Ultrametric tree of spin glasses: predictions for magnetic chaos in finite-dimensional systems

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The article

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Small field chaos in spin glasses: Universal predictions from the ultrametric tree and comparison with numerical simulations

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Plan for the talk

1. Mean Field Spin Glasses
2. RSB Predictions
3. Finite Dimensions
4. Our work

Sherrington-Kirkpatrick Model (1975)[1]

$$\mathcal{H}_J = \sum_{i<j} J_{ij} s_i s_j$$

- The spins are Ising variables $s_i = \pm 1$.
- Simplification: the disorder is introduced directly into the J_{ij}
- The J_{ij} are random variables with a given distribution: Gaussian ($\mathbb{E}[J] = 0$, $\mathrm{var}[J] = 1/N$).
- The spins live in a complete graph (all-to-all interactions, Mean-Field, $D = \infty, \ldots$).

[1] *Solvable Model of a Spin-Glass*, D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 35, 1792 – 29 December 1975

Notation

Disoder Averages:

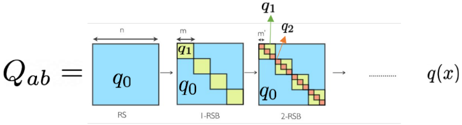
- A set of $\{J_{ij}\}$ is called a sample.
- Physical observables are obtained by averaging over samples:

$$\overline{(\dots)} = \int DJP[J](\dots) = \prod_{i<j} \Big[\sqrt{\frac{N}{2\pi}} \int \mathrm{d}J_{ij} \exp\Big(-\frac{N}{2}J_{ij}^2\Big)\Big](\dots)$$

Replicas:

- Replicas are non-interacting identical copies of system (same sample) with independent thermal histories.

Full Replica Symmetry Breaking (Parisi, 1979)



$$Q_{ab} = \frac{1}{N} \sum_i \langle s_i^a s_i^b \rangle$$

- Exact in $D = \infty$.
- Infinite number of pure states not related by any spin symmetry.
- The pure states are organized following an ultrametric tree structure.
- Spin glass phase is stable under a small magnetic field (de Almeida-Thouless line).
- Spin glass phase is chaotic (vanishing similarity).
- Spin glasses shows stochastic stability.

Validity of RSB picture

- The importance of RSB picture to describe disordered systems has been recognized by the Nobel committee (Nobel Prize in Physics for Giorgio Parisi, 2021).
- The validity of the RSB solution to the SK model has been mathematically and rigorously proven by F. Guerra (2003), M. Talagrand (2011) and D. Panchenko (2013) (Abel Prize to M. Talagrand, 2024).

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RSB and Physics: Pure States

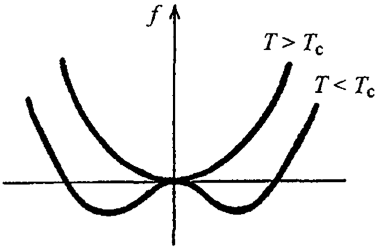
- Ferromagnetic Ising model:

$$\langle\cdot\rangle = \frac{1}{2}\langle\cdot\rangle_+ + \frac{1}{2}\langle\cdot\rangle_-$$

- In the limit $N \to \infty$ and under ergodicity breaking, the Gibbs measure can be decomposed into pure states [a]:

$$\langle\cdot\rangle = \sum_\alpha w_\alpha \langle\cdot\rangle_\alpha$$

$$w_\alpha = \frac{\exp(-\beta F_\alpha)}{\sum_\gamma \exp(-\beta F_\gamma)}$$



(a)

[a] Pure states are defined by the clustering property: $\langle s_i s_j\rangle \to \langle s_i\rangle\langle s_j\rangle$ for $|i-j| \to \infty$

RSB and Physics: Pure states

- SK Spin Glass:
  - The replica free energy is invariant under permutations of replicas.
  - The free energy proportional to the volume of the system.

$$\Downarrow$$

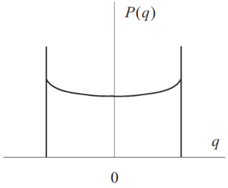
Infinitely many pure states!!

