Numerical construction of the Aizenman-Wehr metastate

J. J. Ruiz-Lorenzo

with A. Billoire (Paris), L. A. Fernández, V. Martín-Mayor (Madrid)
E. Marinari, A. Maiorano, G. Parisi, F. Ricci-Tersenghi (Rome),
J. Moreno-Gordo (Zaragoza)

Dep. Física & ICCAEx (Univ. de Extremadura) & BIFI (Zaragoza)
http://www.eweb.unex.es/eweb/fisteor/juan/juan_talks.html

Leipzig, December 1st, 2017

Outline of the Talk

- What are spin glasses?
- Different Theories and Models (Droplet, Chaotic Pairs and RSB).
- Phases and Thermodynamic limit in Pure systems.
- Phases and Thermodynamic limit in Disordered systems: The Metastate.
- Numerical Construction of the Aizenman-Wehr Metastate
  - Construction of the Aizenman-Wehr Metastate
  - Observables and Numerical Simulations.
  - Results.
- Conclusions.
What are Spin glasses

- Materials with disorder and frustration.
- Quenched disorder.
- Canonical Spin Glass: Metallic host (Cu) with magnetic impurities (Mn). RKKY interaction between magnetic moments:
  \[ J(r) \sim \frac{\cos(2k_F r)}{r^3}. \]
Some Definitions

- The typical Spin Glass Hamiltonian:

\[ H = - \sum_{i,j} J_{ij} \sigma_i \sigma_j \]

\( J_{ij} = \pm 1 \) with equal probability.

- The order parameter is:

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

Using two real replicas:

\[ H = - \sum_{i,j} J_{ij} (\sigma_i \sigma_j + \tau_i \tau_j) \]

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

[More in previous talks by Schnabel and Landau.]
The Droplet Model

- Based on the Migdal-Kadanoff implementation (approximate) of the Renormalization Group (exact in $D = 1$).
- *Disguished 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 $L^{\theta}$.
- Any amount of magnetic field destroys the spin glass phase (even for Heisenberg spin glasses).
- Trivial probability distributions of the overlaps.
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.
- The excitations of the ground state are space filling.
- Overlap equivalence: All the definitions of the overlap are equivalent.
- Stochastic Stability. The Spin Glass Hamiltonian is “generic” under Random Perturbations.

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

A

B

C
A state is a probability distribution (or an average, or a linear functional).

In the non disordered Ising model, we can define two pure states

$$\langle (\cdots) \rangle_+ = \lim_{h \to 0^+} \lim_{L \to \infty} \langle (\cdots) \rangle(L,h),$$

$$\langle (\cdots) \rangle_- = \lim_{h \to 0^-} \lim_{L \to \infty} \langle (\cdots) \rangle(L,h)$$

Mixtures can be analyzed via the decomposition:

$$\langle (\cdots) \rangle = \alpha \langle (\cdots) \rangle_+ + (1 - \alpha) \langle (\cdots) \rangle_-$$

In particular,

$$\lim_{L \to \infty} \langle (\cdots) \rangle(L,h=0) = \frac{1}{2} \langle (\cdots) \rangle_+ + \frac{1}{2} \langle (\cdots) \rangle_-$$
Dobrushin-Lanford-Ruelle states (locally equilibrium states).

Finite volume pure states (conditional probabilities of DLR states).

The states form a convex set. $\Gamma = \sum_i \alpha_i \Gamma_i$ with $\sum_i \alpha_i = 1$, $\alpha_i > 0$. (Mixtures)

Pure states (phases): extremal points of the convex set.

Inside a pure state, intensive magnitudes do not fluctuate, equivalently, the connected correlation functions verify the clustering property.
Phases and Thermodynamic limit in Disordered systems: The Metastate.

- Chaotic Size Dependence: The state $\Gamma_{L,J}$ does not approach a unique limit $\Gamma_J = \lim_{L \to \infty} \Gamma_{L,J}$ (when we increase the size we add additional random bonds to the Hamiltonian).

  1. Non-disordered Ising model with fixed boundary conditions (the values of the spins on the boundary change with $L$).
  2. The magnetization in the RFIM at low temperatures does not converge. (It is given by $\text{sign}(\sum_i h_i)$ which is a random variable).
  3. Chaotic Pairs scenario. The model presents two states (spin flip related) for any large but finite size. This pair of states changes chaotically with $L$.

- Newman-Stein Metastate.
  Despite the lack of limit of $\Gamma_{L,J}$, one can compute the frequency of a given state appears as $L \to \infty$. The set of these frequencies is the Newman-Stein metastate.
Construction of the Aizenman-Wehr Metastate

- Internal disorder $\mathcal{I}$ in the region $\Lambda_R$.
- Outer disorder $\mathcal{O}$ in the region $\Lambda_L \setminus \Lambda_R$.
- We will measure in $\Lambda_W \in \Lambda_R$.
- The wanted limit: $\Lambda_W \ll \Lambda_R \ll \Lambda_L$. 

J. J. Ruiz-Lorenzo (UEx&BIFI) Numerical Construction Metastate CompPhys17
Construction of the Aizenman-Wehr Metastate

- Let us compute

\[ \kappa_{\mathcal{I}, R}(\Gamma) = \lim_{L \to \infty} \mathbb{E}_\mathcal{O} \left[ \delta^{(F)} (\Gamma - \Gamma_{\mathcal{I}, L}) \right] \]

- If the limit

\[ \kappa(\Gamma) = \lim_{R \to \infty} \kappa_{\mathcal{I}, R}(\Gamma) \]

exists, it does not longer depend on the internal disorder \( \mathcal{I} \) and provides the AW metastate.

