

The metastate construction and its
application to $3D$ spin glasses.

Enzo Marinari

(*Sapienza*, Rome, Italy)

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Summary

1. The concept of metastate.
2. Different types of metastate.
3. Metastate Averaged State (MAS) and correlation functions.
4. The numerical construction and analysis of Aizenman-Wehr metastate.
5. A “complex” picture of finite dimensional spin glass like systems.

Numerical Construction of the Aizenman-Wehr Metastate, A. Billoire, L. A. Fernandez, A. Maiorano, EM, V. Martin-Mayor, J. Moreno-Gordo, G. Parisi, F. Ricci-Tersenghi and J.J. Ruiz-Lorenzo, Phys. Rev. Lett. 119, 037203 (2017), [arXiv:1704.01390](#).

After Aizenman-Wehr, Newman-Stein and the recent work by Read.

We consider the standard model for spin-glasses, the Edwards - Anderson model with Ising spins $s_i = \pm 1$, on a size L cube, $\Lambda_L \subset \mathbb{Z}^d$.

Nearest neighbor, bond disordered and strongly frustrated Hamiltonian:

$$H_{\mathcal{J},L}(\underline{s}) = - \sum_{\langle i,j \rangle} J_{ij} s_i s_j .$$

Quenched couplings J_{ij} are independent and identically distributed random variables, $J_{ij} = \pm 1$ with 50%. $\mathcal{J} \equiv \{J_{ij}\}$ is a disorder sample.

The finite- L Gibbs state

$$\Gamma_{\mathcal{J},L}(\underline{s}) = \frac{\exp(-H_{\mathcal{J},L}(\underline{s})/T)}{Z_{\mathcal{J},L}}$$

is a random state, as it depends on the set of random couplings \mathcal{J} .

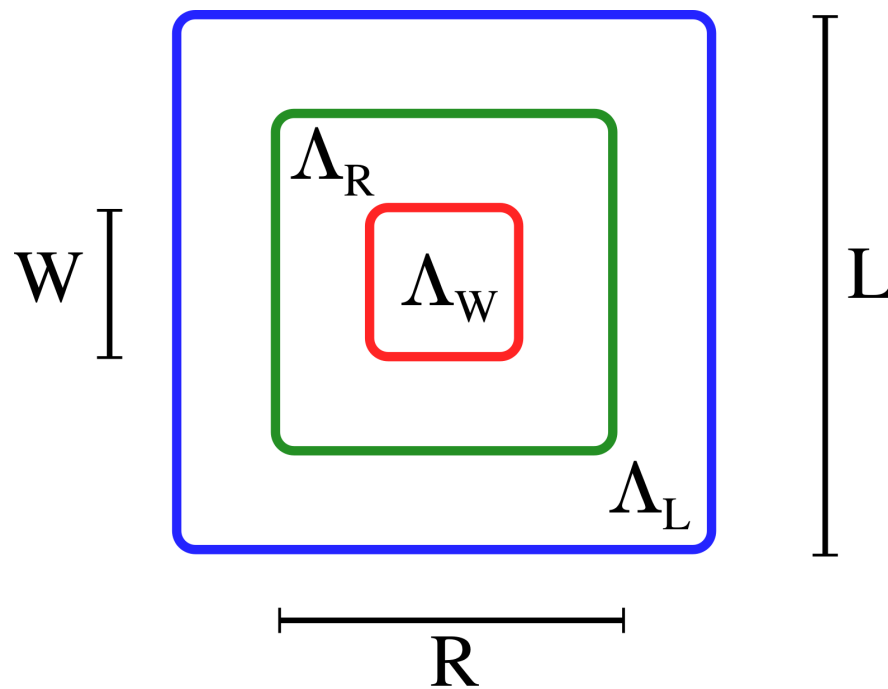
As discussed by Newman and Stein chaotic size-dependence (CSD) makes difficult to take the large L limit of spin glass systems.

Take a fixed, arbitrary yet finite region (e.g. the *measuring window*).

The Gibbs measure over Λ_W changes chaotically when the system grows by the addition of new couplings at the boundaries, while keeping previous couplings unaltered.

This extreme sensibility to changes at the boundaries motivated the introduction of the *metastate*, a probability distribution over states with a (hopefully) smoother $L \rightarrow \infty$ limit.

The construction of the Aizenman-Wehr metastate.



We will use in the following the **Aizenman-Wehr definition of metastate**, since it is easier to implement it numerically.

The lattice Λ_L is divided into an **inner region** Λ_R , a cube of linear size R , and an **outer region**.

Internal couplings:

$$\mathcal{I} \equiv \{J_{ij} | i, j \in \Lambda_R\}$$

Outer couplings:

$$\mathcal{O} = \mathcal{J} \setminus \mathcal{I}.$$

- (i) we restrict our attention to the measuring window Λ_W of size W ,
- (ii) we average over the outer couplings, with *fixed* internal couplings
- (iii) we “send to infinity” all three length scales while $W \ll R \ll L$

If the limit exists it is independent of the arbitrary choice for the fixed internal couplings.

Definition of the Newman-Stein metastate.

The set of couplings \mathcal{J} over the *infinite* lattice \mathbb{Z}^d is fixed.

One considers a sequence of growing finite regions Λ_L .

The Hamiltonian is truncated to the cube Λ_L . Use for example free boundary conditions.

Consider the Gibbs state, $\Gamma_{\mathcal{J},L}$ as restricted to the measuring window Λ_W .

The Newman and Stein metastate records the frequency by which each state appears while the system size grows.

If this sequence of states converges, when the size W of the measuring window gets large, the resulting metastate is expected to be independent of the initial choice of couplings \mathcal{J} (for typical \mathcal{J}).

Recent progresses from a rigorous point of view have been substantial, and different techniques have been very useful.

Talagrand, building on work by Guerra has proven that Parisi solution of the Sherrington Kirkpatrick mean field theory is correct (that was not sure before one proved it. Obviously.).

Also, many recent results by Panchenko, about ultrametricity, stability properties, Potts and p -spin spin glasses.

There is at least a stable foundation on which one can build.

Already for $\infty > d \geq d_c^u$ there are no proofs about what happens. For $d_c^u > d > d_c^u$ the situation is even more difficult. Intrinsic complexity of the systems is resilient both to analytic and, maybe a bit less, to numerical analysis.

Here I will not try to reach any generality, but only to show a single, precise numerical result, with all the issues that can always affect the implications of such results.

The “droplet” description is valid on hierarchical lattices (i.e. in the Migdal-Kadanoff approximation) and it provides a much simpler scenario for the low temperature phase, where the Gibbs measure is a mixture of two spin-flip related pure states.

This is a typical **Scilla and Cariddi** problem. What looks relevant, and it is recognized by all researchers in the field, is the intrinsic **complexity** of the model, that makes dramatically difficult treatments like the ones that have allowed to reach a detailed understanding of “usual” critical phenomena.

As matter of principle the metastate approach can not only allow to define states in a mathematically consistent way, but can also allow to distinguish among these different physical behaviors.

Read recent work has given us the tool to use the metastate approach in a numerical setting. We know about three mathematically consistent pictures for the spin-glass phase.

First, the **Droplet Model metastate** is concentrated on a state which is a mixture of two pure states related by the global spin-flip symmetry, that we call “trivial”.

Second, the **Chaotic Pairs picture**, predicting a *disperse* metastate (there is a large number of states to choose from), where each state is **trivial**. This non-trivial metastate is connected to chaotic size-dependence: by increasing L , one obtains different states.

Finally, the **RSB-metastate** is *disperse* and every state drawn from it contains the Parisi hierarchical tree of pure states.

Alternatives to these three pictures are much limited by recent rigorous results.

After Read one can at least partially discriminate between these competing pictures for the metastate by studying the decay of a correlation function (that we will define later) averaged over the metastate

$$C_\rho(x) \sim |x|^{-(d-\zeta)}$$

for large distances $|x|$.