RSB and Physics: The physical order parameter $P(q)$

The overlap between pure states is $q_{\alpha\beta} = \frac{1}{N}\sum_i \langle s_i\rangle_\alpha \langle s_i\rangle_\beta \in [0,1]$.
Its probability distribution for a given sample is

$$P_J(q) = \sum_{\alpha\beta} w_\alpha w_\beta \delta(q_{\alpha\beta} - q)$$

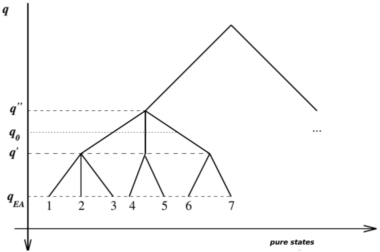
and the 'observable' distribution $P(q) = \overline{P_J(q)} \longrightarrow x(q) = \int_0^q \mathrm{d}q' P(q')$.



$$P(|q|) = \tilde{P}(|q|) + (1 - x(q_{EA}))\delta(q - q_{EA})$$

RSB and Physics: Ultrametricity

Ultrametric space: $d(A,B) = \max(d(A,C); d(B,C))$
Distance: $d(A,B) = \frac{1}{2}(q_{EA} - q_{AB})$, $(q_{EA} = q_{\alpha\alpha})$



$$P(q_1, q_2, q_3) = \frac{1}{2}P(q_1)x(q_1)\delta(q_1 - q_2)\delta(q_1 - q_3) + \frac{1}{2}[P(q_1)P(q_2)\theta(q_1 - q_2)\delta(q_2 - q_3) + \text{permutations}]$$

RSB and Physics: Chaos

- Spin Glasses are chaotic systems: when the system is subjected to a small perturbation δp of an external parameter p (like the temperature or the magnetic field) the states at p and $p + \delta p$ are as different as possible in the thermodynamic limit.
- Magnetic chaos can be studied by looking at the probability distribution $P_C^N(q, h)$ of the overlaps between two replicas, one at $h = 0$ and other one at $h \neq 0$.

Finite Dimensions

Experimental spin glasses are better described by models with:

- Short-range interactions
- Finite dimensions

A simple model with these characteristics is the Edwards-Anderson model[2] (1975)

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} s_i s_j + h \sum_i s_i$$

[2] S. F. Edwards and P. W. Anderson, *Theory of spin glasses*, J. Phys. F: Met. **5** 965, 13 February 1975

Finite Dimensions

The following results have been rigorously proven:

- If ultrametricty holds at finite D, it should have the same properties as one finds at $D = \infty$ (D. Iñiguez, G. Parisi, J.J. Ruiz-Lorenzo, 1996).
- Stochastic stability implies Ultrametricity (D. Panchenko, 2013).

There is numerical evidence for stochastic stability in finite dimensional systems (Janus Colaboration, 2010), so this systems should have ultrametricty of the mean-field kind.

Our work: Objectives

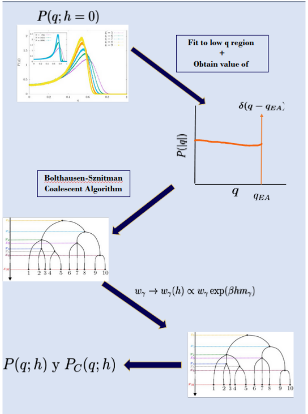
- We want to compare the predictions from RSB theory with simulations of two systems with spin glass behavior:
  - Bethe Lattice SG.
  - 4D Edwads-Anderson SG.
- The theoretical predictions from RSB will be obtained by generating ultrametric trees with the proper statistics via the Bolthausen-Sznitman coalescent algorithm [3].
- The numerical results are obtained via MC simulations supplemented with Parallel Tempering and Multi-Spin Coding.
- We will compare the results for the following observables:

$$P_C^N(q;h) \quad \text{and} \quad P^N(q;h)$$

[3] E. Bolthausen, A. S. Sznitman, On Ruelle's probability cascades and an abstract cavity method. Commun. Math. Phys. 197, 247–276 (1998)

Our work: The strategy

1. Compute through numerical MC simulations the $P(q,0)$.
2. Extract the necessary information for generating the trees:
   - $\tilde{P}(q) \to x(q) \to q(x)$
   - The value of the peak: q_{EA}
3. Generate the trees at $h = 0$ according to the Bolthausen-Sznitman coalescent algorithm.
4. Generate the trees at $h \neq 0$ via a reshuffling of the weights w_α.
5. Measure the desired observables from the trees.
6. Compare the results with numerical MC simulations at $h \neq 0$.



