Thermodynamic States in Finite Dimensional Spin Glasses

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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.

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)

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: \( J(r) \sim \frac{\cos(2k_F r)}{r^3} \).
- 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).
RKKY interaction

Simplification: We take the $J_{ij}$ as random variables! For instance, Gaussian or from a bimodal probability distribution.
Energy:

\[ E = - \sum_{\langle ij \rangle} J_{ij} S_i S_j \]
We compute the partition function for a given realization of the couplings:

$$Z_J = \sum_{[S_i]} \exp(-\beta \mathcal{H}_J) = \sum_{[S_i]} \exp(\beta \sum_{ij} J_{ij} S_i S_j)$$

Next, we compute its free energy:

$$F_J = -\frac{1}{\beta} \log Z_J$$

Finally, we average the different free energies

$$F = \overline{F_J} = \int d[J] p[J] F_J$$

Annealed average:

$$F = -\frac{1}{\beta} \log \int d[J] p[J] \sum_{[S_i]} \exp(-\beta \mathcal{H}_J)$$
Free energy landscape (Disorder + Frustration)
Some experiment (ZF and F-cooled susceptibility)
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: \( q_{EA} = \langle \sigma_i \tau_i \rangle \).
The Droplet Model

- 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 $L^\theta$.
- Any amount of magnetic field destroys the spin glass phase (even for Heisenberg spin glasses).
- Trivial probability distributions of the overlaps.
Replica Symmetry Breaking

\[ \log Z_J = \lim_{n \to 0} \frac{Z^n_J - 1}{n}. \]

\[ Z_n = \overline{Z^n_J} = \sum_{\{s^a\}} \int \text{d}[J] \exp \left( \beta \sum_{a=1}^{n} \sum_{i<j} J_{ij} s_i^a s_j^a - \frac{1}{2} N \sum_{i<j} J_{ij}^2 \right). \]

\[ Z_n = \sum_{\{s^a\}} \exp \left[ \frac{1}{4} \beta^2 N n + \frac{1}{2} \beta^2 N \sum_{a<b} ^n \left( \frac{1}{N} \sum_i s_i^a s_i^b \right)^2 \right]. \]

Linearising the sum over the sites by introducing the so-called replica matrix \( Q_{ab} \),

\[ Z_n = \int \text{d}[Q_{ab}] \sum_{\{s^a\}} \exp \left[ \frac{1}{4} \beta^2 N n - \frac{1}{2} \beta^2 N \sum_{a<b} ^n Q_{ab}^2 + \beta^2 \sum_{a<b} ^n \sum_i Q_{ab} s_i^a s_i^b \right]. \]
Replica Symmetry Breaking

\[ Z_n = \int d[Q_{ab}] e^{-\mathcal{H}_n\{Q_{ab}\}}, \]

where the effective Hamiltonian is

\[ \mathcal{H}_n\{Q_{ab}\} = -\frac{Nn}{4} \beta^2 + \frac{N}{2} \beta^2 \sum_{a<b} Q_{ab}^2 N \log \left[ \sum_{\{s^a\}} \exp \left( \beta^2 \sum_{a<b} Q_{ab} s^a s^b \right) \right]. \]

The Mean Field solution is given by

\[ \delta \mathcal{H}_n / \delta Q_{ab} = 0 \]

which can be written as

\[ Q_{ab} = \frac{1}{N} \sum_i \langle s^a_i s^b_i \rangle \mathcal{H}_n , \ a \neq b, \quad (1) \]
0-step: $Q_{ab} = (1 - \delta_{ab}) q$

\[
\hat{Q}_{0\text{-step}} = \begin{pmatrix}
0 & & & q_0 \\
& \ddots & & \\
q_0 & & 0
\end{pmatrix}
\]

\[
q = \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} \exp(-z^2/2) \tanh^2(\beta z \sqrt{q}).
\]

Problem: Negative Entropy!!
Replica Symmetry Breaking \((D < \infty)\)

\[
H_n = \int d^D x \left[ (\partial_\mu Q_{ab})^2 + \tau \text{Tr} Q^2 + g_3 \text{Tr} Q^3 + g_4 \text{Tr} Q^4 + \lambda \sum Q_{ab}^4 \right]
\]

- \(\lambda \neq 0\). The symmetry group is \(S_n\).
- When \(\lambda = 0\), \(S_n \rightarrow O(n)\).
- \((\lambda = 0)\), \(Q_{ab} = (1 - \delta_{ab})q\). \(O(n)\) Spontaneously broken: Goldstone Bosons.
- But when \(\lambda \neq 0\), \(O(n)\) explicitly broken. Goldstone bosons acquire mass (negative!). Unstable solution.
Replica Symmetry Breaking

\[ \hat{Q}_{0\text{-step}} = \begin{pmatrix} 0 & q_0 \\ q_0 & 0 \end{pmatrix} \]

\[ \hat{Q}_{1\text{-step}} = \begin{pmatrix} 0 & q_1 & \ldots & q_0 \\ \vdots & q_1 & \ldots & q_0 \\ q_0 & 0 & \ldots & q_1 \\ q_0 & q_0 & \ldots & q_1 \end{pmatrix} \]
$n > m_1 > m_2 > \ldots > 1.$
Replica Symmetry Breaking

The matrix elements can be described by the probability distribution

\[ P(q) = \frac{1}{n(n-1)} \sum_{a \neq b} \delta(Q_{ab} - q) \]

\[ = \frac{n}{n(n-1)} \left[ (n - m_1)\delta(q - q_0) + (m_1 - m_2)\delta(q - q_1) \right. \]
\[ + (m_2 - m_3)\delta(q - q_2) + \ldots \]

Finally, we have to take the limit \( n \to 0 \),

\[ P(q) = m_1\delta(q - q_0) + (m_2 - m_1)\delta(q - q_1) + (m_3 - m_2)\delta(q - q_2) + \ldots \]

Notice that now (after \( n \to 0 \)): \( 0 < m_1 < m_2 < \ldots < 1 \).

In the limit of infinite RSB steps we obtain a continuous variation, so \( q_k \to q(x) \), with \( x \in [0, 1] \).

Hence, the spin-glass order parameter is a function,

\[ \frac{dx}{dq} = P(q). \]
Ultrametricity

- Metric Space: \( d(A, B) \leq d(A, C) + d(B, C) \).
- Ultrametric Space: \( d(A; B) \leq \max(d(A, C), d(B, C)) \).

Replica Symmetry Breaking (Ultrametricity)

\[ D(A, B) = \frac{1}{2} (q_{EA} - q_{AB}). \]
Different Theories

- Field Theory of the Replica Symmetry Breaking (RSB) Theory.
- Hamiltonian

\[ H_n = \int d^D x \left[ (\partial_\mu Q_{ab})^2 + \tau \text{Tr}Q^2 + g_3 \text{Tr}Q^3 + g_4 \text{Tr}Q^4 + \lambda \sum Q_{ab}^4 \right] \]

\( a, b = 1, \ldots, n. \) At the end, \( n \to 0! \) (The replica trick)
- Propagator \((T > T_c)\):

\[ G(p) = \frac{1}{p^2 + m^2} \]
- Propagator \((T = T_c, \lambda, g_4 \text{ are irrelevant: } \phi^3 \text{ theory, and the upper critical dimensions is } D = 6)\):

\[ G(p) = \frac{1}{p^{2-\eta}} \]
Different Theories.

- Propagators (Parisi Matrix) ($T < T_c$ and $\lambda$ is relevant):
  \[ G_q(r) \simeq q^2 + A(q)r^{-\theta(q)} \]

  where
  - $\theta(q_M) = D - 2$. This result may be exact (some kind of Goldstone theorem).
  - $\theta(q) = D - 3$ for $q_M > q > q_m$. This result should be modified below $D = 6$.
  - $\theta(q_m) = D - 4$ for $q_m = 0$.

- In the droplet/scaling Theory:
  \[ G(r) \simeq q_{EA}^2 + Ar^{-\theta} \]

  where $\theta$ is the standard droplet exponent.
Different Theories: External Magnetic Field

RG from the paramagnetic phase:

- The upper critical dimension in a field is still six (Bray and Moore).
- Due to a dangerous irrelevant variable, some observables change behavior at eight dimensions (Fisher and Sompolinsky).
- Projecting the theory (replicon mode) no fixed points were found (Bray and Roberts).
- However, starting with the most general Hamiltonian of the RS phase and relaxing the $n = 0$ condition a stable fixed point below six dimensions was found (Dominicis, Temesvári, Kondor and Pimentel).
- Temesvári is able to build the dAT slightly below $D = 6$ (but Bray and Moore, Temesvári and Parisi, Moore,...)
Renormalization group predictions (from Temesvári and Parisi):

\[ T^2 \]

(a) (b)

RSB

AT-line

RS

\[ h^2 \]

\[ h_c^2 \]

\[ T_c \]

\[ T \]
Replica Symmetry Breaking

Summary

- 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,

\[ \lim_{L \to \infty} \langle (\cdots) \rangle_{(L,h=0)} = \frac{1}{2} \langle (\cdots) \rangle_+ + \frac{1}{2} \langle (\cdots) \rangle_- \]
Phases and Thermodynamic limit in Pure systems

- 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 (CP) 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 $\Lambda_L \setminus \Lambda_R$.
- Measurements in $\Lambda_W \subset \Lambda_R$.
- The wanted limit: $\Lambda_W << \Lambda_R << \Lambda_L$. 

\[
\begin{array}{c}
\Lambda_R \\
\Lambda_L \\
\Lambda_W \\
\end{array}
\]
Construction of the Aizenman-Wehr Metastate

- Let us compute

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

- If the limit

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

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

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

\[ \langle \cdots \rangle_\rho \equiv \langle \cdots \rangle_\Gamma_\kappa \]

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

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

- The metastate is a probability distribution on this hyperplane.

- The MAS \( \rho(s) \) 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:

\[
C_\rho(x) = \left[ \langle s_0 s_x \rangle \Gamma \right]_\kappa^2 = \frac{1}{N_I} \sum_i \left( \frac{1}{N_O} \sum_o \langle s_0^{i;o} s_{x}^{i;o} \rangle \right)^2 = \\
= \frac{1}{N_I} \sum_i \frac{1}{N_O^2} \sum_{o,o'} \langle s_0^{i;o} s_{x}^{i;o} s_0^{i;o'} s_{x}^{i;o'} \rangle \sim |x|^{-(d-\zeta)},
\]

- Remember \( \langle \cdots \rangle_\rho \equiv \left[ \langle \cdots \rangle \Gamma \right]_\kappa \).
- \( \zeta \) is the Read’s exponent.
- \( i = 0, \ldots, N_I. \ N_I = 10 \) instances of internal disorder (\( I \)).
- \( o = 0, \ldots, N_O. \ N_O = 1280 \) instances of outer disorder (\( O \)).
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 $q_{i;o,o'}$:

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

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

- $P(q)$ is the standard probability distribution of the overlap.
Although $P_\rho(q) \rightarrow \delta(q)$ as $L \rightarrow \infty$, 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 $W/R = 0.75$. 
Results: Scaling

\[ \rho = \frac{L}{2}, \quad T = 0.698 \]

\[ \chi \frac{\rho}{R^{2.3}} \]

\[ \frac{W}{R} \]

\[ L = 8 \]
\[ L = 12 \]
\[ L = 16 \]
\[ L = 24 \]

\[ \zeta = 0.76 \left( \frac{W}{R} \right)^{2.3} \]

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

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

\[ \zeta = d \]

\[ d_U = 6 \]

\[ d_L \approx 2.5 \]

\[ \zeta_{q=0} \]
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: