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)

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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.

- Materials with disorder and fustration.
- 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:

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

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

• The order parameter is:

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

Using two real replicas:

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

Let $q_i = \sigma_i \tau_i$ be the normal overlap, then: $q_{\text{EA}} = \langle \sigma_i \tau_i \rangle$. [More in previous talks by Schnabel and Landau.] J. J. Ruiz-Lorenzo (UEx&BIFI) Numerical Construction Metastate

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 $\pm q_{\rm EA}$ (related by spin flip).
- Compact Excitations of fractal dimension d_f . The energy of a excitation of linear size L grows as L^{θ} .
- 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, α , the clustering property holds: $\langle S_i S_j \rangle_{\alpha} - \langle S_i \rangle_{\alpha} \langle S_j \rangle_{\alpha} \to 0$ as $|i - j| \to \infty$.

Different Theories and Models (Comparison).



Phases and Thermodynamic limit in Pure systems

- 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,

$$\lim_{L \to \infty} \langle (\cdots) \rangle_{(L,h=0)} = \frac{1}{2} \langle (\cdots) \rangle_{+} + \frac{1}{2} \langle (\cdots) \rangle_{-}$$

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- 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).
 - 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 $sign(\sum_i h_i)$ which is a random variable).
 - Chaotic Paits 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.

- Internal disorder \mathcal{I} in the region Λ_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: $\Lambda_W << \Lambda_R << \Lambda_L.$



Construction of the Aizenman-Wehr Metastate

• Let us compute

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

• 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), $\rho(\underline{s})$, is defined via $\langle \cdots \rangle_{\rho} \equiv [\langle \cdots \rangle_{\Gamma}]_{\kappa}$
- Restricted to Λ_W , a state $\Gamma(\underline{s})$ is a set of probs. $\{p_{\alpha}\}_{\alpha=1,\dots,2^{W^d}}$. This is a point of the hyperplane $\sum_{\alpha} p_{\alpha} = 1$.
- The metastate is a probability distribution on this hyperplane.
- The MAS $\rho(\underline{s})$ is the average of this distribution, and it is itself a point on the hyperplane (hence, the MAS is a state itself).

• The MAS spin glass correlation function:

$$\begin{split} C_{\rho}(x) &= \overline{\left[\langle s_0 s_x \rangle_{\Gamma}\right]_{\kappa}^2} = \frac{1}{\mathcal{N}_{\mathcal{I}}} \sum_{\mathbf{i}} \left(\frac{1}{\mathcal{N}_{\mathcal{O}}} \sum_{\mathbf{o}} \langle s_0^{\mathbf{i};\mathbf{o}} s_x^{\mathbf{i};\mathbf{o}} \rangle \right)^2 = \\ &= \frac{1}{\mathcal{N}_{\mathcal{I}}} \sum_{\mathbf{i}} \frac{1}{\mathcal{N}_{\mathcal{O}}^2} \sum_{\mathbf{o},\mathbf{o}'} \langle s_0^{\mathbf{i};\mathbf{o}} s_x^{\mathbf{i};\mathbf{o}'} s_0^{\mathbf{i};\mathbf{o}'} s_x^{\mathbf{i};\mathbf{o}'} \rangle \sim |x|^{-(d-\zeta)} \;, \end{split}$$

- Remember $\langle \cdots \rangle_{\rho} \equiv [\langle \cdots \rangle_{\Gamma}]_{\kappa}$.
- ζ is the Read's exponent.

• $\mathbf{i} = 0, \dots, \mathcal{N}_{\mathcal{I}}$. $\mathcal{N}_{\mathcal{I}} = 10$ instances of internal disorder (\mathcal{I}) .

• $o = 0, \ldots, \mathcal{N}_{\mathcal{O}}$. $\mathcal{N}_{\mathcal{O}} = 1280$ instances of outer disorder (\mathcal{O}).

Physics behind the ζ -exponent

- $\log \mathcal{N}_{\text{states}}(W) \sim W^{d-\zeta}$. $\zeta \ge 1$.
- 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:

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

• 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: $G_d(\mathbf{r}, q, t) \equiv \overline{\langle q(\mathbf{r}, t)q(0, t) \rangle}$ plays the role of $C_{\rho}(\mathbf{r})$, with $R \sim \xi(t)$. [Manssen, Hartmann and Young].

• The (generalized) overlap on the box Λ_W :

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

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

$$P(q) = \frac{\sum_{\mathbf{i}} P_{\mathbf{i}}(q)}{\mathcal{N}_{\mathcal{I}}} \quad , \qquad P_{\mathbf{i}}(q) = \frac{1}{\mathcal{N}_{\mathcal{O}}} \sum_{\mathbf{o}} \langle \delta(q - q_{\mathbf{i};\mathbf{o},\mathbf{o}}) \rangle,$$
$$P_{\rho}(q) = \frac{\sum_{\mathbf{i}} P_{\rho,\mathbf{i}}(q)}{\mathcal{N}_{\mathcal{I}}} \quad , \qquad P_{\rho,\mathbf{i}}(q) = \frac{1}{\mathcal{N}_{\mathcal{O}}^2} \sum_{\mathbf{o},\mathbf{o}'} \langle \delta(q - q_{\mathbf{i};\mathbf{o},\mathbf{o}'}) \rangle.$$

• P(q) is the standard probability distribution of the overlap.

• 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 $T_{\min} = 0.698 = 0.64T_c$

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.

Results: Scaling



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



P(q) and $P_{\rho}(q)$ are different: Dispersed Metastate.

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Results: ζ -exponent



- 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:

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