- The metastate-averaged state (MAS), \( \rho(s) \), is defined via

\[ \langle \cdots \rangle_\rho \equiv \left[ \langle \cdots \rangle_\Gamma \right]_\kappa \]

- Restricted to \( \Lambda_W \), a state \( \Gamma(s) \) is a set of probs. \( \{p_\alpha\}_{\alpha=1,...,2^{Wd}} \).

This is a point of the hyperplane \( \sum_\alpha p_\alpha = 1 \).

- The metastate is a probability distribution on this hyperplane.

- The MAS \( \rho(s) \) is the average of this distribution, and it is itself a point on the hyperplane (hence, the MAS is a state itself).
Some Observables

- The MAS spin glass correlation function:

\[ C_\rho(x) = \left[ \frac{\langle s_0 s_x \rangle}{\Gamma} \right]^2 = \frac{1}{\mathcal{N}_I} \sum_i \left( \frac{1}{\mathcal{N}_O} \sum_o \langle s_i^{i.o} s_x^{i.o} \rangle \right)^2 = \frac{1}{\mathcal{N}_I} \sum_i \frac{1}{\mathcal{N}_O^2} \sum_{o,o'} \langle s_0^{i.o} s_x^{i.o} s_0^{i.o'} s_x^{i.o'} \rangle \sim |x|^{-(d-\zeta)} , \]

- Remember \( \langle \cdots \rangle_\rho \equiv \left[ \langle \cdots \rangle \right]_\kappa \).
- \( \zeta \) is the Read's exponent.
- \( i = 0, \ldots, \mathcal{N}_I. \mathcal{N}_I = 10 \) instances of internal disorder (\( \mathcal{I} \)).
- \( o = 0, \ldots, \mathcal{N}_O. \mathcal{N}_O = 1280 \) instances of outer disorder (\( \mathcal{O} \)).
Physics behind the $\zeta$-exponent

- $\log N_{\text{states}}(W) \sim W^{d-\zeta}$. $\zeta \geq 1$.
- If $\zeta < d$ we have a dispersed metastate.
- Reid's conjecture $\zeta = \zeta_{q=0}$.
- The constrained (on $q$) equilibrium overlap-overlap correlation function is defined as:

$$G(r, q) \equiv \langle q(r)q(0) \rangle_q - q^2 \sim \frac{1}{r^{d-\zeta_q}}$$

- Above the upper critical dimension (de Dominicis et al.):
  - $\zeta_{q=0} = 4$.
  - $\zeta_q = 3$, $0 < q < q_{\text{EA}}$.
  - $\zeta_{q_{\text{EA}}} = 2$.
- Dynamical interpretation: $G_d(r, q, t) \equiv \langle q(r,t)q(0,t) \rangle$ plays the role of $C_\rho(r)$, with $R \sim \xi(t)$. [Manssen, Hartmann and Young].
Some Observables

- The (generalized) overlap on the box $\Lambda_W$:

$$q_{i;o,o'} \equiv \frac{1}{W^3} \sum_{x \in \Lambda_W} \sigma_x^{i;o} \tau_x^{i;o'}.$$ 

- Probability density functions of $q_{i;o,o'}$:

$$P(q) = \frac{\sum_i P_i(q)}{N_I} , \quad P_i(q) = \frac{1}{N_O} \sum_o \langle \delta(q - q_{i;o,o'}) \rangle ,$$

$$P_\rho(q) = \frac{\sum_i P_{\rho,i}(q)}{N_I} , \quad P_{\rho,i}(q) = \frac{1}{N_O^2} \sum_{o,o'} \langle \delta(q - q_{i;o,o'}) \rangle.$$ 

- $P(q)$ is the standard probability distribution of the overlap.
Some Observables

- Although $P_\rho(q) \to \delta(q)$ as $L \to \infty$, the scaling of its variance provides us with useful information:

  $$\chi_\rho = \sum_{x \in \Lambda_W} C_\rho(x) = W^d \int q^2 P_\rho(q) \, dq \sim W^\zeta.$$

- $P_\rho(q/(W^{-(\zeta-d)/2}))$ is Gaussian.
**Numerical Simulations**

- We have simulated the three-dimensional Edwards-Anderson model with periodic boundary conditions and bimodal disorder.
- We have implemented the Parallel Tempering Method (with Metropolis single spin-flip).
- We have used multispin coding (128 bits).
- Equilibration was assessed on a sample-by-sample basis.
- For large systems, the worse samples were simulated using multisite multispin coding.
- We have run on conventional supercomputers.
- We have simulated $L = 8, 12, 16$ and $24$.
- The lowest temperature $T_{\text{min}} = 0.698 = 0.64T_c$
Results: the MAS overlap probability distribution

Notice that for $R/L = 3/4$ there are no finite size effects. We will take in the following the safe ratio $R/L = 1/2$. 
The scaling regime extends to \( W/R = 0.75 \).
$R = L/2$, $T = 0.698$

$\chi_\rho / R^{2.3}$

$L = 8$
$L = 12$
$L = 16$
$L = 24$

$0.76(W/R)^{2.3}$

$\zeta = 2.3(3)$, to be compare with $\zeta_{q=0} = 2.62(2)$
Results: Comparison $P(q)$ and $P_\rho(q)$

$P(q)$ and $P_\rho(q)$ are different: Dispersed Metastate.
Results: $\zeta$-exponent

\[ d_U = 6 \]
\[ d_L \approx 2.5 \]
\[ \zeta = d \]
\[ \zeta_{q=0} \]
Conclusions

- We have constructed numerically the Aizenman-Wehr metastate.
- We have found strong evidences for a dispersed metastate.
- Only RSB and CP have a dispersed metastate.
- Strong numerical support on the Reid’s conjecture $\zeta = \zeta_{q=0}$. 
Some (additional) References: