Challenging Problems in Disordered Systems

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Orsay, April 2004.

Overwiew of the talk

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5. The droplet model
6. The Parisi Solution (Replica Symmetry Breaking)
7. Phase transition in three dimensions
8. Low temperature properties. Equilibrium numerical simulations.
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Disorder

One can introduce two different kinds of disorder: Annealed and Quenched.

- Annealed Disorder. In this case the impurities (I) are in thermal equilibrium with the atoms of the material (S). Hence, the partition function of the systems is:

$$\mathcal{Z} = \mathrm{Tr}_{\{S\},\{I\}} \exp(-\beta \mathcal{H}(\mathcal{S};\mathcal{I}))\,,$$

  and the free energy is

$$F_a = -\frac{1}{\beta} \log \mathcal{Z}\,.$$

- Quenched Disorder. Now the impurities are completely frozen. The response of the atoms is quicker than the response of the impurities. So, the partition function is

$$\mathcal{Z}(\mathcal{I}) = \mathrm{Tr}_{\{S\}} \exp(-\beta \mathcal{H}(\mathcal{S};\mathcal{I}))\,,$$

$$F(I) = -\frac{1}{\beta} \log \mathcal{Z}(\mathcal{I})\,,$$

  and the free energy is

$$F_q = \int F(I) P(I) d\mu[I]\,.$$

The quenched disorder is analogous to the Born-Oppenheimer approximation in Molecular Physics. There are two different time scales: that of nucleus (impurities) and the one of the electrons (atoms). Also used (mainly in the past) in lattice QCD: the degrees of freedom of the quarks are frozen.

Frustration

$$\mathcal{H} = -\sum J_{ij} S_i S_j$$

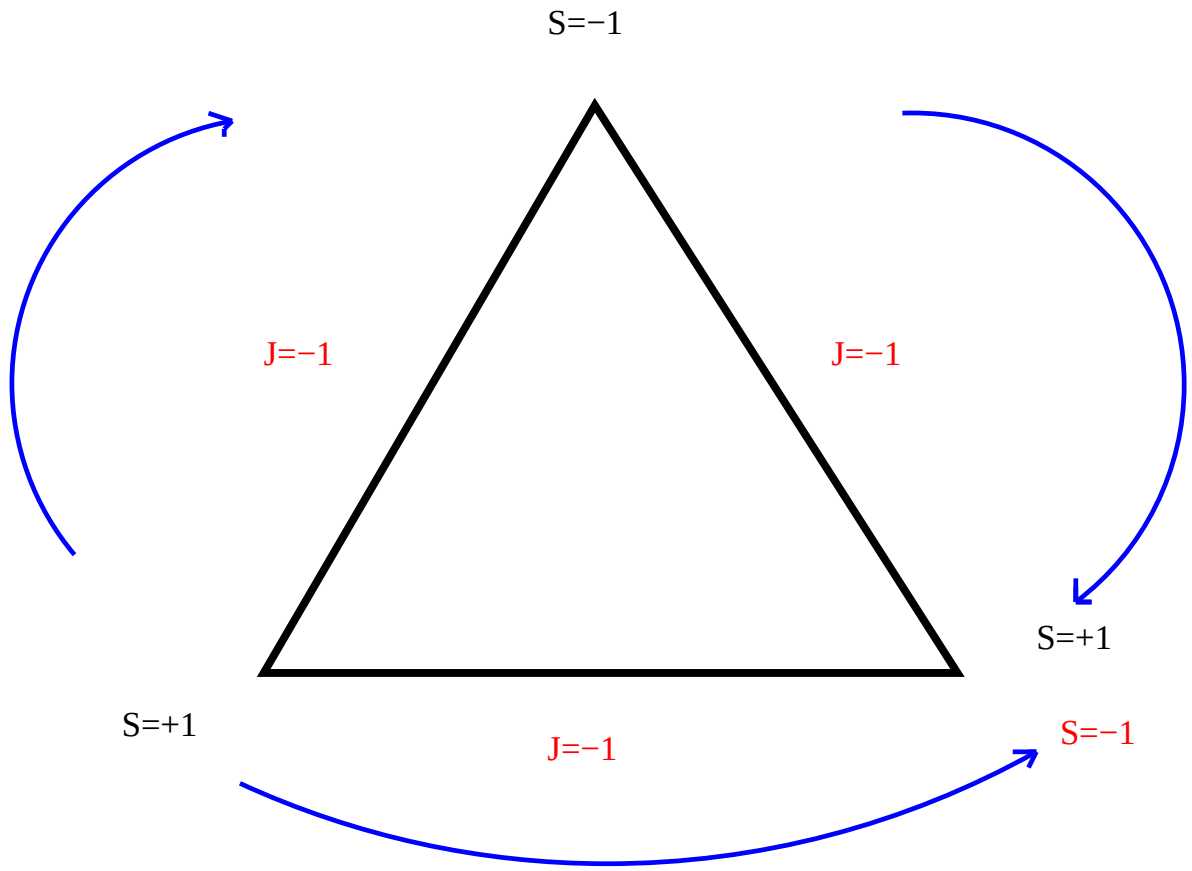

Figure 1: Frustrated triangle. For instance, an antiferromagnetic system on a triangular lattice.

