte Carlo sweep:

- Usual MC sweeps on all copies of the system at fixed temperature.
- Swap two values of T. Consider $C(T_0)$ and $C(T_1)$. Propose them to swap T values.



Selection of T values range and spreading is the freedom of the method. If equidistributed T values and T_{min} is fixed from physics parameters are N_T and ΔT.
Use Metropolis to swap

$$\Delta S \equiv S' - S = \Big(\beta' E + \beta E\Big) - \Big(\beta E + \beta' E'\Big)$$

- do previous point for all configuration couples $C(T_1)$ and $C(T_2)$, $C(T_2)$ and $C(T_3)$ etcetera.

Choice of

- T_{min}: interesting physics + reasonable CPU time.
- T_{max}: "$\gg$" T_c.
- N_T: keep high acceptance factor for tempering swap.

Check thermalization

- Symmetry of $P_J(q)$ (here this is not as a strong check as in normal Monte Carlo: spin flip is not the slowest mode anymore).
- Check convergence of observables on logarithmic time scale.
- Check that acceptance rate for tempering has been kept high (see earlier).
- Each of the N_T copies of the system must have covered the $T_{(\alpha)}$ space with "many visits".

Ultrametricity

Here a few basic issues, toward a numerical approach.

Ultrametricity (UM) needs lot of space to emerge: it is really difficult to verify it on finite lattices. Cacciuto, EM, Parisi 1996, Franz, Ricci-Tersenghi 1999.

In our 1996 paper we tried to find an effective procedure to detect ultrametricity. Ultrametricity:

$$d_{13} \leq d_{12} + d_{23} \longrightarrow d_{13} \leq \max\left(d_{12}, d_{23}\right),$$

from triangular to (stronger) ultrametrical.

UM is an absolutely crucial feature of Parisi continuous RSB scheme. Consider two spin configurations α and β. Define a distance d from:

$$d^2_{\alpha,\beta} = \frac{1}{2}\left(1 - \frac{q_{\alpha,\beta}}{q_{EA}}\right)$$

equal to zero if $q = q_{EA}$, equal to 1 if $q = -q_{EA}$. Overlap:

$$q_{\alpha,\beta} = \frac{1}{V}\sum_{i=1}^{V} \sigma_i^\alpha \sigma_i^\beta \ .$$

In mean field:

$$
\begin{aligned}
& \overline{P_J\left(q_{12}, q_{13}, q_{23}\right)} \\
= \quad & \frac{1}{2}\, P(q_{12}) x(q_{12}) \delta(q_{12} - q_{23}) \delta(q_{12} - q_{13}) \\
+ \quad & \frac{1}{2} \{ P(q_{12}) P(q_{23}) \theta(q_{12} - q_{23}) \delta(q_{23} - q_{13}) \\
+ \quad & \text{two permutations } \}
\end{aligned}
$$

i.e. UM holds. How can we verify that?

Constrained Monte Carlo procedure. For one given realization of the disorder consider three copies of the system, and fix

$$
q_{\alpha,\beta} = \overline{q} \ , \quad q_{\beta,\gamma} = \tilde{q}
$$

(smooth constraint, with some given allowance ϵ). A good choice of $\overline{q}$ and $\tilde{q}$ is crucial: they must be in the support of $P(q)$ of the unconstrained model, and such to make the UM bound as different as possible from the triangular one.

$4D$ EA SG, $T_{\text{min}} \sim 0.7\ T_c$. Select

$$
\overline{q} = \tilde{q} = \frac{2}{5} q_{EA} \simeq 0.21 \ .
$$

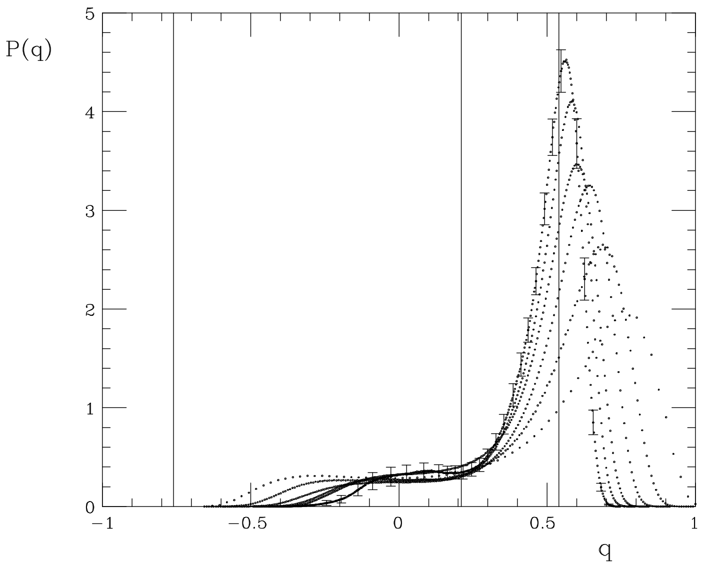
1. triangular $\Longrightarrow q \geq -\frac{7}{5} q_{EA}$
2. ultrametric $\Longrightarrow q \geq \frac{2}{5} q_{EA}$

from left to right

triangular lower bound

UM lower bound

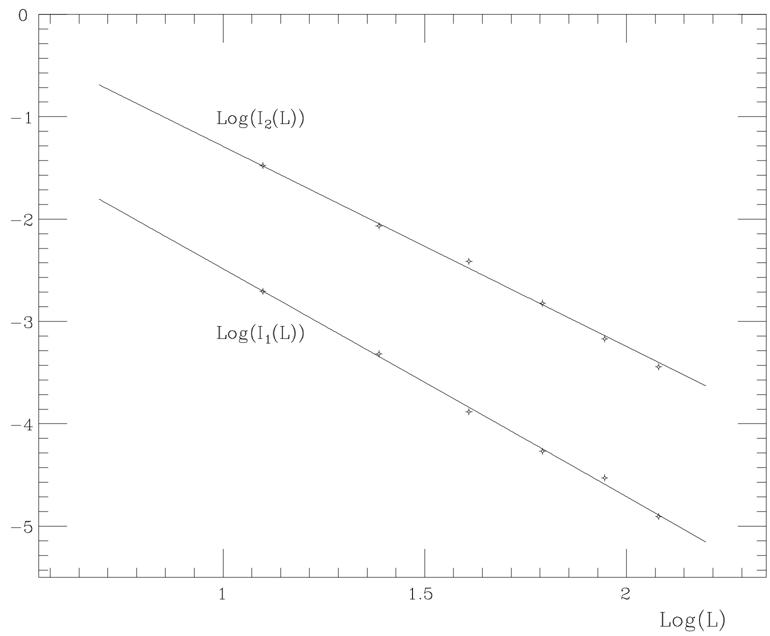
Edwards Anderson infinite volume upper bound



Far from triangular bound, but very large finite volume effects

Probability for a configuration not to be ultrametric:

$$I^L \equiv \int_{-1}^{q_{min}} (q(L) - q_{min})^2 P(q) dq$$
$$+ \int_{q_{MAX}}^{1} (q(L) - q_{MAX})^2 P(q) dq \ ,$$



Best fit:

$$I^L \simeq (-.0001 \pm .0005) + (0.76 \pm 0.03) L^{-2.21 \pm 0.04} \ .$$

Reasonable but not perfect (mainly clear problems with finite volume).

Nice dynamic UM analysis Franz, Ricci-Tersenghi. Evolve two copies of the system at fixed overlap $\overline{q}$ (as usual keep $\overline{q}$ in the support of $P(q)$).

autocorrelation:

$$C(t,t') = \frac{1}{V}\sum \sigma_i(t)\sigma_i(t')$$

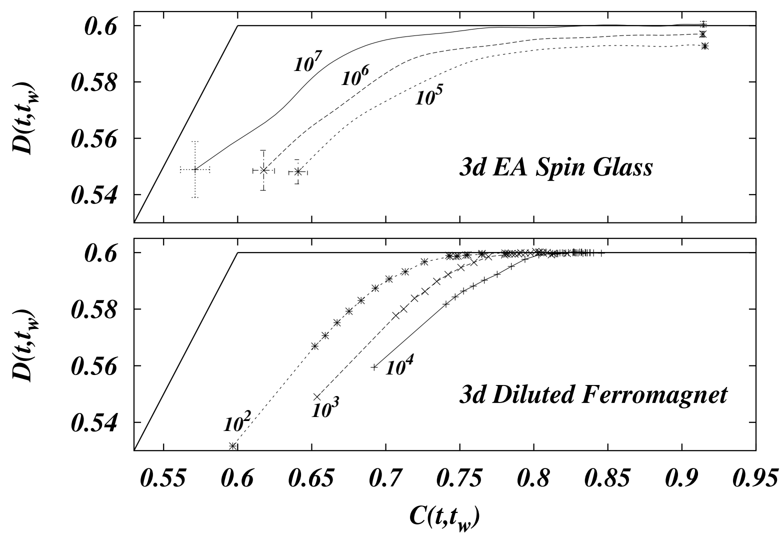
cross-correlation:

$$D(t,t') = \frac{1}{V}\sum \sigma_i(t)\tau_i(t')$$

(Dynamic) ultrametricity implies that

$$D(t,t') = \min\left\{C(t,t'),\overline{q}\right\}$$

(based on approach by Franz, Parisi and Virasoro). The main point is in the fact that $\overline{q}$ fixes two of the correlations over the ones you can form using $\sigma(t)$, $\sigma(t')$, $\tau(t)$, $\tau(t')$,



Sum Rules

Parisi; Guerra; Aizenman, Contucci; EM, Parisi, Ricci-Tersenghi, Ruiz-Lorenzo, Zuliani. We can define sum rules by starting from a crucial property of systems that are "generic enough". Define:

$$H^{(\epsilon)} \equiv H^0 + \epsilon H_{\text{random}}$$

H^0 is for the original system, for example an EA SG, while H_{random} is a (further) random perturbation.

Stochastic stability:
after averages over the original H^0 and over H_{random} all the properties of the original system are smooth functions of ϵ around $\epsilon = 0$.

A typical H_{random} is

$$H_{\text{random}} = \mathcal{N}(N) \sum_{i_1 \dots i_A} R_{\text{random}}(i_1 \dots i_A)$$
$$\sigma(i_1) \dots \sigma(i_A)$$

R: random uncorrelated Gaussian variables. If there is a symmetry, no stochastic stability (for example need $h \sim \epsilon$). Sum rules can be derived from stochastic stability. For example:

$$P(q_1, q_2) \equiv \overline{P_J(q_1) P_J(q_2)} = \frac{2}{3} P(q_1) P(q_2) + \frac{1}{3} P(q_1) \delta(q_1 - q_2)$$

that in turn implies $\overline{\langle q^2 \rangle^2} = \frac{1}{3} \overline{\langle q \rangle} + \frac{2}{3} \overline{\langle q^2 \rangle}^2$

To check these ideas compute numerically joint overlaps of real replicas.

Here $3D$, EA SG, binary couplings.

$$E(\cdot) \equiv \overline{\langle \cdot \rangle}$$

So what we wrote before can be written as

$$E\left(q_{12}^2 q_{34}^2\right) = \frac{2}{3} E\left(q_{12}^2\right)^2 + \frac{1}{3} E\left(q_{12}^4\right)$$

and both sides of the relation can be obtained by only two copies of the system. This is not true for example for a second relation:

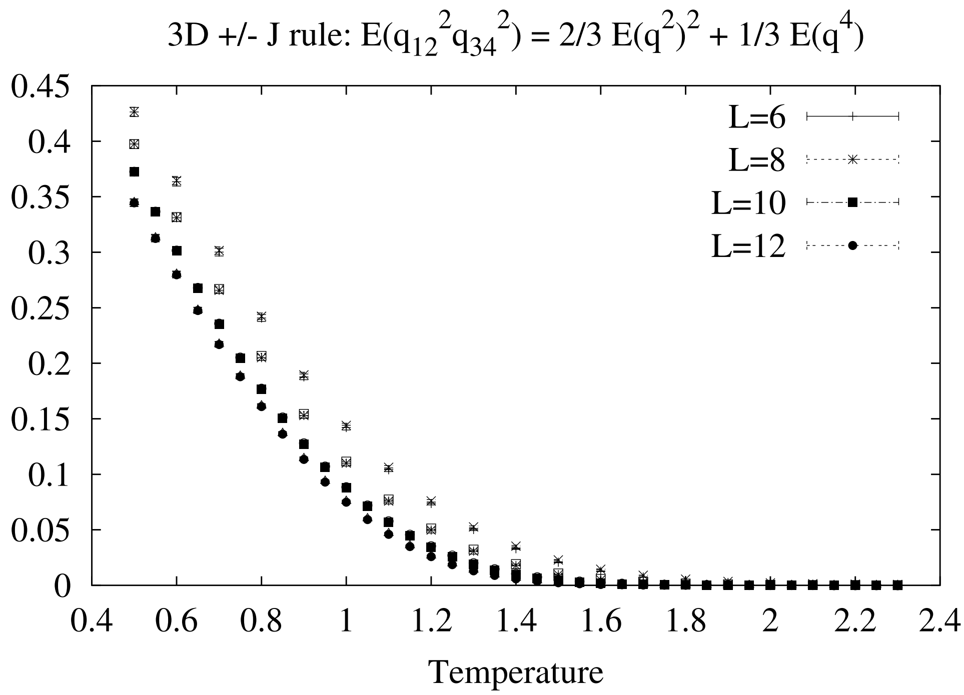
$$E\left(q_{12}^2 q_{23}^2\right) = \frac{1}{2} E\left(q_{12}^2\right)^2 + \frac{1}{2} E\left(q_{12}^4\right)$$

where you need at least three copies.

This second relation is very interesting, since it contains the effect of correlated replicas.

Left and right hand side. They cannot be distinguished on this scale.

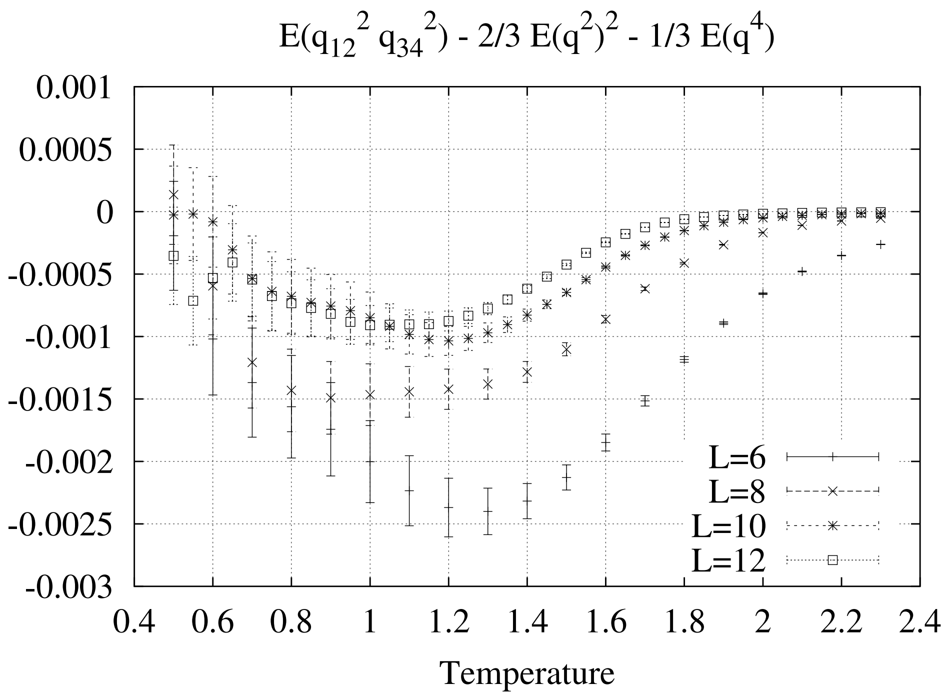
The sum rule is satisfied (since points are perfectly superposed) and in a non-trivial way (i.e. not by 0=0) (since the values are non-zero for $T < T_c$).



Size of the violation on a finite lattice.

The corrections are already small on small lattices.

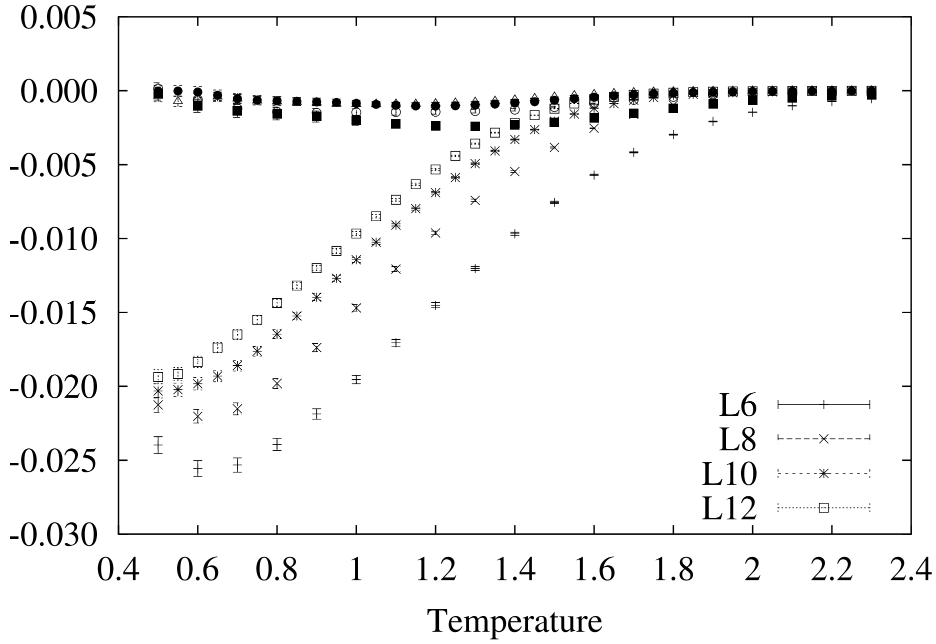
They are maximum close to T_c and decrease far away.



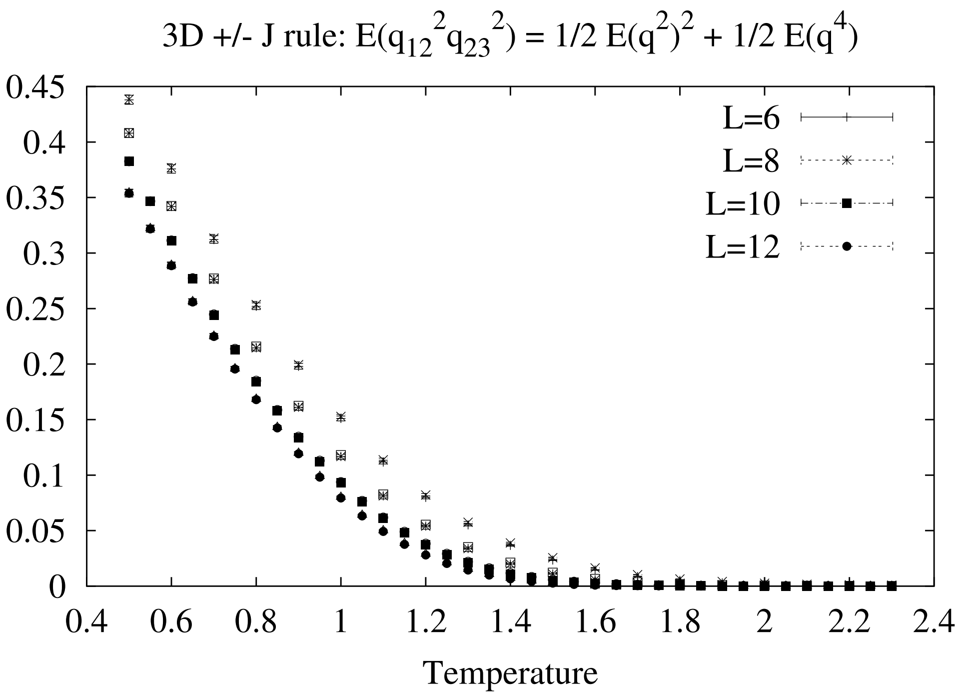
Maybe you doubt. Indeed even for a droplet like, delta like probability distribution, the sum rule would be satisfied.

So we sum the two factors with wrong coefficients:

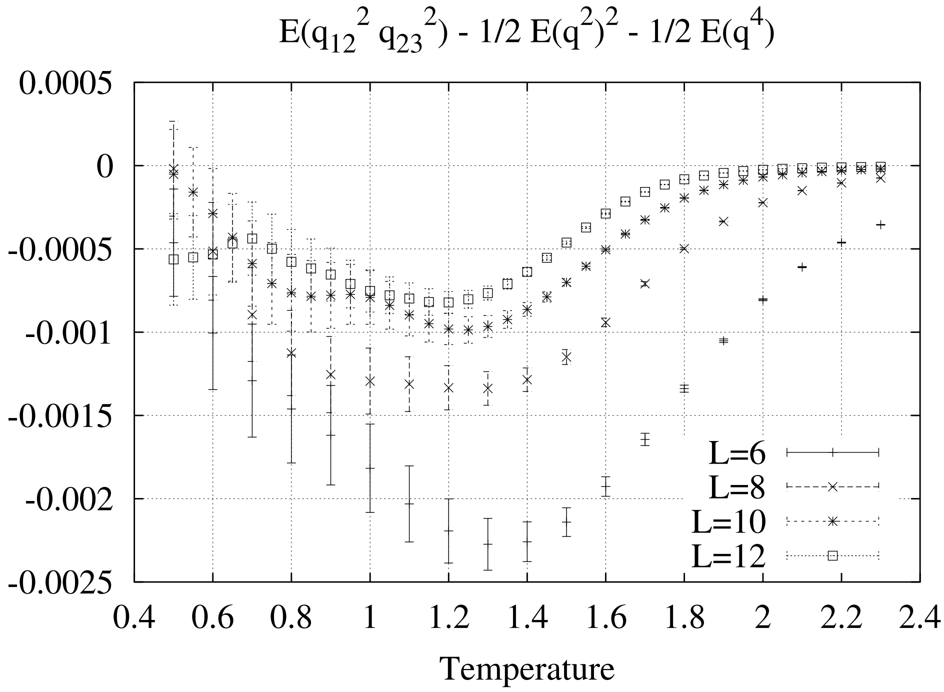
$$E(q_{12}^2 q_{34}^2) - \frac{1}{3}E(q^2)^2 - \frac{2}{3}E(q^4)$$



Also for the 3 replicas sum rule there is a perfect agreement of right hand side and left hand side.



Same pattern than before for finite size effects.



Analysis of spin-spin correlation functions in the framework of replica field theory $\longrightarrow$ sum rules. Bray and Moore 1987, De Dominicis, Giardina, EM, Martin, Zuliani, tbp.

A cancellation mechanism leads to an exponential decay for a particular correlation function. This mechanism is connected to the existence of a sum rule.

Define

$$C_\alpha(i,j) = \overline{\langle\sigma_i\sigma_j\rangle^2} - 2\alpha\overline{\langle\sigma_i\rangle\langle\sigma_i\sigma_j\rangle\langle\sigma_j\rangle} + (2\alpha-1)\overline{\langle\sigma_i\rangle^2\langle\sigma_j\rangle^2}$$

(notice that here you need $h \sim \epsilon$ or, better, to partion configuration space). $\alpha = 1$: usual spin glass susceptibility

$$(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle)^2$$

At large distance:

$$\lim_{|i-j|\to\infty} C_\alpha(i,j) = \overline{q_{12}^2} - 2\alpha\overline{q_{12}q_{23}} + (2\alpha-1)\overline{q_{12}q_{34}}$$

$\alpha = 2$: expect exponential decay. This a precise prediction of Mean Field, not shared by droplet picture. Also in this case plateau is zero because of the sum rule:

$$\overline{q_{12}^2} - 4\overline{q_{12}q_{23}} + 3\overline{q_{12}q_{34}} = 0$$

We have find numerically that this decay is indeed exponential, and plateau goes to zero when $L \to \infty$.

Back to ultrametricity is via an interesting result by Parisi and Ricci-Tersenghi.

(1) stochastic stability + 2) overlap equivalence) $\Longrightarrow$ ultrametricity

1) stochastic stability, that we have already discussed, is equivalent to replica equivalence, i.e. the fact that observables which depend only on one replica are replica symmetric.

2) overlap equivalence is connected to separability:

$$Q_{ab} = Q_{cd} \Longrightarrow f(Q_{ab}) = f(Q_{cd}) \ ,$$

for example Q^*_{ab}, $\sum_c Q_{ac} Q_{bc}$.

For a generic observable $w_i(\{\sigma\})$ define a generalized overlap $w_i(\{\sigma\}) w_i(\{\tau\})$. Typical example is the link overlap.

In MF $q_{\rm link} \sim q^2$. In the fixed q ensemble fluctuations due to RSB disappear.

Testing UM with Clustering

Clustering results of numerical simulations.
Domany, Hed, Hartmann, Stauffer 2001, Domany, Hed, Palassini, Young 2001.

We try to apply quantitative testing techniques Ciliberti, Marinari. We test MF: we know detecting UM is very difficult.

We find that the Z_2 symmetry has to be removed before any quantitative testing. This is very important: the ± 1 degeneracy completely obfuscates the results of the UM tests (see later).

Clustering (here for SK model with Gaussian couplings).

First you produce independent configurations (save $\forall 1000$ full MC plus tempering sweeps) configurations at different (low) T values. N up to 512. T down to 0.2 (very low).

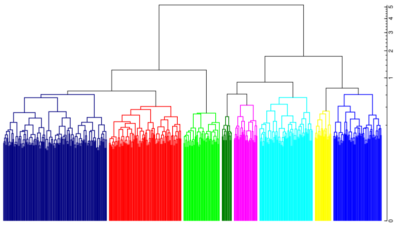
Set of configurations $\{C_t^{\tilde{T}}\}$. Compute overlaps at $T = \tilde{T}$ from $\sigma_{t'}^{\tilde{T}}(i)\sigma_{t''}^{\tilde{T}}(j)$, and since we are at equilibrium and configurations are uncorrelated this is a stationary sequence.

Clustering: partition data in "natural classes"':

- impose an ultrametric structure;
- check it it is natural.

Partion N objects into K clusters so that two points that belong to the same group are more similar than objects belonging to different groups.

Here we use, for the case $q \in (-1, +1)$ the definition $d \sim \frac{1-q}{2} \in (0, 1)$.

Hierarchical cluster algorithm $\longrightarrow$ dendogram.  There are many clustering algorithms one could use. Ward algorithm looks very suitable.

Fuse two clusters (individual objects are initial clusters).

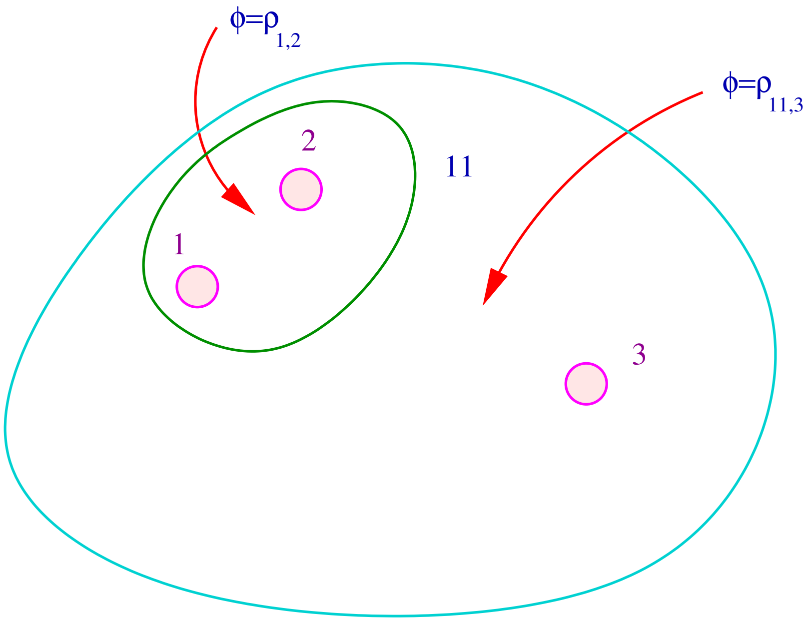
Initial partition: one object per cluster. Compute $D_{\alpha,\beta}$ among all "clusters". Fuse the two closer clusters:

$$\gamma = \text{``}\alpha \cup \beta''$$

Now define effective distance from this cluster to other clusters. For the process $\alpha + \beta \longrightarrow \gamma$, let n_α be the number of objects in cluster α. For all other cluster η we define $\mathcal{N} \equiv n_\alpha + n_\beta + n_\eta$. and

$$d_{\gamma\eta} = \frac{n_\alpha + n_\eta}{\mathcal{N}} d_{\alpha\eta} + \frac{n_\beta + n_\eta}{\mathcal{N}} d_{\beta\eta} - \frac{n_\eta}{\mathcal{N}} d_{\alpha\beta}$$

$$\phi(\gamma) \equiv d_{\alpha,\beta} \quad (\phi_{\text{initial configuration}}(\alpha) = 0)$$



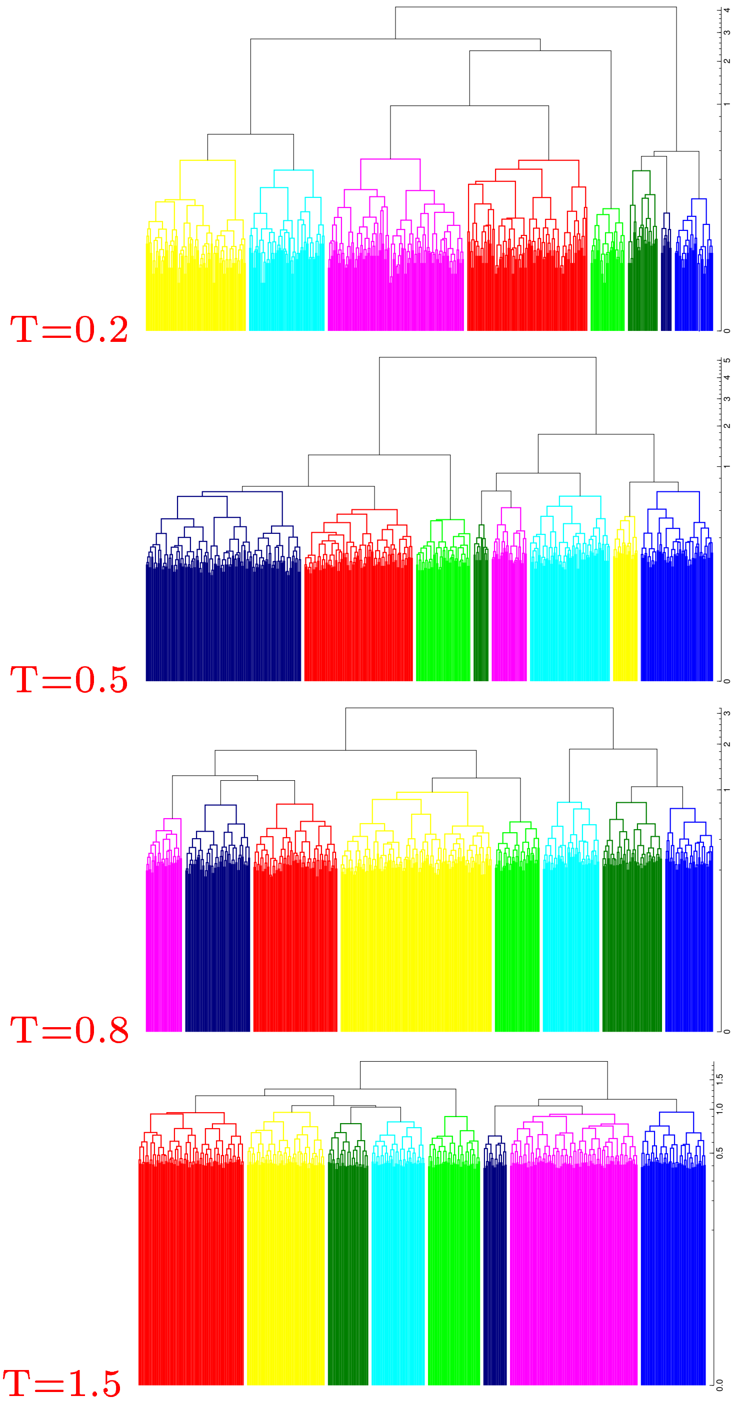
$$\delta(\gamma) = \sum_{\alpha,\beta\in\gamma} D^2_{\alpha,\beta}$$

distance of all couples of configurations in a cluster. Clusters formed earlier have lower ϕ and δ.

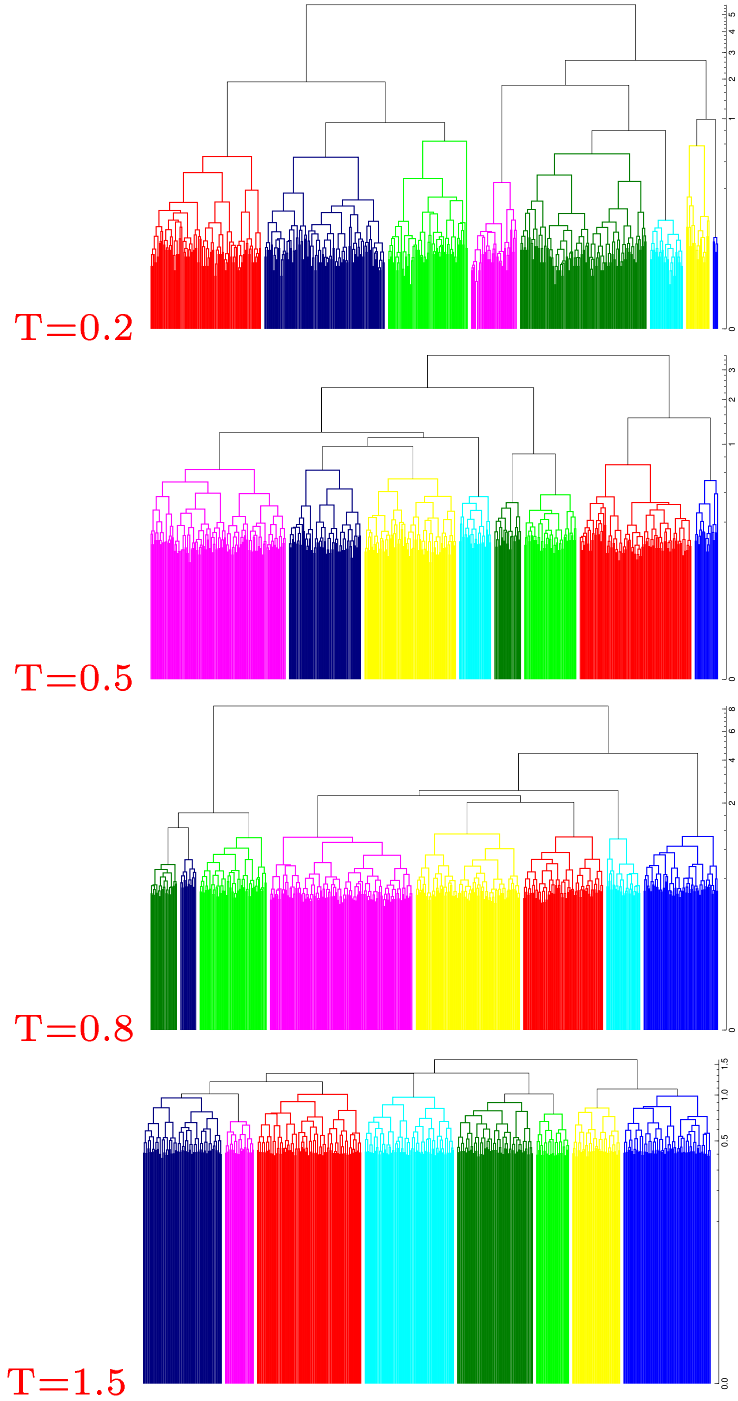
Output of the procedure is a dendogram. Leaves are configurations. Ascending the tree you coarsen. UM is built in.

Testing: are we detecting a real UM? A valid clustering is equivalent to the presence of an ultrametric structure. So, we have to check validity of the clustering.

Visual observation does not help much... (but scale is different).



A different disorder sample.



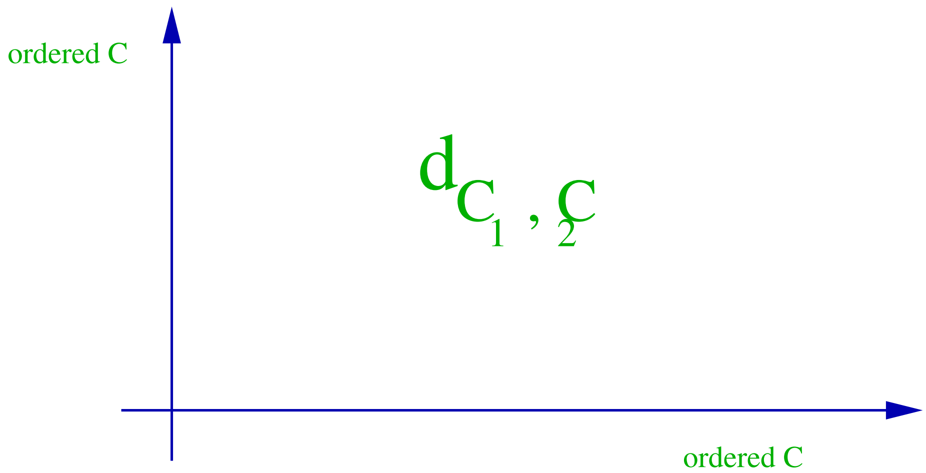
We summarize:

$$d_{\alpha,\beta} = \frac{1 - q_{\alpha,\beta}}{2}$$

by application of a cluster algorithm we obtain a

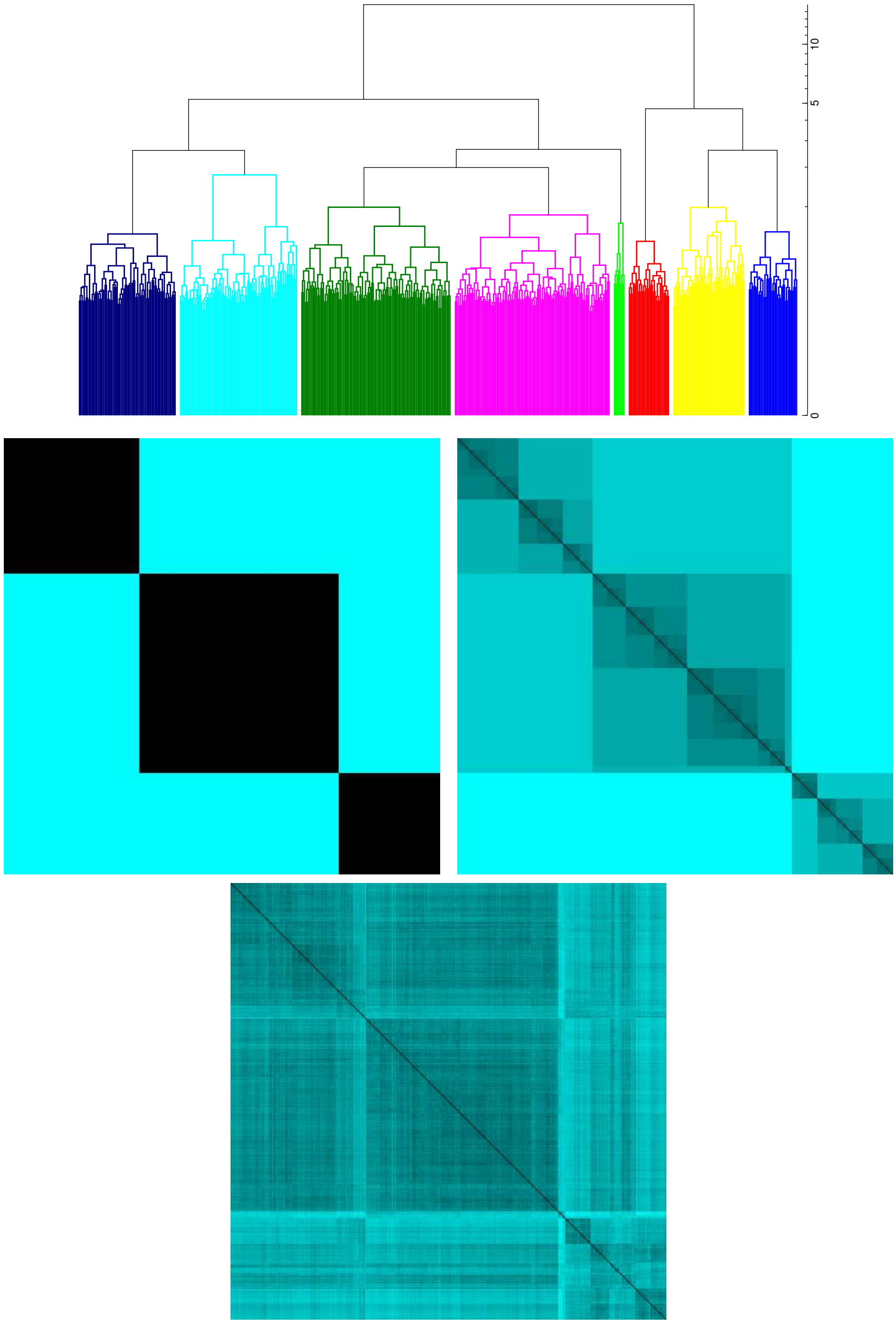
DENDOGRAM

i.e. an ordering of the configurations enriched by a (cophenetic) distance



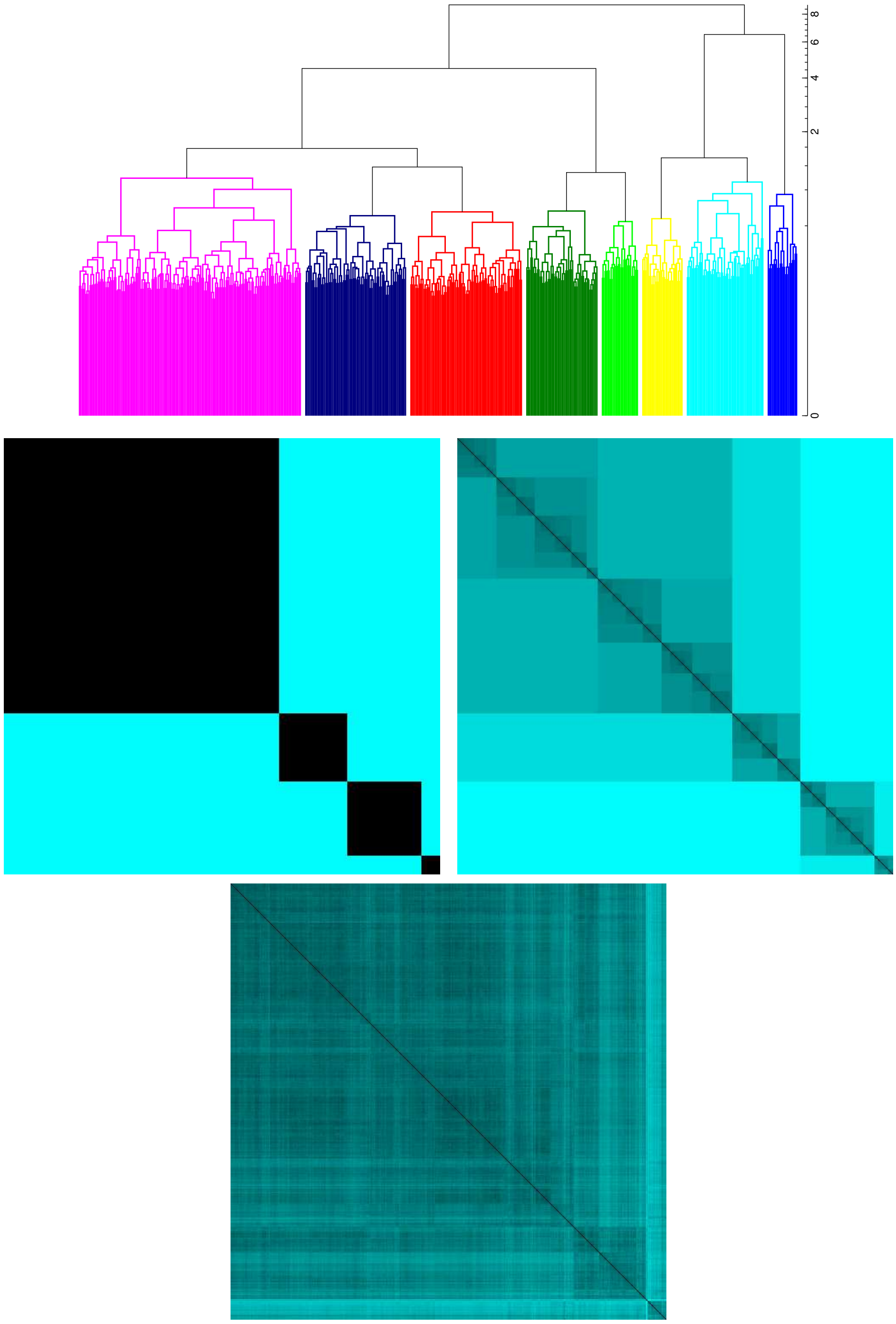
And now we can look at some figures.

SK, N=512, $T = T_c/2$



There is something good here.

SK, N=512, $T = T_c/2$



But much less here.

Before testing clustering. Classical analysis for ultrametricity detection. Order

$$d_{\alpha,\beta} \geq d_{\alpha,\gamma} \geq d_{\beta,\gamma}$$

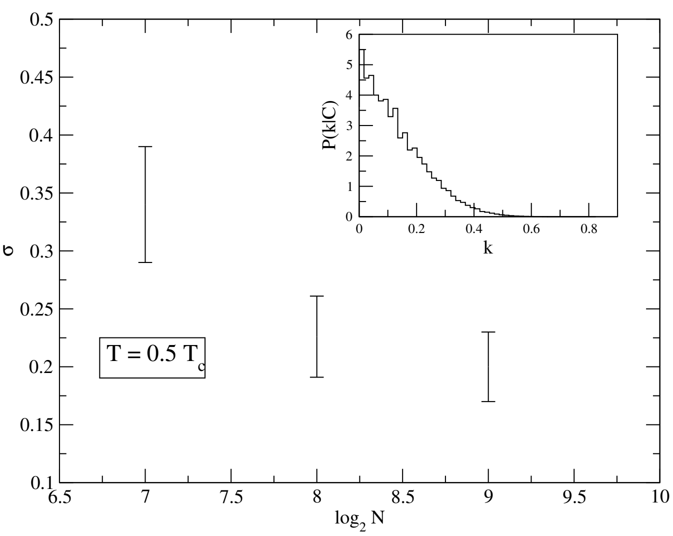
and define

$$W_{\alpha,\beta,\gamma} = \frac{d_{\alpha,\beta} - d_{\alpha,\gamma}}{d_{\beta,\gamma}}$$

$$\text{UM} \Longrightarrow \rho_{\alpha,\beta} = \rho_{\alpha,\gamma} \Longrightarrow P(W) \longrightarrow \delta(W) \text{ for } L \to \infty .$$

$$P_L(W) \sim e^{-\frac{W^2}{2\sigma^2}\theta(W)} \ , \quad \sigma \to 0$$

Very slow decrease (see Cacciuto, EM, Parisi before).



Standard techniques fo a quantitative test of clustering Jain and Dubes, Algorithms for Clustering Data, Prentice Hall (1998).

Two hypothesis: R_0 randomness (no UM), R_1 structures (our clustering is ok, UM structure is not a dream).

We define some variable r, small under the null hypothesis R_0. We define a threshold R_α such that

$$P(r \geq r_\alpha | R_0) = \alpha$$

Measure $r = r^*$ in our data.

- $r^* \geq r_\alpha \Longrightarrow$ reject R_0 at level α;
- $r^* < r_\alpha \Longrightarrow$ accept R_0 at level α.

Hubert Γ statistics.

You want to compare two proximity matrices for the same object.

- $d_{\alpha,\beta}$ true distance among configurations.
- $f_{\alpha,\beta}$ is zero if α and β are in the same valley (defined under a threshold level), is 1 if it is not.

$$m_d \equiv \frac{1}{M^2}\sum_{\alpha,\beta} d_{\alpha,\beta}\ ;\quad m_f \equiv \frac{1}{M^2}\sum_{\alpha,\beta} f_{\alpha,\beta}$$

$$s_d^2 \equiv \frac{1}{M^2}\sum_{\alpha,\beta}\left[d_{\alpha,\beta}^2\right] - m_d^2$$

$$s_f^2 \equiv \frac{1}{M^2}\sum_{\alpha,\beta}\left[f_{\alpha,\beta}^2\right] - m_f^2$$

$$\Gamma \equiv \frac{1}{M^2}\sum_{\alpha,\beta}\frac{(d_{\alpha,\beta}-m_d)\,((f_{\alpha,\beta}-m_f)}{s_d s_f}$$

Testing the hypothesis. Compute the probability level. Select a number of random permutations of integers $\pi(\alpha)$ and compute

$$\Gamma(\pi) \equiv \frac{1}{M^2}\sum_{\alpha,\beta}\frac{(d_{\alpha,\beta}-m_d)\left((f_{\pi(\alpha),\pi(\beta)}-m_f\right)}{s_d s_f}$$

Build up an histogram and check how probable it is the clustering you obtained (larger than 95% ok?)

Results are positive (for valley threshold we have seen in the figure) even after removing the ± 1 symmetry. There is some structure!

We discuss last a second indicator. This is crucial, since it tells us about the validity of the hierarchical structure.

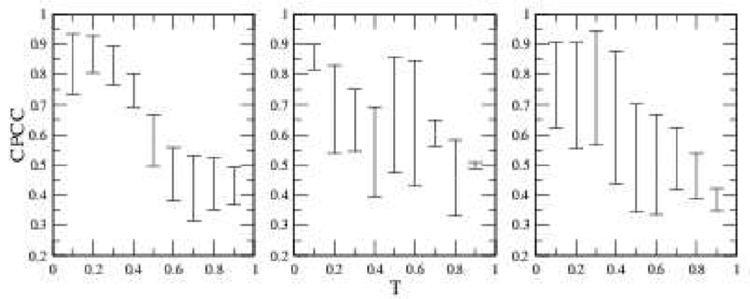
$d^C_{\alpha,\beta}$ cophenetic distance (UM by definition), i.e. the distance on the dendogram. $d_{\alpha,\beta}$ is the true distance.

$$\mathcal{K} \equiv \frac{\frac{1}{M^2}\sum_{\alpha,\beta} d^C_{\alpha,\beta} d_{\alpha,\beta} - \overline{d^C}\ \overline{d}}{\sigma_d \sigma_c}$$

It must be close to one to support the presence of a hierarchical structure (here there is not arbitrary threshold in the definition).

K is very used in numerical taxonomy. Empirically 0.9 is not enough (can establish accurately levels with MC as before).

Again, in presence of the Z_2 symmetry, K is very high and misleading. After removing it:



low, large errors, not very N dependent.

Detection on UM on “medium” size lattices is, even for MF models, very difficult or, better, impossible.