Thermodynamic States in Finite Dimensional Spin Glasses

J. J. Ruiz-Lorenzo

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

Instituto Gregorio Millán Barbany
Universidad Carlos III
Leganés, January 23rd, 2018

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.

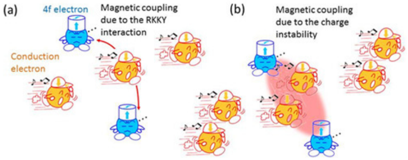
with A. Billoire (Paris), L. A. Fernández, V. Martín-Mayor (Madrid), E. Marinari, A. Maiorano, G. Parisi, F. Ricci-Tersenghi (Rome), J. Moreno-Gordo (Zaragoza)

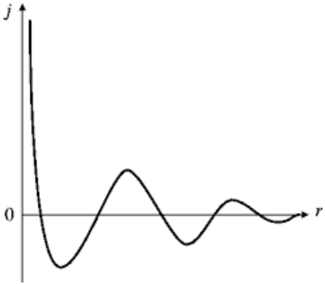
Phys. Rev. Lett. 119, 0327203(2017) (arXiv:1704.01390).

What are Spin glasses

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



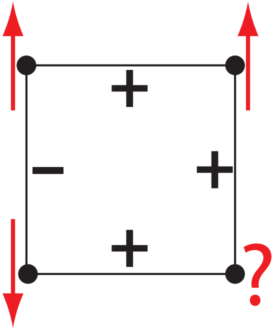


Simplification: We take the J_{ij} as random variables! For instance, Gaussian or from a bimodal probability distribution.

Frustration

Energy:

$$E = -\sum_{<ij>} J_{ij} S_i S_j$$



Quenched and Annealed Disorder

- We compute the partition function for a given realization of the couplings:

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

- Next, we compute its free energy:

$$F_J = -\frac{1}{\beta} \log \mathcal{Z}_J$$

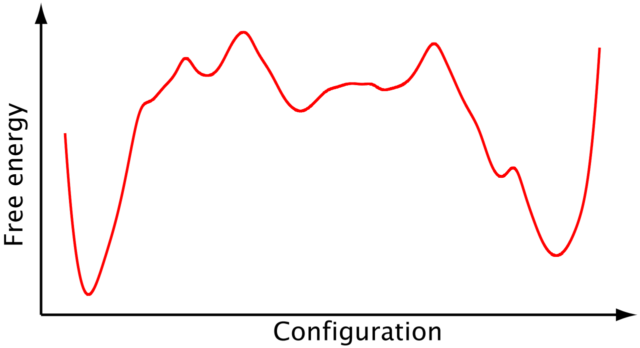
- Finally, we average the different free energies

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

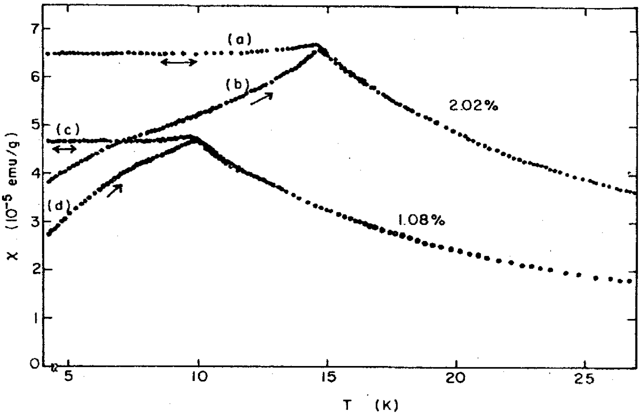
- Annealed average:

$$F = -\frac{1}{\beta} \log \int d[J] p[J] \sum_{[S_i]} \exp(-\beta \mathcal{H}_{\mathcal{J}})$$

Free energy landscape (Disorder+Frustration)



Some experiment (ZF and F-cooled susceptibility)



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:

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

  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: $q_{\mathrm{EA}} = \overline{\langle \sigma_i\tau_i \rangle}$.

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 $\pm q_{\mathrm{EA}}$ (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

$$\log Z_J = \lim_{n\to 0} \frac{Z_J^n - 1}{n} .$$

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

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

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

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

Replica Symmetry Breaking

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

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

$$Q_{ab} = \frac{1}{N} \sum_i \langle s_i^a s_i^b \rangle_{\mathcal{H}_n} \ , \ a \neq b, \qquad (1)$$

0-step: $Q_{ab} = (1 - \delta_{ab})q$

$$\hat{Q}_{0-\mathrm{step}} = \begin{pmatrix} 0 & & q_0 \\ & \ddots & \\ q_0 & & 0 \end{pmatrix}$$

$$q = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp(-z^2/2) \tanh^2(\beta z \sqrt{q}).$$

Problem: Negative Entropy!!

Replica Symmetry Breaking ($D < \infty$)

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

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

Replica Symmetry Breaking

$$\hat{Q}_{0-\mathrm{step}} = \begin{pmatrix} 0 & & q_0 \\ & \ddots & \\ q_0 & & 0 \end{pmatrix}$$

$$\hat{Q}_{1-\mathrm{step}} = \begin{pmatrix} \overbrace{0 \quad\quad q_1}^{m_1} & & & & & & \\ \ddots & & q_0 & & \cdots & & q_0 \\ q_1 \quad\quad 0 & & & & & & \\ & 0 & & q_1 & & & \\ q_0 & & \ddots & & \cdots & & q_0 \\ & q_1 & & 0 & & & \\ \vdots & & \vdots & & \ddots & & \vdots \\ & & & & 0 & & q_1 \\ q_0 & & q_0 & & \cdots & \ddots & \\ & & & & q_1 & & 0 \end{pmatrix}$$

Replica Symmetry Breaking

$$\begin{pmatrix} \overbrace{\begin{matrix} \overbrace{\begin{matrix}0 & & q_2\\ & \ddots & \\ q_2 & & 0\end{matrix}}^{m_2} & \cdots & q_1 \\ \vdots & \ddots & \vdots \\ q_1 & \cdots & \begin{matrix}0 & & q_2\\ & \ddots & \\ q_2 & & 0\end{matrix}\end{matrix}}^{m_1} & \cdots & q_0 \\ \vdots & \ddots & \vdots \\ q_0 & \cdots & \begin{matrix} \begin{matrix}0 & & q_2\\ & \ddots & \\ q_2 & & 0\end{matrix} & \cdots & q_1 \\ \vdots & \ddots & \vdots \\ q_1 & \cdots & \begin{matrix}0 & & q_2\\ & \ddots & \\ q_2 & & 0\end{matrix}\end{matrix} \end{pmatrix}$$

$n > m_1 > m_2 > \ldots > 1.$

Replica Symmetry Breaking

The matrix elements can be described by the probability distribution

$$
\begin{aligned}
P(q) &= \frac{1}{n(n-1)} \sum_{a \neq b} \delta(Q_{ab} - q) \\
&= \frac{n}{n(n-1)} \big[(n - m_1)\delta(q - q_0) + (m_1 - m_2)\delta(q - q_1) \qquad (2) \\
&\qquad + (m_2 - m_3)\delta(q - q_2) + \ldots \big] \qquad (3)
\end{aligned}
$$

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,

$$
\frac{\mathrm{d}x}{\mathrm{d}q} = P(q).
$$

Ultrametricity

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

M. C. Espejo et al. Biochemical Systematics and Ecology, 22, 894 (1994)

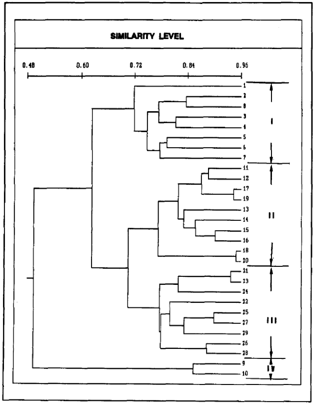
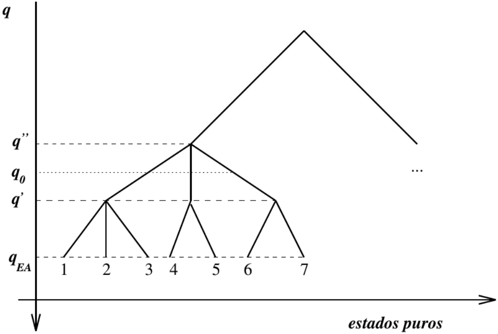


FIG. 2. UPGMA DENDROGRAM OF *PHASEOLUS VULGARIS* ACCESSIONS BASED ON ISOENZYMATIC SYSTEM DATA ANALYZED.

Replica Symmetry Breaking (Ultrametricity)

$D(A, B) = \frac{1}{2}\,(q_{\mathrm{EA}} - q_{AB}).$



Different Theories

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

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

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

$$G(p) = \frac{1}{p^2 + m^2}$$

- Propagator ($T = T_c$, λ, g_4 are irrelevant: ϕ^3 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 λ 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:

$$G(r) \simeq q_{EA}^2 + A r^{-\theta}$$

  where θ is the standard droplet exponent.

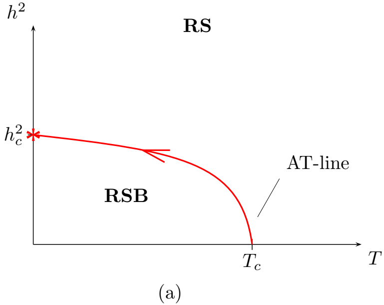
Different Theories: External Magnetic Field

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,...)

Different Theories: External Magnetic Field

Renormalization group predictions (from Temesvári and Parisi):



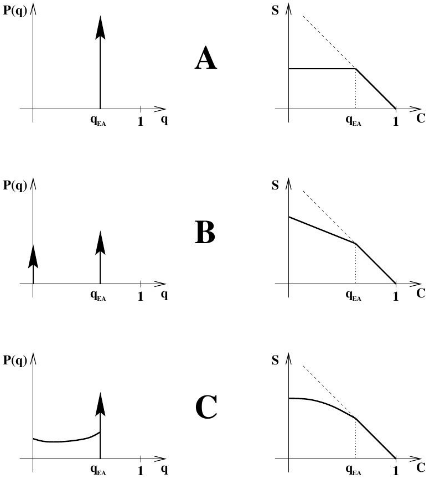
Replica Symmetry Breaking

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, 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,

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

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.

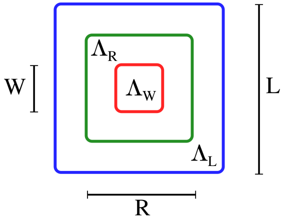
Phases and Thermodynamic limit in Disordered systems: The Metastate.

- 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 temperaures does not converge. (It is given by $\mathrm{sign}(\sum_i h_i)$ 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 Λ_R.
- Outer disorder $\mathcal{O}$ in the region $\Lambda_L \backslash \Lambda_R$.
- Measurements in $\Lambda_W \subset \Lambda_R$.
- The wanted limit: $\Lambda_W << \Lambda_R << \Lambda_L$.



Construction of the Aizenman-Wehr Metastate

- Let us compute

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

- 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), $\rho(\underline{s})$, 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. $\{p_\alpha\}_{\alpha=1,\ldots,2^{W^d}}$. 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).

Some Observables

- The MAS spin glass correlation function:

$$C_\rho(x) = \overline{[\langle s_0 s_x \rangle_\Gamma]_\kappa^2} = \frac{1}{\mathcal{N_I}} \sum_{\mathtt{i}} \left(\frac{1}{\mathcal{N_O}} \sum_{\mathtt{o}} \langle s_0^{\mathtt{i;o}} s_x^{\mathtt{i;o}} \rangle \right)^2 =$$

$$= \frac{1}{\mathcal{N_I}} \sum_{\mathtt{i}} \frac{1}{\mathcal{N_O}^2} \sum_{\mathtt{o,o'}} \langle s_0^{\mathtt{i;o}} s_x^{\mathtt{i;o}} s_0^{\mathtt{i;o'}} s_x^{\mathtt{i;o'}} \rangle \sim |x|^{-(d-\zeta)} \,,$$

- Remember $\langle \cdots \rangle_\rho \equiv [\langle \cdots \rangle_\Gamma]_\kappa$.
- ζ is the Read's exponent.
- $\mathtt{i} = 0, \ldots, \mathcal{N_I}$. $\mathcal{N_I} = 10$ instances of internal disorder ($\mathcal{I}$).
- $\mathtt{o} = 0, \ldots, \mathcal{N_O}$. $\mathcal{N_O} = 1280$ instances of outer disorder ($\mathcal{O}$).

Physics behind the ζ-exponent

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

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

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

Some Observables

- The (generalized) overlap on the box Λ_W:

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

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

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

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

- $P(q)$ 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:

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

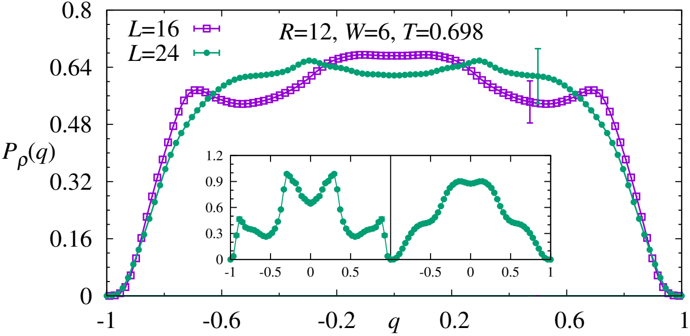
- $P_\rho\big(q/(W^{-(\zeta-d)/2})\big)$ is Gaussian.