Disorder + Frustration

- Free energy landscape with a large number of metastable states, large free energy barriers and maybe a large number of absolute minima (pure states).
- Glassy Behavior.

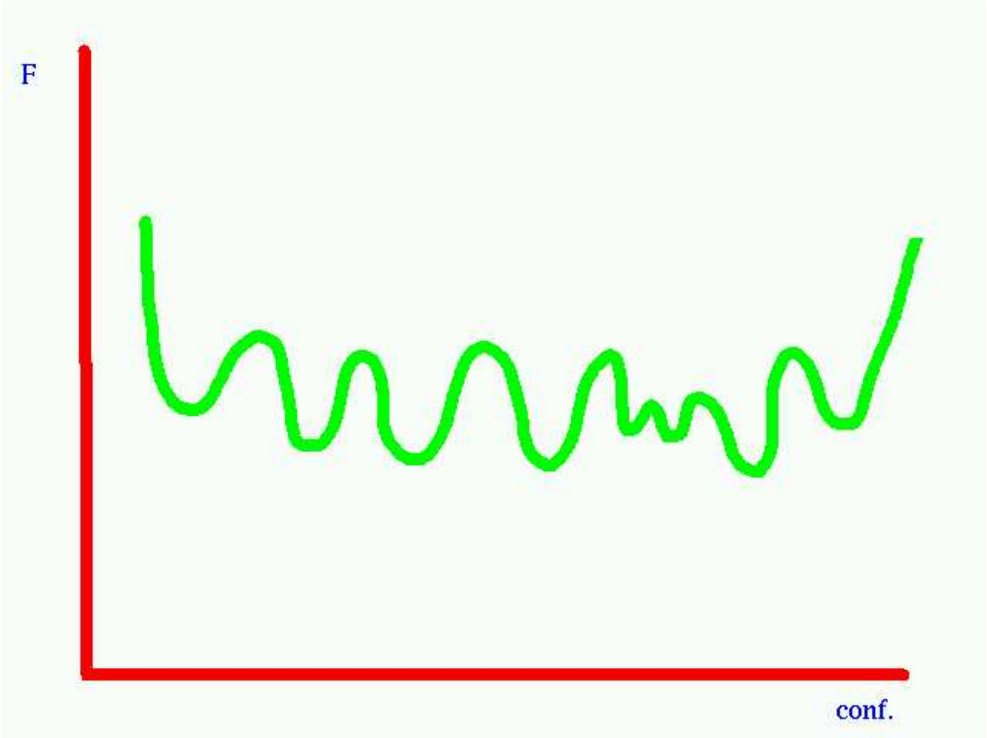

Figure 2: Free energy landscape of a system with disorder and frustration.

Spin Glasses: The Edwards-Anderson Model

- Metals with magnetic impurities. For example, Cu or Ag with impurities of Fe or Mn. ($\simeq 1\%$).
- The interaction between the magnetic moments of the magnetic impurities is mediated by the electrons of the conduction band, inducing an oscillating interaction (RKKY):

$$J(r) \simeq \frac{\cos(2k_{\mathrm{F}}r)}{r^3} \quad \text{as} \quad k_{\mathrm{F}}r \gg 1 \ .$$

- All these properties induce disorder and frustration.
- In general the spins are Heisenberg, but the spins in CuMn can be considered as Ising in a good approximation.
- The Edwards-Anderson Hamiltonian is:

$$\mathcal{H} = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - \sum_{<i,j>} J_{ij}\tau_i\tau_j$$

  J_{ij} Gaussian distributed or ± 1 with equal probability. σ and τ are Ising spins.
- Order parameter: Overlap between two independent replicas of the system, q:

$$q = \overline{\langle \sigma_i\tau_i \rangle}$$

- Goal: Compute $P(q)$.

The droplet model

- "Disguised" ferromagnet.
- High temperature phase paramagnetic: $\overline{\langle m_i \rangle^2} = 0$.
- $h = 0$: Low temperature (spin glass) phase composed by two states related by a global spin-flip: $q_{\rm EA} = \overline{\langle m_i \rangle^2} \neq 0$. Phase transition paramagnetic-spin glass.
- $h > 0$: The spin glass phase is unstable under the magnetic field, so, the low temperature phase in presence of a magnetic field is paramagnetic. There is no phase transition.
- $P(q)$ trivial.

The Parisi Solution (RSB)

- **High temperature phase paramagnetic.**
- **Low temperature phase spin glass:**
  - **Infinite number (uncountable) of finite volume pure states not related by symmetry (modulo the global spin-flip symmetry).**
  - **These states could be organized in an ultrametric fashion.**
- **Phase Transition both at $h = 0$ as well as at $h \neq 0$.**
- **$P(q)$ non trivial.**

There exists a third scenario: TNT (Trivial Not Trivial): $P(q)$ Non Trivial but $P(q_{\text{link}})$ Trivial (Martin).

Phase transition in three dimensions

Is dimension three above the lower critical dimension of the model?

Definition of a correlation length in a finite Volume (for instance, Caracciolo et al.):

$$C(\boldsymbol{r}) = \frac{1}{V} \sum_i \overline{\langle q_i q_{i+\boldsymbol{r}} \rangle}$$

$$\xi^2 = \frac{1}{4\left[\sin^2(k^x_{\rm m}/2) + \sin^2(k^y_{\rm m}/2) + \sin^2(k^z_{\rm m}/2)\right]} \left[\frac{\chi_q}{\hat{C}(\boldsymbol{k}_{\rm m})} - 1\right] ,$$

$\boldsymbol{k}_{\rm m}$ is the minimum wave-vector allowed for the used boundary conditions (e.g. $\boldsymbol{k}_{\rm m} = (2\pi/L, 2\pi/L^2, 2\pi/L^3)$ for helicoidal boundary conditions) and $\chi_q = \hat{C}(0)$.

SUE + Parallel tempering + Spectral density method + Correlation length.

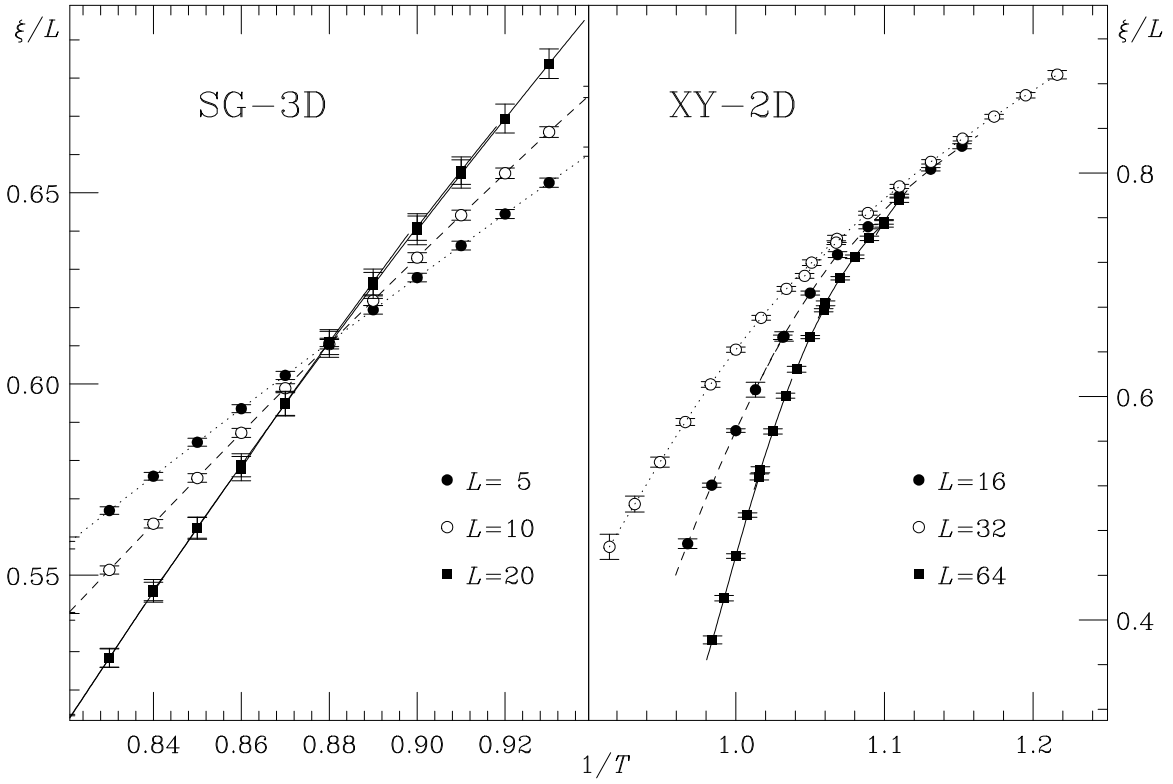

Figure 3: ξ/L for the $3d$ ± 1 Ising spin glass (left) and for the $2d$ XY (non disordered) model (right).

Some low temperature properties in equilibrium

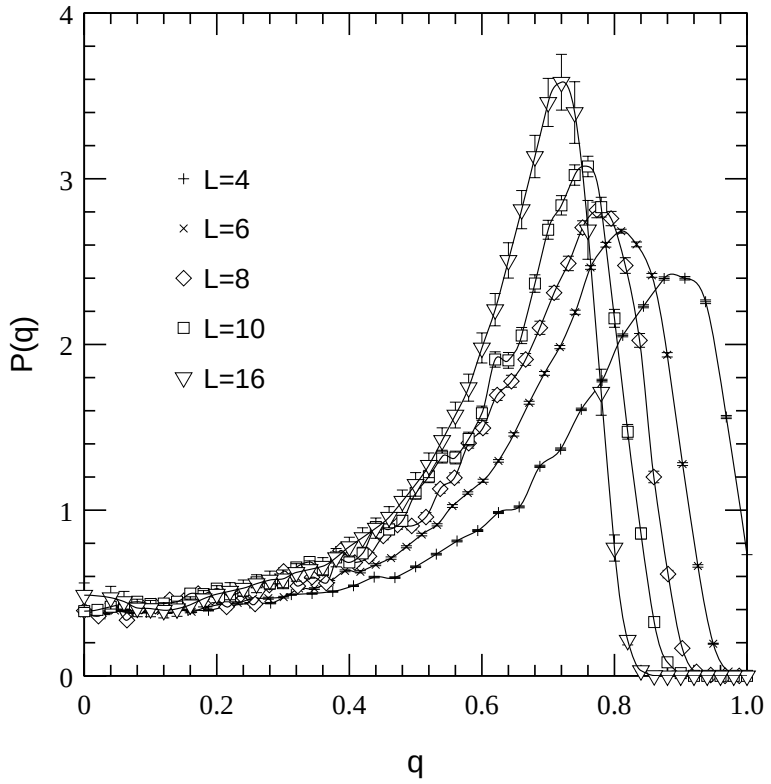

Figure 4: Overlap probability distribution, $P_L(q)$, for $L = 4$, 6, 8, 10 and 16 at $T \simeq 0.7 T_c$.

We can define $q_{\rm EA}$ as the value in which $P_L(q)$ shows a maximum. We obtained:

$$q_{\rm EA}(L) = 0.7 + O(L^{-1.5})\,.$$

Notice $P_L(0) \to$ Constant $\neq 0$ as L grows.

Out of equilibrium simulations: FDT.

If one perturb a Hamiltonian $\mathcal{H}$:

$$\mathcal{H}' = \mathcal{H} + \int \Delta h(t) A(t)\, dt \ ,$$

one can define the correlation function C and the response one, R,:

$$C(t_1, t_2) \equiv \langle A(t_1) A(t_2) \rangle \ .$$

$$R(t_1, t_2) \equiv \left. \frac{\delta \langle A(t_1) \rangle}{\delta \Delta h(t_2)} \right|_{\Delta h = 0} \ .$$

Usually $A(t) = \sigma_i(t)$.

At equilibrium C and R are related by

$$R(t_1, t_2) = \frac{1}{T} \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2} \ ,$$

which is the Fluctuation-Dissipation Theorem.

Out of equilibrium and in Mean Field it is possible to show (Cugliandolo and Kurchan) $(t_1 > t_2)$

$$R(t_1, t_2) = \frac{1}{T} X(C(t_1, t_2)) \frac{\partial C(t_1, t_2)}{\partial t_2} \ ,$$

In addition, when $t_2 \to \infty$, $q = C(t_1, t_2)$:

$$X(q) \to x(q) \equiv \int_{q_{\min}}^{q} dq' P(q') \ \ ,$$

which is the dynamic-static relation.

This relation also holds in systems which are stochastically stables (Franz, Mezard, Parisi and Peliti).

In the linear regime:

$$m[h+\Delta h](t) = m[h](t) + \int_{-\infty}^{t} dt' \left.\frac{\delta m[h'](t)}{\delta h'(t')}\right|_{h'(t)=h(t)} \Delta h(t') + \mathcal{O}(\Delta h^2)$$

Putting the definition of R:

$$\Delta m[h,\Delta h](t) = \int_{-\infty}^{t} dt' \; R(t,t')\Delta h(t') + \mathcal{O}(\Delta h^2) \; ,$$

Using the off equilibrium fluctuation-dissipation relation:

$$\Delta m[h,\Delta h](t) \simeq \Delta h \beta \int_{t_{\rm w}}^{t} dt' \; X[C(t,t')] \frac{\partial C(t,t')}{\partial t'}$$

Performing the following change of variable $u = C(t,t_{\rm w})$:

$$\Delta m[h,\Delta h](t) \simeq \Delta h \beta \int_{C(t,t_{\rm w})}^{1} du \; X[u] \; ,$$

By defining

$$S(C) \equiv \int_{C}^{1} dq \; x(q) \; ,$$

we can finally write ($t_{\rm w} \gg 1$):

$$\boxed{\frac{\Delta m[\Delta h](t) \; T}{\Delta h} \simeq S(C(t,t_{\rm w}))}$$

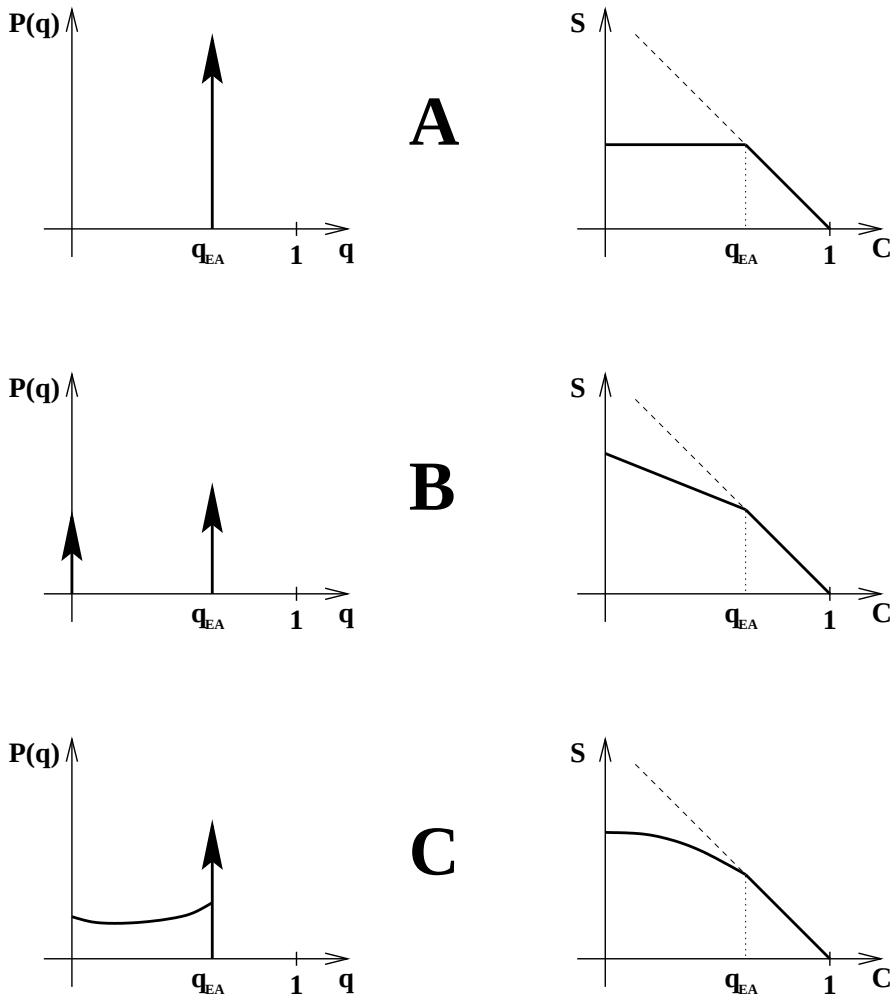

Figure 5: Three possible scenarios for spin glasses.

Numerical Simulations

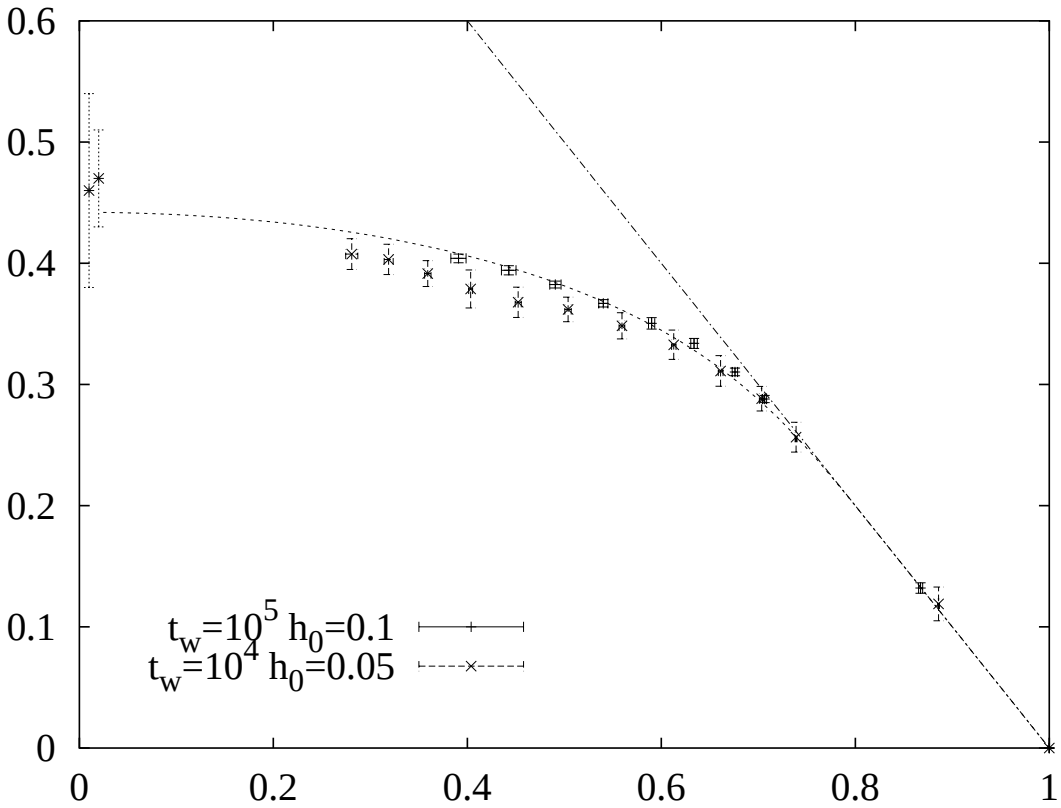

Figure 6: $L = 64$, $T = 0.7T_c$, $3d$ Gaussian spin glass.