Vanishing fields

We want to study the situation where the perturbation $\delta\mathcal{H}$:

- Change the relative weight of the pure states.
- Do **NOT** change the properties inside a given state.

We choose to add a perturbation (magnetic field)

$$H = h/\sqrt{N} \quad h \in \{1, 2, 4, 6, 8, 10\}$$

that vanishes in the thermodynamic limit.

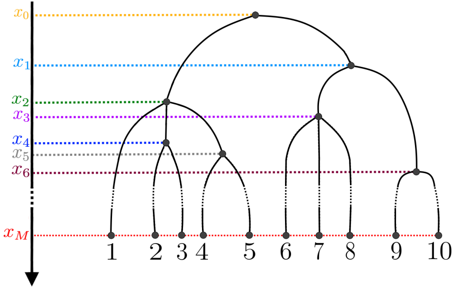
Generating the trees: Algorithm

The structure of the tree:

1. Start with $b = M$ nodes (the leaves) at time t=0.
2. Chose a number k in $\{2, 3, \ldots, b\}$ with probability

$$P(k|b) = \frac{b}{(b-1)(k-1)}$$

   and merge k nodes into a single one.
3. Now $t \to t + \Delta t$, with Δt a random number following $f(\Delta t, b) = (b-1)e^{-(b-1)\Delta t}$.
4. Repeat [2-3] until $b = 1$ (the root of the tree).



Generating the trees: Algorithm

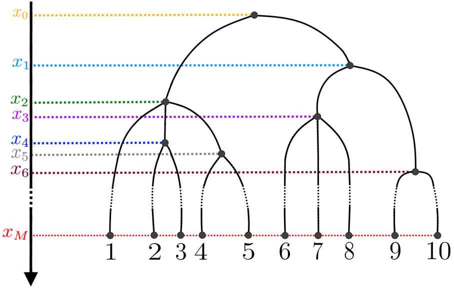
The overlaps:

- $t \longrightarrow x(t) = x_M \exp(-t)$.
- At each level of the tree we have an overlap $q = q(x(t))$.

Assigning the weights:

- We generate M i.i.d. random numbers u with the distribution $p(u) = x_M \theta(u-1) u^{-1-x_M}$.
- The weight for each pure state are given by

$$w_\alpha = \frac{u_\alpha}{\sum_\gamma u_\gamma}$$



Generating the trees: Algorithm

The magnetization:

1. Start with the root and assign it a magnetization equal to $r_g\sqrt{q_{\mathrm{root}}}$ with $r_g \sim \mathcal{N}(0,1)$ a random Gaussian number.
2. Scan the tree from top to bottom and assign to each node a magnetization

$$m_{\mathrm{node}} = m_{\mathrm{parent}} + r_g\sqrt{q_{\mathrm{node}} - q_{\mathrm{parent}}}$$

In this way, the magnetization of the pure states are random Gaussian numbers with covariance $\overline{m_\alpha m_\beta} = q_{\alpha\beta}$.

Generating the trees: The effects of the field h

- In the presence of a field h, the weights are reshuffled as $w_\gamma(h) \propto w_\gamma \exp(\beta h m_\gamma)$
- The observables of interest can be computed as:

$$P_J^C(q;h) = \sum_{\alpha\beta} w_\alpha w_\beta(h)\delta(q - q_{\alpha\beta}) \quad \text{and} \quad P_J(q;h) = \sum_{\alpha\beta} w_\alpha(h) w_\beta(h)\delta(q - q_{\alpha\beta})$$

- And the magnetization in a field is computed as:

$$m(h) = \beta h\left(1 - \int_{-1}^{1} \mathrm{d}q P(q;h) q\right)$$

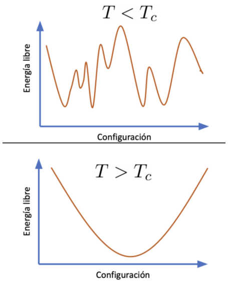
Simulations of Spin Glasses

Simulations of Spin Glasses are hard (in fact, NP-hard[4]).

- It is hard to reach equilibrium via MC updates due to the multi-valley structure of the free energy.
- One needs to simulate many realizations of the disorder (samples).

To overcome these problems, we follow two strategies:

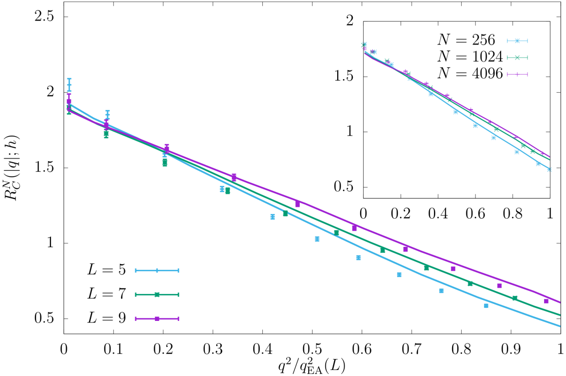
- Parallel Tempering
- Multi-Spin Coding



	Sample 1	Sample 2	Sample 3		Sample 126	Sample 127	Sample 128
s[0]	1	0	1	···	0	0	1
s[1]	0	1	1	···	1	0	1
···							
s[V]	0	1	0	···	1	1	1

[4] F Barahona, *On the computational complexity of Ising spin glass models* J. Phys. A: Math. Gen. 15 3241, 1982

Results: Finite size effects



$$R_c^N(|q|;h) = \frac{P_C^N(|q|;h)}{P_C^N(|q|,0)}$$

Results: Bethe Lattice

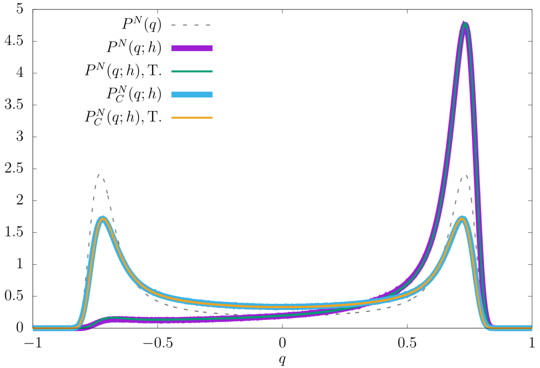


Figure: $P^N(q)$, $P_C^N(q;h)$ and $P^N(q;h)$ at $T = 0.5T_c$ for $h = 4$ for the largest volume $N = 4096$ of the Bethe Lattice.

Results: 4D EA

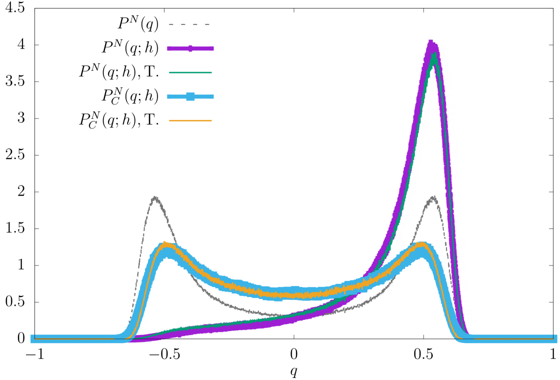


Figure: $P^N(q)$, $P^N_C(q;h)$ and $P^N(q;h)$ at $T = 0.7T_c$ for $h = 10$ for the largest volume $N = 9^4$ of the 4D Edwards-Anderson model.

Conclusions and Perspectives

- RSB provides universal predictions for the behavior of the system under a small perturbation, that only depends on the overlaps statistics at zero field $P(q)$.
- We have found excellent agreement between simulations of the EA 4D model and predictions from the ultrametric trees, what constitutes evidence of RSB in these systems.
- This method could enable us to test the validity of RSB in experimental spin glasses.

Thanks!

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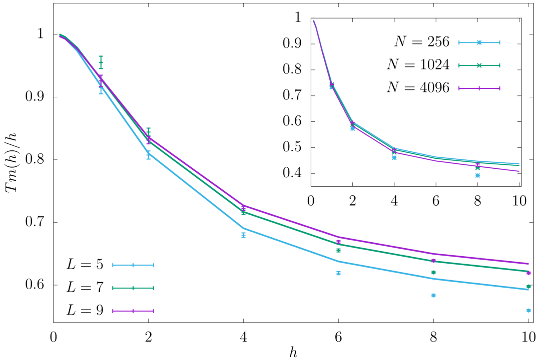
Extra: Magnetization



Extra:cutting leaves

We do not generate infinite trees. We neglect trees that have a weight $w < \epsilon$, so the pruned tree has M leaves where $M = \mathcal{O}(\epsilon^{x_M})$.
The minimum weight is of order $\epsilon_M \sim M^{1/x_M}$