Numerical Simulations and Observables

Numerical Simulations

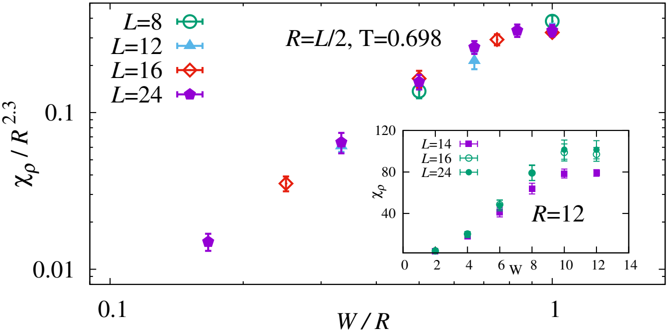
- We have simutated the three-dimensional Edwards-Anderson model with periodic boundary conditions and bimodal disorder.
- We have implemented the Parallel Tempering Method (with Metropolis single spin-flip).
- We have used multispin coding (128 bits).
- Equilibration was assessed on a sample-by-sample 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 $T_{\text{min}} = 0.698 = 0.64 T_c$

Results: the MAS overlap probability distribution



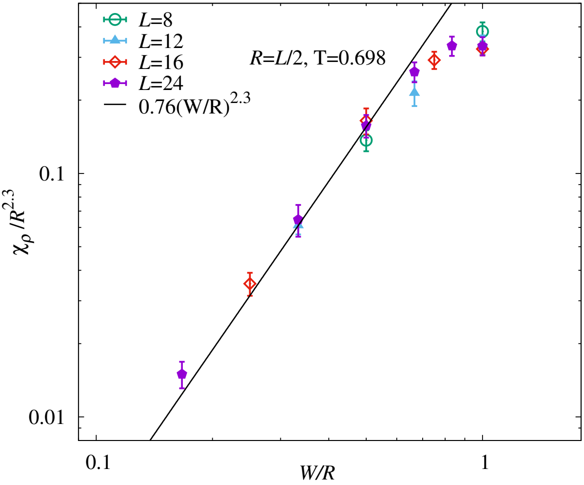
Notice that for $R/L = 3/4$ there are no finite size effects. We will take in the following the safe ratio $R/L = 1/2$.

Results: Scaling



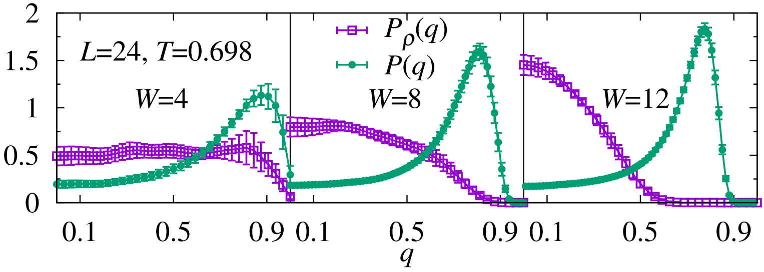
The scaling regime extends to $W/R = 0.75$.

Results: Scaling



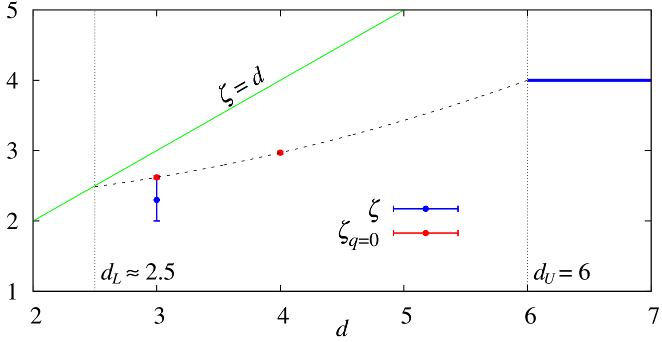
$\zeta = 2.3(3)$, to be compare with $\zeta_{q=0} = 2.62(2)$

Results: Comparison $P(q)$ and $P_\rho(q)$



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

Results: ζ-exponent



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 (additonal) References:

- M. Aizenman and J. Wehr, Comm. Math. Phys. **130**, 489 (1990).
- C. M. Newman and D. L. Stein, Phys. Rev. B **46**, 973 (1992); Phys. Rev. Lett. **76**, 4821 (1996); Phys. Rev. E **55**, 5194 (1997); Phys. Rev. E **57**, 1356 (1998).
- E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. J. Ruiz-Lorenzo and F. Zuliani, J. Stat. Phys. **98**, 973 (2000).
- N. Read, Phys. Rev. E **90**, 032142 (2014).
- M. Manssen, A. K. Hartmann, A. P. Young, Phys. Rev. B **91**, 104430 (2015).
- W. Wang, J. Machta, H. Munoz-Bauza, H. G. Katzgraber. Phys. Rev. B 96, 184417 (2017).