Experiments

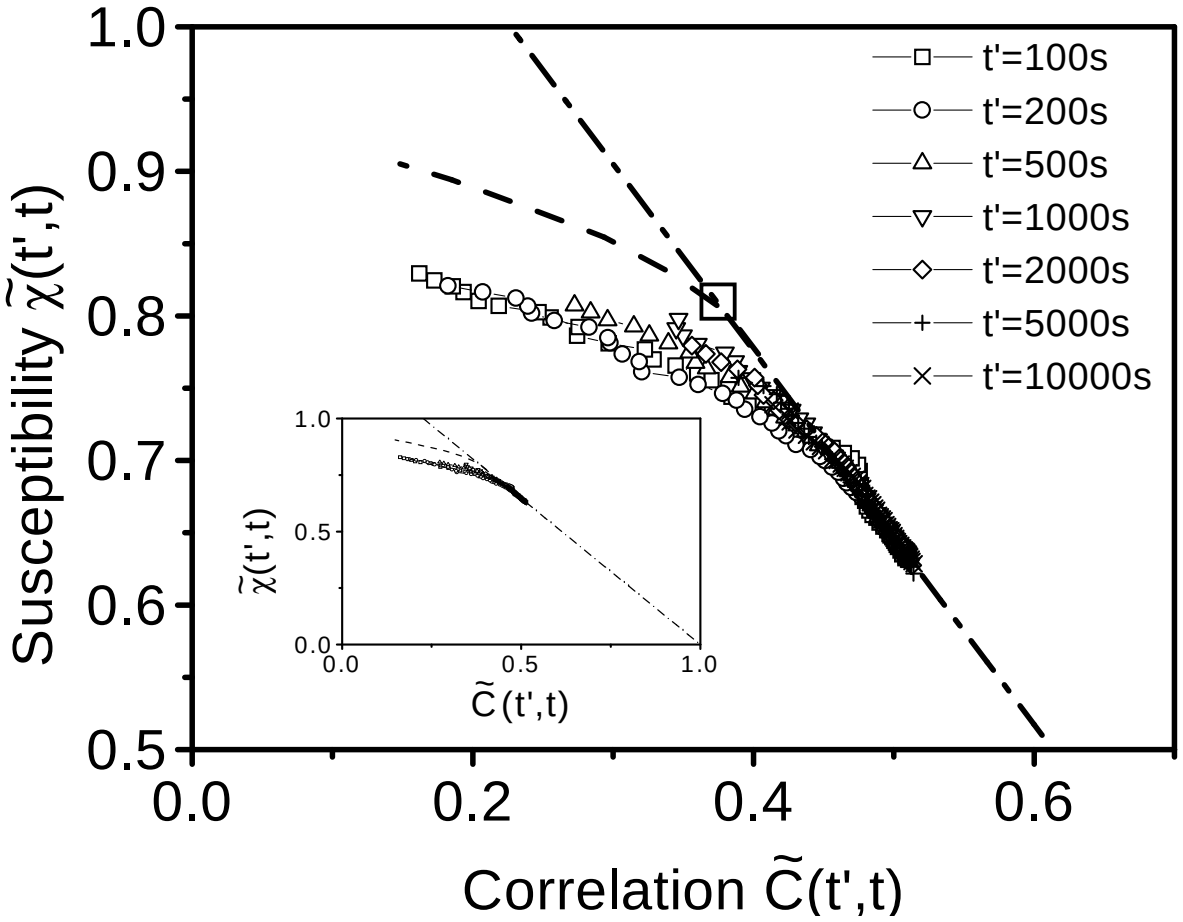

Figure 7: $CdCr_{1.7}In_{0.3}S_4$. $T_g = 16.2$K. $T = 0.8T_g$. Hérisson and Ocio.

Computational Effort

To do a Metropolis update in a three-dimensional Gaussian spin glass we need:

1. Read seven spin variables (short int).
2. Read six couplings (float).
3. Perform seven products and five sums.
4. Generate a random number in the interval [0,1).
5. Compute an exponential.
6. Do a comparison.

For instance:

$$\Delta E = S_i \sum_{j(\mathrm{nn})(i)} J_{ij} S_j \, .$$

We perform the change $S_i \to -S_i$ iff

$$\exp(-\Delta E) > \mathrm{random} \, .$$

Hence

- The total amount of memory is 14 L^3 byte.
- Single precision is enough.

The ± 1 Ising spin glass can be simulated using a multispin coding (32 systems in parallel in a 32 bit processor) with a memory amount of $16L^3$ byte.

Where are the difficulties??

1. Very large thermalization times. At the critical point the dynamical exponent (z) is near 6 to confront with that of the pure Ising model which is near 2. ($t_{\text{thermalization}} \simeq L^z$). At $T = T_c/2$ the effective dynamical exponent is near 12!!
2. To average over the disorder, we need to simulate a large number of samples (realizations of the disorder) of the system. From 40000 samples in small lattices to order 7000 samples in 20^3 lattices. There are some observables, like $P(q)$ which are not self-averaging!!

To simulate large lattices (for example in dynamical studies) parallelization is mandatory!!

We can choose to run these systems commercial computers (PC-based Linux farm) with MPI tools or computers designed to achieve a maximum performance in other fields of the Science (like APE machine and QCD: In APE-100 it was easy to parallelize a program!).

Another strategy is to build a dedicated machine.

Numerically it was obtained for an effective dynamical exponent

$$z(T) = 6.5(5)\frac{T_c}{T} \ .$$

And experimentally:

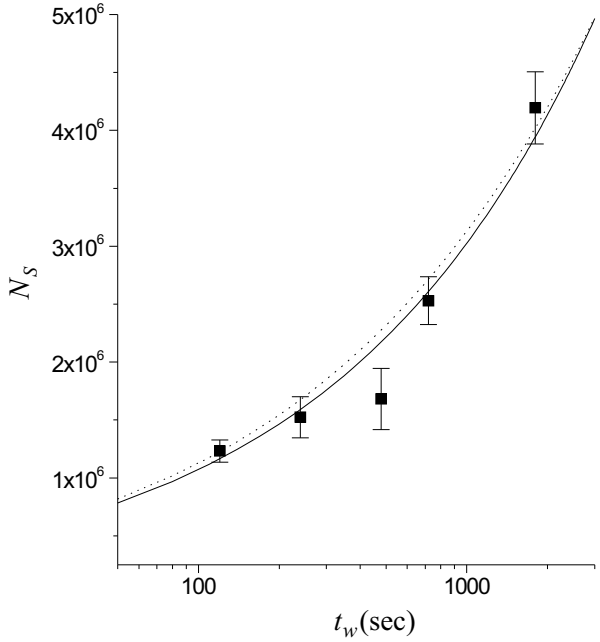

Figure 8: N_s, number of spin participating in barrier quenching (and hopping) as a function of $\log t_w$ at $T = 0.78T_g = 28$ K for CuMn. Orbach et al.

$$\xi(t_w, T) \propto N_s^{1/3} = 0.653 \left(\frac{t_w}{\tau_0}\right)^{0.169T/T_g}$$

where $\tau_0 = 4.1 \times 10^{12}$. So, the effective dynamical exponent is

$$z(T) = 5.9\frac{T_g}{T} \ .$$

Spin Update Engine

[Cruz, Pech, Tarancón, Téllez, Ullod and Ungil]

- Three dimensional Spin Glass model dedicated machine.
- The machine consists in 12 boards.
- Designed using Programmable Electronic Components (ALTERAS).
- Each single board can simulate 8 replicas, updating all the systems at every clock cycle. The update speed of the whole machine is 217 ps/spin with 48 MHz clock frequency.
- A device to generate Random numbers has been designed.
- The machine uses the Heat Bath algorithm.
- Built in 2000. Price one board: 2400 euros: 500 for PCB and 1900 for components. Price 12 boards: 29000 euros (of course, no salaries included!!).

