Fluctuation-dissipation relations in finite dimensional spin glasses.

J. J. Ruiz-Lorenzo

Dep. Física,
Instituto de Computación Científica Avanzada (ICCAEx),
Universidad de Extremadura
Janus Collaboration (Ferrara-Rome-Extremadura-Madrid-Zaragoza)
http://www.eweb.unex.es/eweb/fisteor/juan/juan_talks.html

Madrid, March 10th, 2016
Plan of the Talk

- What are spin glasses?
- Different Theories: Droplet/Scaling and RSB.
- Relations of fluctuation-dissipation (FDR):
  1. Definitions
  2. Analytical Results.
  3. Experiments.
- Conclusions.
What are Spin glasses

- Materials with disorder and frustration.
- Quenched disorder (similar to the Born-Oppenheimer in Molecular Physics).
- Canonical Spin Glass: Metallic host (Cu) with magnetic impurities (Mn).
- RKKY interaction between magnetic moments: $J(r) \sim \frac{\cos(2k_F r)}{r^3}$.
- Role of anisotropy: Ag:Mn at 2.5% (Heisenberg like), CdCr$_{1.7}$In$_{0.3}$S$_4$ (also Heisenberg like) and Fe$_{0.5}$Mn$_{0.5}$TiO$_3$ (Ising like).
Some equations

- Edwards-Anderson Hamiltonian:

\[ \mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \]

\( J_{ij} \) are random quenched variables with zero mean and unit variance, \( \sigma = \pm 1 \) are Ising spins.

- The order parameter is:

\[ q_{EA} = \langle \sigma_i \rangle^2 \]

Using two real replicas:

\[ \mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} (\sigma_i \sigma_j + \tau_i \tau_j) \]

Let \( q_i = \sigma_i \tau_i \) be the normal overlap, then: \( q_{EA} = \langle \sigma_i \tau_i \rangle \).

We also define the link overlap: \( q_{i,\mu}^l = q_i q_{i+\mu} \).
The Droplet/Scaling Theory.

- Based on the Migdal-Kadanoff implementation (approximate) of the Renormalization Group (exact in $D = 1$).
- *Disguised Ferromagnet*: Only two pure states with order parameter $\pm q_{EA}$ (related by spin flip).
- Compact Excitations of fractal dimension $d_f$. The energy of a excitation of linear size $L$ grows as $L^\theta$. The free energy barriers (in the dynamics) grow as $L^\psi$. $\theta < (D - 1)/2 < D - 1 < d_f < D$ and $\psi \geq \theta$.
- Any amount of magnetic field destroys the spin glass phase (even for Heisenberg spin glasses).
- Trivial probability distributions of the overlaps (both normal overlap and link one).
Different Theories.

Replica Symmetry Breaking (RSB) Theory.

- Exact in $D = \infty$.
- Infinite number of phases (pure states) not related by any kind of symmetry.
- These (pure) states are organized in a ultrametric fashion.
- The spin glass phase is stable under (small) magnetic field. Phase transition in field: the de Almeida-Thouless line.
- The excitations of the ground state are space filling: e.g. the interface between two pure states is space filling.
- Overlap equivalence: All the definitions of the overlap are equivalent.

Note: In a pure state, $\alpha$, the clustering property holds:
$$\langle S_i S_j \rangle_\alpha - \langle S_i \rangle_\alpha \langle S_j \rangle_\alpha \rightarrow 0 \text{ as } |i - j| \rightarrow \infty.$$
Different Theories (Comparison).

A model is stochastically stable under a given class of random perturbations

\[ \mathcal{H} \rightarrow \mathcal{H} + \epsilon \mathcal{H}_R \]

if its averaged free energy is differentiable with respect to \( \epsilon \) and the thermodynamical limit commutes with \( \partial / \partial \epsilon \).

If we change the free energies of the states \( (F_\alpha) \) by a random amount: \( G_\alpha = F_\alpha + \epsilon r_\alpha \) (\( r_\alpha \) are uncorrelated random numbers), then the probability distribution of the free energies is invariant:

\[ \rho(F) = \rho(G) \]

The weight of the state \( \alpha \) is \( w_\alpha \propto \exp(-\beta F_\alpha) \).

It is equivalent to the replica equivalence property of the Parisi’s matrices \( Q_{ab} (D = \infty) \).

Exact in \( D = \infty \), and strongly tested in numerical simulations \( (D = 3 \text{ and } 4.) \)
In experiments the magnetization ($M$) and susceptibility ($\chi$) are measured.

One can extract the spin glass susceptibility, $\chi_{SG} = V\langle q^2 \rangle$ via

$$\chi - \frac{M}{H} = \chi_2 H^2 + \chi_4 H^4 + O(H^6)$$

$$\chi_{SG} \propto \chi_2$$

But:

- We need to compute the equilibrium susceptibility (low frequencies).

- In order to extract $P(q)$ we need to know the microscopic structure of the spins (the configurations). Solution: → FDR out of equilibrium!
We start with the perturbed Hamiltonian $\mathcal{H}'$:

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

We can define the autocorrelation function, $C(t_1, t_2)$ and the response function $R(t_1, t_2)$,

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

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

In spin models: $A(t) = \sigma_i(t)$.

### Equilibrium (Fluctuation-Dissipation Theorem)

$$R(t_1, t_2) = \frac{1}{T} \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2}$$
FDR: Out of equilibrium

\[ R(t_1, t_2) = X(C(t_1, t_2)) \left( \frac{1}{T} \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2} \right) \]

- At equilibrium \( X = 1 \).
If \( C(t_1, t_2) = q \), then \( X(C(t_1, t_2)) \rightarrow x(q) \)

Where \( x(q) \) is the cumulative distribution of the overlap computed in the equilibrium regime:

\[
x(q) = \int_{-1}^{q} dq' \ P(q')
\]

\[
m(t, t_w) = h \int_{t_w}^{t} dt' R(t, t') \ , \ h(t) = h\theta(t - t_w)
\]

\[
m(t, t_w) \simeq h\beta \int_{t_w}^{t} dt' X[C(t, t')] \frac{\partial C(t, t')}{\partial t'} = h\beta \int_{C(t, t_w)}^{1} du X[u] \equiv h\beta S[C]
\]

\[
T \chi(t, t_w) = T \frac{m(t, t_w)}{h} = S[C(t, t_w)]
\]
CdCr$_{1.7}$In$_{0.3}$S$_4$. $T_g = 16.2$K. $T = 0.8T_g$.
Hérisson and Ocío. PRL 88, 257202 (2002)

\[ P(C) = -\frac{\partial^2 S(C)}{\partial C^2} \]
Different Theories (Comparison).

A

B

C

J. J. Ruiz-Lorenzo (UEx)

FDT in Spin glasses

NonEq. Cond. Mat. and Bio.
$P(q)$ from FDR

Marinari et al. JPA 33, 2373 (2000).
Dedicated Computers: Janus.

Some figures

- Ferrara-Rome-Madrid-Extremadura-Zaragoza scientific collaboration.
- Dedicated computer optimized to simulate a wide variety of spin models.
- 16 boards of 16 FPGA’s each (Virtex 4).
- Performance. For Ising models: Janus is equivalent to 10000 PC.
- Parallelization inside the boards.
- Previous numerical simulations simulated the $10^{-5}$ sec region (SSUE).
- Janus allows us to simulate in the 0.1 second time region. Note: Experimental times range from 1 sec to 3000 sec.

Some figures

- Built in 2015.
- ～5 times most powerful than Janus.
- Still a dedicated computer optimized to simulate a wide variety of spin models.
- More flexible topology.
- 16 boards of 16 FPGA’s each (one IOP and PC integrated on each board) (Virtex 7).
- Janus II will allow us to simulate in the 1 second time region.

Janus II

J. J. Ruiz-Lorenzo (UEx)  FDT in Spin glasses  NonEq. Cond. Mat. and Bio.
Comparing MC times (Janus) with real times
(Experiments)

How to extract the coherence length ($\xi(t_w)$)?

- Numerical Simulations.

$$C_4(r, t_w) = \langle q_x(t_w) q_x + r(t_w) \rangle = \frac{1}{r^a} f(r/\xi(t_w))$$

- Experiments (Joh et al. PRL 82, 438 (1999)). They compute the Zeeman Energy at a given $t_w$:

$$E_Z(t_w) = N_s(t_w) \chi_{fc} H^2$$

and then they extract $N_s(t_w) \propto \xi(t_w)^b$, $b \simeq 2.5$ (Berthier and Young, PRB 69, 184423 (2004)).

$$\xi(T, t_w) = \xi_0(T) t^{1/z(T)} , \quad z(t) = 6.86 \frac{T_c}{T} ,$$
Comparing MC times (Janus) with real times (Experiments)

Nakamae et al. (APL 101, 242409(2012))
Comparing MC times (Janus) with real times (Experiments)

\[ \frac{\xi(t_w, T)}{\xi_0(T)} / \frac{T}{T_c \log(t_w/\tau_0)} \]

Ising SG Universality Class

Experimental Data
Fit JANUS data
JANUS: \( T=0.54T_c \), time=0.9 s
GPUs: \( T=T_c \), time=\( 2 \times 10^{-5} \) s

Nakamae et al. (APL 101, 242409(2012) with Janus Coll. data (PRL 101, 157201 (2008) and PRL 105, 177202 (2010)).

In numerical simulations \( t_w/\tau_0 \) is just the number of sweeps.
FDT: Numerical Results

Janus Coll. (in preparation).

J. J. Ruiz-Lorenzo (UEx) FDT in Spin glasses NonEq. Cond. Mat. and Bio.
Static-Dynamics Dictionary:

\[ \chi_{L_{\text{eff}}} = S(C_{L_{\text{eff}}}(t, t_w), L_{\text{eff}}(t, t_w)) \]

Length Scales: \( L, \xi(t_w) \) and \( \xi(t + t_w) \).

Janus Coll. (in preparation).
FDT: Numerical Results: Synthetic $P(q)$

\[ P_{\text{syn}}(q, L) = (P(0, L) + P_1q^2)\theta(q_{\text{EA}}^{(L)}) + [1 - x(q_{\text{EA}}^{(L)})]\delta(q - q_{\text{EA}}^{(L)}) \]

\[ q_{\text{EA}}^{(L)} = q_{\text{EA}}^{(L=\infty)} + \frac{A}{L^{0.38}} \]

\[ S_{\text{syn}}(C, L) = \min[1 - C, S(0, L) - P_0C^2 - P_1C^4] \]

Janus Coll. (in preparation).
Conclusions

FDR in spin glasses

- Solid analytical base both in Mean Field and also at finite dimensions.
- It has been implemented in (difficult) experiments.
- Numerical simulations are reaching the experimental time region.
- The emerging picture points out a low temperature spin glass phase with Replica Symmetry Breaking properties.