Fluctuation-dissipation relations in finite dimensional spin glasses.

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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.
	- ⁴ Numerical Simulations.
- Conclusions.
- 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: $J(r) \sim \frac{\cos(2k_F r)}{r^3}$ $\frac{2\kappa_F T)}{r^3}$.
- 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).

Edwards-Anderson Hamiltonian:

$$
\mathcal{H} = -\sum_{} J_{ij} \sigma_i \sigma_j
$$

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

• The order parameter is:

$$
q_{\text{EA}} = \overline{\langle \sigma_i \rangle^2}
$$

Using two real replicas:

$$
\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \left(\sigma_i \sigma_j + \tau_i \tau_j \right)
$$

Let $q_i = \sigma_i \tau_i$ be the normal overlap, then: $q_{EA} = \overline{\langle \sigma_i \tau_i \rangle}$. 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 $D = 1$).
- Disquised Ferromagnet: Only two pure states with order parameter $\pm q_{\text{EA}}$ (related by spin flip).
- Compact Excitations of fractal dimension d_f . The energy of a excitation of linear size L grows as L^{θ} . The free energy barriers (in the dynamics) grow as L^{ψ} . $\theta < (D-1)/2 < D-1 < d_f < D$ and $\psi > \theta$.
- 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, α , the clustering property holds: $\langle S_i S_j \rangle_\alpha - \langle S_i \rangle_\alpha \langle S_j \rangle_\alpha \to 0 \text{ as } |i - j| \to \infty.$

Different Theories (Comparison).

Parisi et al., Eur. Phys. J. B 10, 317 (1999).

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

$$
\mathcal{H} \to \mathcal{H} + \epsilon \mathcal{H}_R
$$

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

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

$$
\rho(F)=\rho(G)
$$

The weight of the state α 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 $(D = 3 \text{ and } 4.)$

Order Parameter from Experiments?

- In experiments the magnetization (M) and susceptibility (χ) are measured.
- One can extract the spin glass susceptibility, $\chi_{SG} = V \langle q^2 \rangle$ via

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

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

But:

- We need to compute the equilibrium susceptibility (low frequencies).
- \bullet In order to extract $P(q)$ we need to know the microscopic structure of the spins (the configurations). Solution: \rightarrow FDR out of equilibrium!

FDR: Definitions.

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 $R(t_1, t_2)$,

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

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

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

Equilibrium (Fluctuation-Dissipation Theorem)

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

.

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

- At equilibrium $X = 1$.
- Mean Field. Cugliandolo and Kurchan. PRL 71, 173 (1993).
- Finite Dimensional spin glasses: Franz et al. PRL 81, 1758 (1998).

FDR: Connection Out of Equilibrium and Equilibrium

- If $C(t_1, t_2) = q$, then $X(C(t_1, t_2)) \to x(q)$
- Where $x(q)$ is the cumulative distribution of the overlap computed in the equilibrium regime:

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

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

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

$$
T\chi(t, t_w) = T \frac{m(t, t_w)}{h} = S[C(t, t_w)]
$$

FDR: Experiments

CdCr_{1.7}In_{0.3}S₄. $T_q = 16.2$ K. $T = 0.8T_q$. Hérisson and Ocio. PRL 88, 257202 (2002)

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Marinari et al. JPA 31, 2611 (1998).

$$
P(C) = -\frac{\partial^2 S(C)}{\partial C^2}
$$

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Different Theories (Comparison).

$P(q)$ from FDR

Dedicated Computers: Janus.

Some figures

- \bullet Built in 2008.
- 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.

Comp. Phys. Comm. 178, 208(2008).

Some figures

- \bullet Built in 2015.
- \sim 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.

Comp. Phys. Comm. 185, 550(2014).

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Comparing MC times (Janus) with real times (Experiments)

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

• Numerical Simulations.

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

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

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

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

$$
\xi(T, t_w) = \xi_0(T) t^{1/z(T)}
$$
, $z(t) = 6.86 \frac{T_c}{T}$,

Comparing MC times (Janus) with real times (Experiments)

Nakamae et al. (APL 101, 242409(2012)

Comparing MC times (Janus) with real times (Experiments)

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/τ_0 is just the number of sweeps.

FDT: Numerical Results

Janus Coll. (in preparation).

FDT: Numerical Results

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 $P(q)$

$$
P_{\text{syn}}(q, L) = (P(0, L) + P_1 q^2) \theta(q_{\text{EA}}^{(L)}) + [1 - x(q_{\text{EA}}^{(L)})] \delta(q - q_{\text{EA}}^{(L)})
$$

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

 $S_{\text{syn}}(C, L) = \min[1 - C, S(0, L) - P_0 C^2 - P_1 C^4]$

Janus Coll. (in preparation).

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.