If we assume that a 60^3 lattice has small finite size effects (far away of the transition point) we are a factor 5×10^7 still off of the Nature (in real materials, in a good approximation, all the spins flips together every 10^{-12} seconds).

We are planning to build a new version of SUE (SSUE) with a speed of 0.5 ps/spin, a factor 400 over SUE.

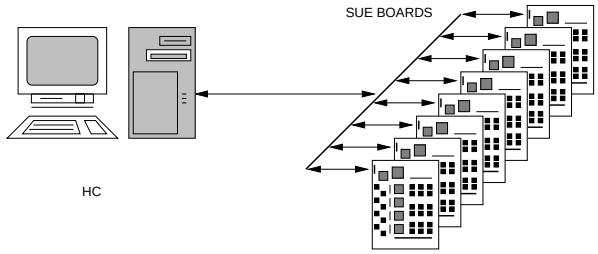

Figure 9: Eight boards SUE machine

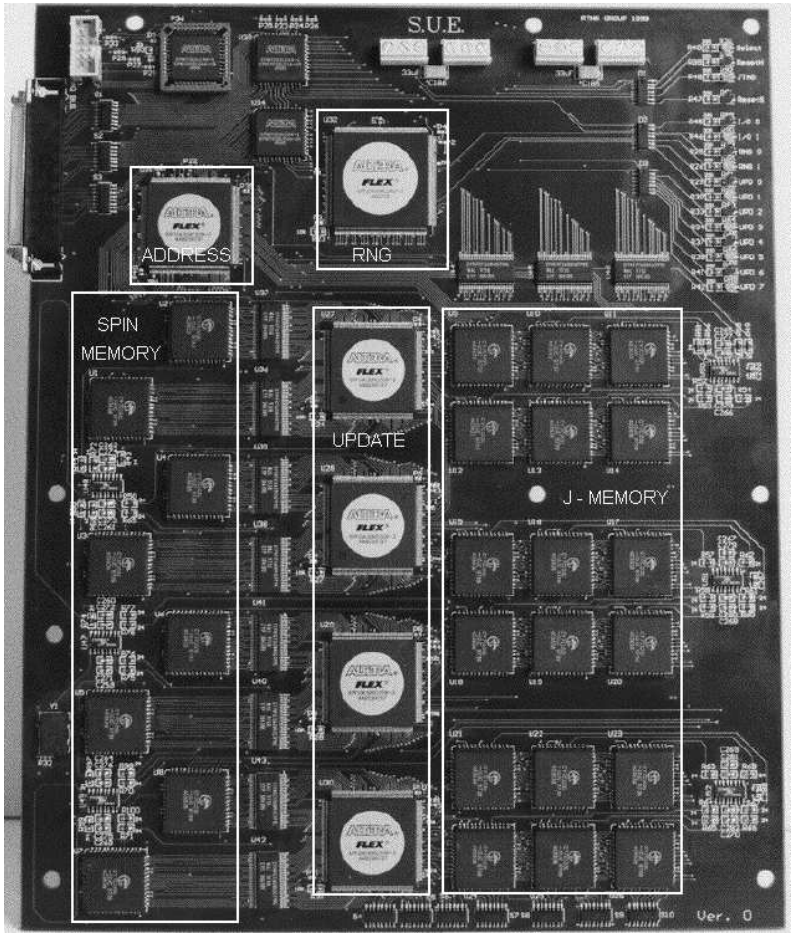

Figure 10: A SUE board.

Conclusions

- I have not discussed (no time) other important disordered systems as Random Field Ising Model, diluted models, rejuvenation and memory, Heisenberg spin glasses, combinatorial problems, type II superconductors with disorder, growth of surfaces in disordered substrates, effect of the disorder in first order phase transitions, etc.
- I have not talked about algorithms (e.g. parallel tempering). It is necessary to improve the algorithms!!
- I have not described other numerical approaches to Ising spin glasses as the exact computation of ground states.
- It is necessary to have a large amount of computer resources to simulate these systems.
- In particular a great level of parallelism is mandatory in order to simulate a large number of samples (using the machine in farm mode) as well for running larger lattices in off equilibrium numerical simulations.