An exponent value $\zeta < d$ implies a disperse metastate.

In the RSB-metastate, the number of pure states that can be resolved by studying a region of size W is exponentially large in $W^{d-\zeta}$.

In 2015 Manssen, Hartmann and Young have tried to use a non-equilibrium approach to implement numerically the metastate construction.

One studies large 3d spin glass systems up to $L = 128$ and up to long times of $t = 10^8$ sweeps.

The authors conclude that the local behavior of a spin glass depends on the spin configurations (and presumably also the bonds) far away.

A connection between the non-equilibrium dynamics and averages computed theoretically using the metastate is an interesting possibility that can only be speculated.

Recent work (November 2017) by Gertler and Machta.

There is no chaotic size dependence on hierarchical lattices, i.e. in Migdal-Kadanoff approximation. This is implied by a bound that guarantees convergence.

The metastate in this case is simple.

This is consistent, since we know that this situation is described by droplet physics.

A numerical construction of the Aizenman and Wehr metastate for the EA model in $d = 3$ is possible with the state of the art available computer power.

Our construction makes precise several hints by Read.

We discuss how large the ratios of length scales L/R and R/W need to be to uncover metastate properties.

We study the dependence on the fixed internal couplings, a crucial issue that has not yet been addressed quantitatively.

We make quantitative computations of overlap distributions and correlation functions averaged over the AW metastate, thus computing the crucial ζ exponent.

We find a value that is, in our estimated statistical and systematic accuracy, definitively smaller than $d = 3$.

3d EA model endowed with periodic boundary conditions (which makes irrelevant the location of Λ_R in Λ_L).

Probability distribution of $\Gamma_{\mathcal{J},L}$ at fixed internal disorder \mathcal{I} , while sending $L \rightarrow \infty$ and averaging over the outer disorder \mathcal{O} :

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

If the limit

$$\kappa(\Gamma) = \lim_{R \rightarrow \infty} \kappa_{\mathcal{I},R}(\Gamma)$$

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

The purpose of the “measuring window” Λ_W is making boundary effects irrelevant. Any measure is taken only inside Λ_W , while bonds are fixed in Λ_R .

Two kind of averages: thermal averages over the Gibbs state $\langle \cdots \rangle_\Gamma$ and averages over the metastate $[\cdots]_\kappa$.

The *metastate averaged state (MAS)*

$$\rho(\underline{s})$$

is defined via the *average* $\langle \cdots \rangle_\rho \equiv [\langle \cdots \rangle_\Gamma]_\kappa$.

As seen from the measuring window Λ_W , a *state* $\Gamma(\underline{s})$ is a set of probabilities $\{p_\alpha\}_{\alpha=1,\dots,2^{W^d}}$ over the spin configurations in Λ_W .

In other words, it is a point on the hyperplane defined by the equation $\sum_\alpha p_\alpha = 1, p_\alpha \geq 0$. The metastate is a probability distribution over 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).

We simulate the EA model with $8 \leq L \leq 24$.

We sample spin configurations at equilibrium by a combination of Metropolis single spin flip Monte Carlo and Parallel Tempering.

Usual Metropolis is not effective for simulating spin glass systems. Multiple free energy barriers (precursors of ergodicity breaking and of the appearance of multiple states) slow down the dynamics, making it completely ineffective for large systems sizes.

Parallel tempering allow systems to trade their temperature. Copies of the system wander in temperature space, always staying at Boltzmann equilibrium when analyzed with respect to a given temperature value (parallel tempering is a very civilized annealing). In this way free energy barriers become lower for increasing temperature and disappear when the system enters the warm phase.

We select a set of temperatures, from a $T_{\min} < T_c$ up to a $T_{\max} > T_c$. We analyze data at $T_{\min} = 0.698 \simeq 0.64T_c$.

Equilibration is a crucially delicate point. We assess it on a sample-by-sample basis.

For improving the computational efficiency of our codes we use multi-spin coding techniques (both multi-sample, MUSA and multi-site, MUSI).

We repeat the computation for $\mathcal{N}_{\mathcal{I}} = 10$ different internal couplings \mathcal{I} samples (indexed by $0 \leq i < \mathcal{N}_{\mathcal{I}}$) and, for each of these, we use $\mathcal{N}_{\mathcal{O}} = 1\,280$ different outer disorder \mathcal{O} realizations (indexed by $0 \leq o < \mathcal{N}_{\mathcal{O}}$). For each sample we simulate $m = 4$ distinct replicas.

We take $\mathcal{N}_{\mathcal{I}} \ll \mathcal{N}_{\mathcal{O}}$ because we expect all inner disorder samples to be “typical” when computing metastate averages at $R \gg 1$. We find however sizable sample to sample fluctuations for the system sizes we consider.

The average over the Gibbs state $\langle \cdots \rangle_\Gamma$ is estimated via Monte Carlo thermal averages $\langle \cdots \rangle$ at fixed disorder \mathcal{J} , i.e. for given indices \mathbf{i} and \mathbf{o} .

The average over the metastate is given by $[\cdots]_\kappa = \sum_{\mathbf{o}} (\cdots) / \mathcal{N}_{\mathcal{O}}$, and the one over the internal disorder by $\overline{(\cdots)} = \sum_{\mathbf{i}} (\cdots) / \mathcal{N}_{\mathcal{I}}$.

The MAS spin correlation function is given by

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

defining Read ζ exponent for $|x| \gg 1$.

Measure in Λ_W the overlaps between any two real replicas $\underline{\sigma}$ and $\underline{\tau}$ sharing the same internal disorder (indexed by \mathbf{i}) and having external couplings indexed by \mathbf{o} and \mathbf{o}'

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

For each $\{\mathbf{i}; \mathbf{o}, \mathbf{o}'\}$, we have $m(m-1)/2$ contributions from different pairs of real replicas if $\mathbf{o} = \mathbf{o}'$ and m^2 otherwise.

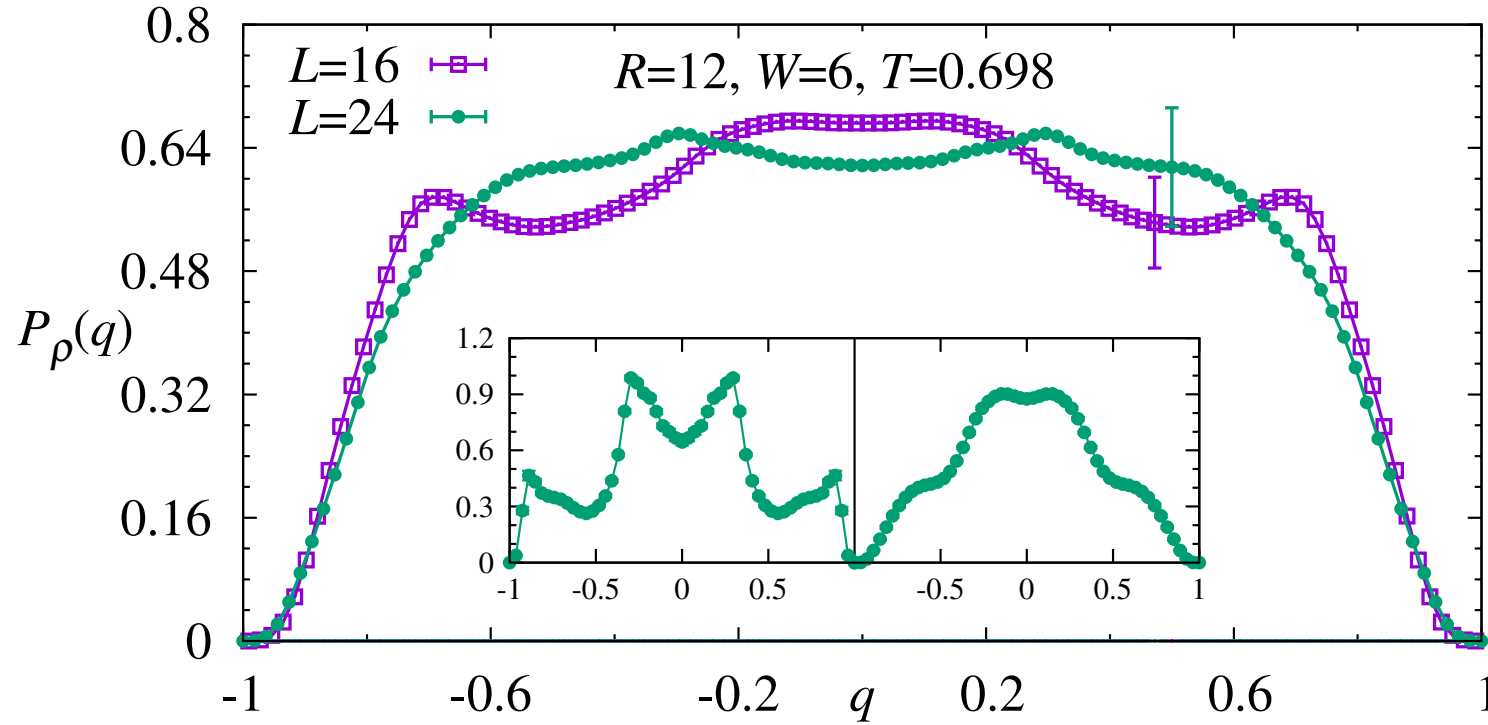
The main objects of our numerical study are the probability density functions of the overlaps:

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

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

$P(q)$ is the usual window pdf already measured in many numerical simulation of spin glasses, $P_{\rho}(q)$ is the pdf of the overlap over the **MAS**. Although $P_{\rho}(q) \rightarrow \delta(q)$ for $W \rightarrow \infty$, the scaling of its variance is informative

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



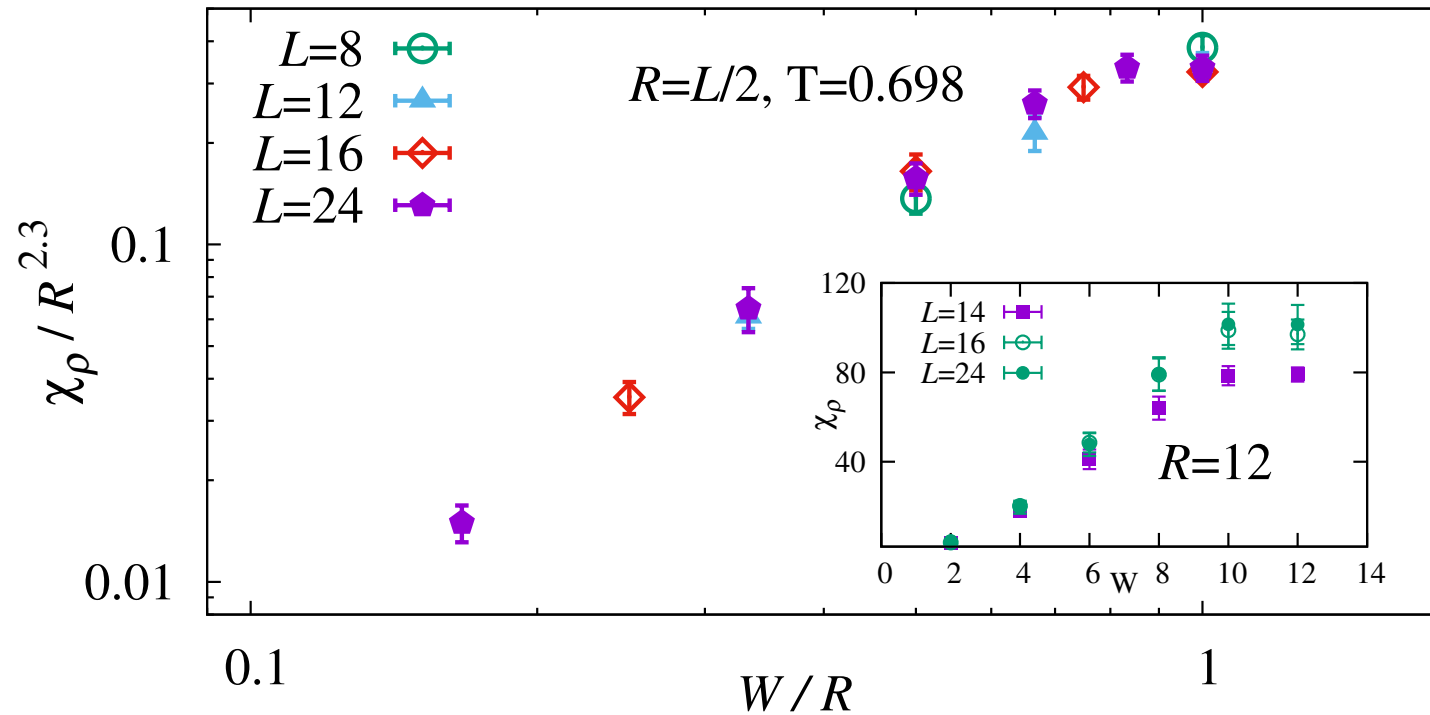
Main plot: The MAS overlap distribution $P_\rho(q)$ with $R = 12$ at $T = 0.698 \simeq 0.64T_c$ shows **no statistical significant dependence on the lattice size L** (the error bars, computed from fluctuations on \mathcal{I} , are shown for one value of q only for sake of clarity).

Insets: $P_{\rho,i}(q)$ for two specific configurations of the inner disorder \mathcal{I} (the error bars, computed from fluctuations on \mathcal{O} , are smaller than the data points).

So, we have some control on finite (total) size effects.

The MAS $P_\rho(q)$ measured with $R = 12$ and both $L = 24$ and $L = 16$ are statistically compatible, suggesting that $R/L = 3/4$ is already a safe choice.

The error bars are large, because the dependence of $P_{\rho,i}(q)$ on the internal disorder sample is very strong for the values of W and R we are using (as shown by the insets).



Main plot: Collapse of MAS susceptibility measured with $R = L/2$ at $T \simeq 0.64T_c$.

Inset: Deviations from the asymptotic behavior only for $R/L > 3/4$.

MAS susceptibility χ_ρ

Inset: fixing $R = 12$, all data with $R/L \leq 3/4$ are statistical compatible, while data with $R/L = 6/7$ show significant deviations even for small W values. We safely fix $R = L/2$.

The **main panel** shows χ_ρ for $R = L/2$ (i.e. $R \ll L$) and different ratios W/R .

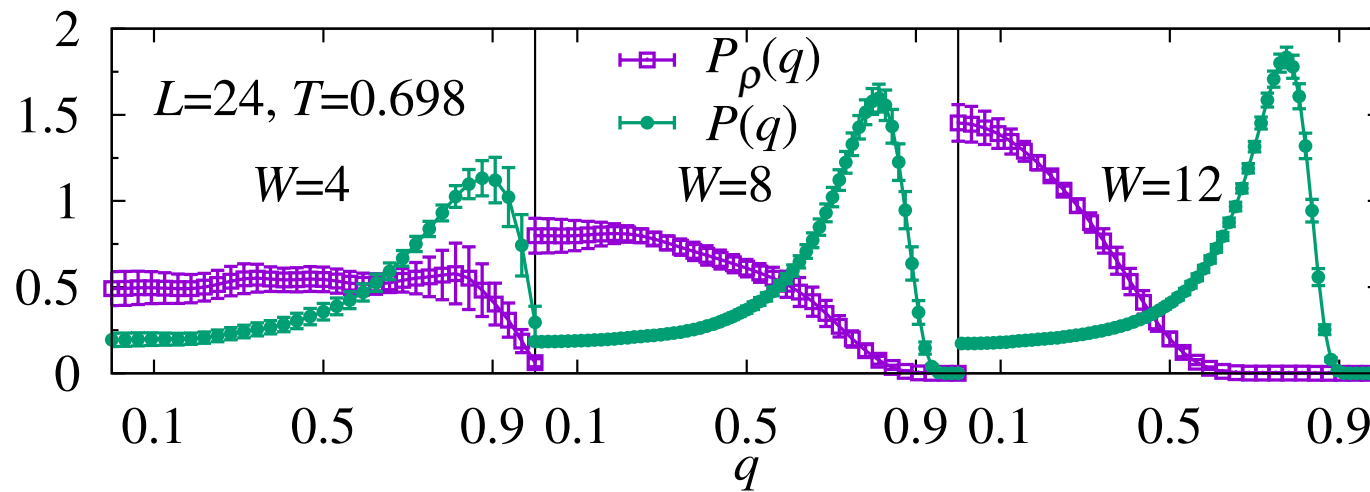
Data have been rescaled as

$$\chi_\rho(W, R) = R^\zeta f(W/R) ,$$

with $f(x) \propto x^\zeta$ for $x \ll 1$.

The physical behavior we expect in the limit $W/R \ll 1$ actually extends up to $W/R \approx 0.75$, where corrections to the asymptotic power law appear. Fitting data with $W/R < 0.75$ we estimate Read exponent

$$\zeta = 2.3 \pm 0.3$$



$P_\rho(q)$ and $P(q)$ for $L = 24$, $R = L/2$, $T = 0.698$ and different values of the measuring window size, $W = 4, 8, 12$.

These would be equal in a trivial metastate... (probably our strongest evidence towards a dispersed metastate).

State-of-the-art numerical simulations of spin glasses in $d = 3$ allow for the construction of the AW metastate.

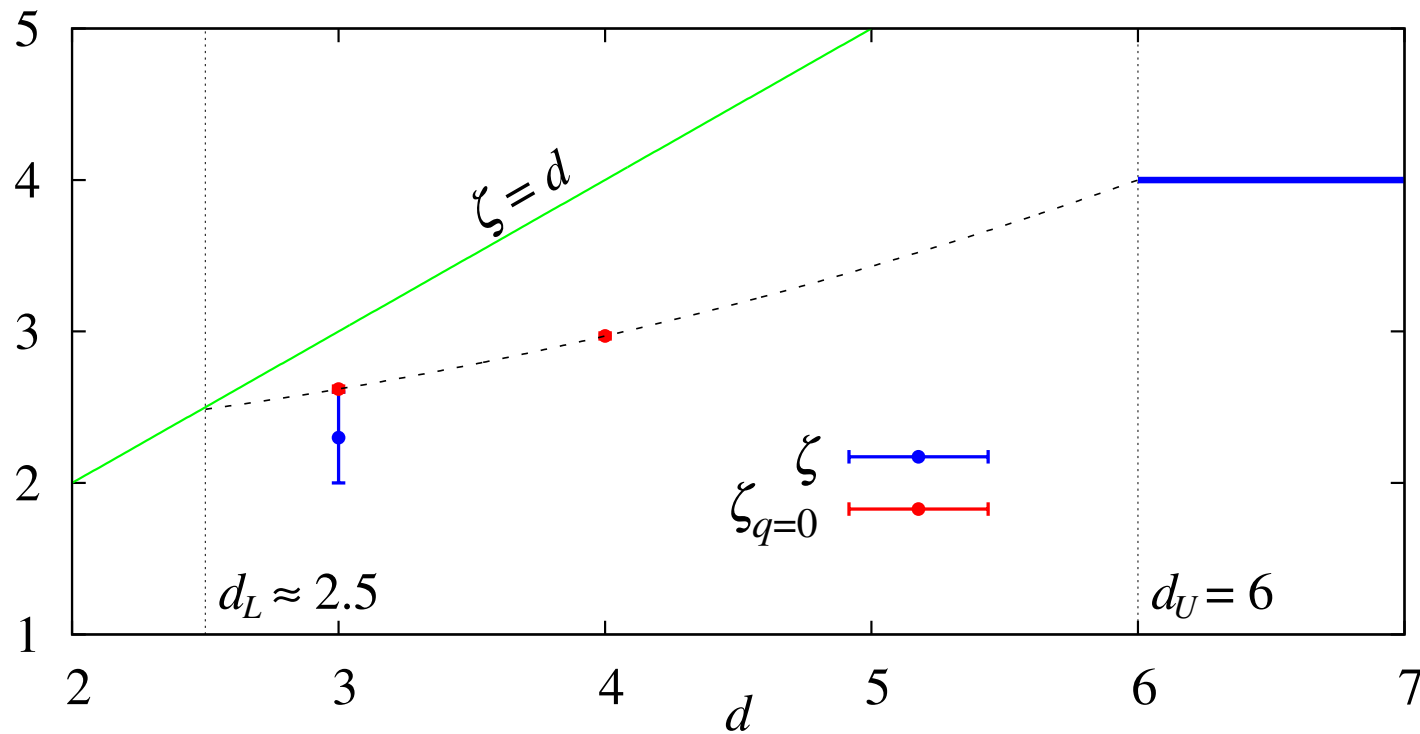
Numerical data suggest that the limiting conditions $1 \ll W \ll R \ll L$ can be implemented as $W/R, R/L \approx 3/4$.

From the numerical construction of the AW metastate we have obtained quantitative information on the nature of the spin glass phase in $d = 3$.

The metastate average overlap distribution $P(q)$ and the MAS $P_\rho(q)$ are significantly distinct objects already at moderate lattice sizes.

We cannot extrapolate safely to the thermodynamic limit, and sample to sample fluctuations are still important at the accessible system sizes.

We have exhibited a convincing scaling law for the MAS susceptibility, and an estimate of $\zeta(d = 3) = 2.3(3)$, suggesting $\zeta < d$.



The exponent ζ as a function of d .

The exponent ζ is related to the number of different states that can be measured in a system of size W as $\log n_{\text{states}} \sim W^{d-\zeta}$.

Such a number diverges in the thermodynamic limit as long as $\zeta < d$, supporting the picture of a metastate with infinitely many states.

In the figure we have summarized our knowledge about the ζ exponent.

At and above the upper critical dimension $d_U = 6$, where mean field exponents are correct, $\zeta = 4$.

Assuming $\zeta(d)$ is a continuous and monotonically non-decreasing function, the inequality $\zeta < d$ still holds slightly below d_U .

We have found $\zeta(d = 3) = 2.3(3)$.

An alternative estimate of the ζ exponent comes from the decay of the 4-spins spatial correlation function conditional to the $q = 0$ sector

$$C_4(x) = \overline{[\langle \sigma_0^{\mathbf{i};\mathbf{o}} \tau_0^{\mathbf{i};\mathbf{o}} \sigma_x^{\mathbf{i};\mathbf{o}} \tau_x^{\mathbf{i};\mathbf{o}} \rangle_{\Gamma|q_{\mathbf{i};\mathbf{o},\mathbf{o}}=0}]_{\kappa}} \sim |x|^{-(d-\zeta_{q=0})}$$

for $|x| \gg 1$: $\zeta_{q=0}(d=3) = 2.62(2)$ and $\zeta_{q=0}(d=4) = 2.97(2)$.

Read conjecture: $\zeta_{q=0} = \zeta$. These estimates are shown by red points.

A gentle interpolation of the ζ estimates (dashed line) seems to meet the $\zeta = d$ condition very close to the current best estimate for the lower critical dimension $d_L \approx 2.5$ (see for example Franz, Parisi and Virasoro 1994, Boettcher, PRL 2005, Maiorano and Parisi, 2017, arXiv:1711.05590, submitted to PNAS).

We have a new tool to analyze systems of very high complexity, like spin glasses.

Both quantitative and qualitative hints can be obtained.

A consistent picture emerges from this study.

Determination of ζ , shape of $P(q)$ and of the MAS averaged $P_\rho(q)$, $\zeta_{q=0}$.

What I believe is clear and important is the inherent high complexity of spin glass like systems.