The case for a three dimensional spin glass phase in presence of a magnetic field

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With Janus Collaboration (Zaragoza-Rome-Madrid-Ferrara-Extremadura)
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and
J. Stat. Mech. P05014 (2014)

Plan of the Talk

- What are spin glasses?
- Different Theories: Droplet/Scaling and RSB.
- Results for the one dimensional Edwards-Anderson (diluted) long range model in field. (see P. Young's talk)
- Experiments. (see R. Orbach's and P. Norblad's talks)
- The Janus' dedicated supercomputers (see V. Martín-Mayor's talk)

1. Janus results for $D = 4$ in a field.
2. Janus results for $D = 3$ in a field.
    - Dynamical studies (Equilibrium and out-of-equilibrium).
    - Thermodynamical studies.
3. Conclusions.

What are Spin glasses

- Materials with disorder and frustration.
- Quenched disorder (similar to the Born-Oppenheimer in Molecular Physics).
- 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).

Some equations

- Edwards-Anderson Hamiltonian:

$$\mathcal{H} = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j$$

J_{ij} are random quenched variables with zero mean and unit variance, $\sigma = \pm 1$ are Ising spins.

- The order parameter is:

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

Using two real replicas:

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

Let $q_i = \sigma_i\tau_i$ be the normal overlap, then: $q_{\mathrm{EA}} = \overline{\langle \sigma_i\tau_i \rangle}$.

Different Theories.

The Droplet/Scaling Theory.

- Based on the Migdal-Kadanoff implementation (approximate) of the Renormalization Group (exact in $D = 1$).
- *Disguised Ferromagnet*: Only two pure states with order parameter $\pm q_{\rm EA}$ (related by spin flip).
- Compact Excitations of fractal dimension d_f. The energy of a excitation of linear size L grows as L^θ. The free energy barriers (in the dynamics) grow as L^ψ. $\theta < (D-1)/2 < D-1 < d_f < D$ and $\psi \geq \theta$.
- Any amount of magnetic field destroys the spin glass phase (even for Heisenberg spin glasses).
- Trivial probability distributions of the overlaps (both normal overlap and link one).

Different Theories.

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. Phase transition in field: the de Almeida-Thouless line.
- The excitations of the ground state are space filling: e.g. the interface between two pure states is space filling.
- Overlap equivalence: All the definitions of the overlap are equivalent.

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 $|i - j| \to \infty$.

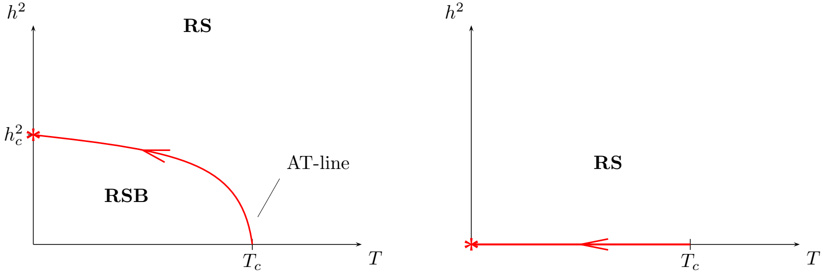
Different Theories: External Magnetic Field

RG from the paramagnetic phase:

1. The upper critical dimension in a field is still six (Bray and Moore).
2. Due to a dangerous irrelevant variable, some observables change behavior at eight dimensions (Fisher and Sompolinsky).
3. Projecting the theory (replicon mode) no fixed points were found (Bray and Roberts).
4. 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)
5. Temesvári is able to build the dAT slightly below $D = 6$ (but Bray and Moore, Temesvári and Parisi, Moore,...)

Different Theories: External Magnetic Field

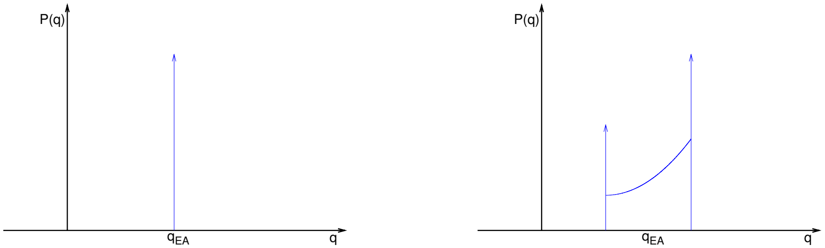
Renormalization group predictions (from Temesvári and Parisi):



(a) (b)

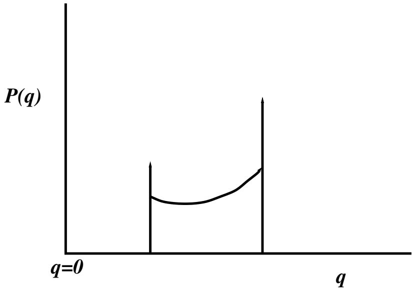
Different Theories: External Magnetic Field

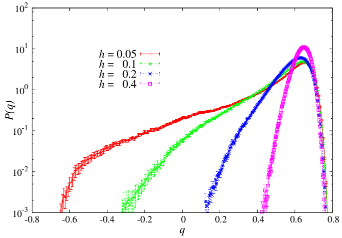
Different behavior of $P(q)$ in a magnetic field:



The negative overlap problem

- $P(q)$ in a magnetic field: SK results and numerical ones.





- The negative overlap region induces large corrections in $\tilde{G}(0)$!!

The correlation length

- Correlation Functions ($D = 4$): The replicon Propagator:

$$
\begin{aligned}
G_1(\boldsymbol{r}) &= \frac{1}{L^4} \sum_{\boldsymbol{x}} \overline{\left(\langle S_{\boldsymbol{x}} S_{\boldsymbol{x}+\boldsymbol{r}} \rangle - \langle S_{\boldsymbol{x}} \rangle \langle S_{\boldsymbol{x}+\boldsymbol{r}} \rangle \right)^2}, \\
G_2(\boldsymbol{r}) &= \frac{1}{L^4} \sum_{\boldsymbol{x}} \overline{\left(\langle S_{\boldsymbol{x}} S_{\boldsymbol{x}+\boldsymbol{r}} \rangle^2 - \langle S_{\boldsymbol{x}} \rangle^2 \langle S_{\boldsymbol{x}+\boldsymbol{r}} \rangle^2 \right)}.
\end{aligned}
$$

- Correlation Length:

$$
\xi_2 = \frac{1}{2 \sin(\pi/L)} \left(\frac{\hat{G}(0)}{\hat{G}(\boldsymbol{k}_1)} - 1 \right)^{1/2},
$$

where $\boldsymbol{k}_1 = (2\pi/L, 0, 0, 0)$ (and three perm.)

Numerical Analysis of the Correlation function

- We will avoid the $k = 0$ value by fitting ($k > 0$):

$$\left(\frac{1}{\tilde{G}(k)}\right)^{\mathrm{fit}} = A(L,T) + B(L,T)[\sin(k/2)]^2$$

- We can analyze the L and T dependence of

$$A(L,T) \equiv \lim_{k \to 0} \frac{1}{\tilde{G}(k)}$$

- We fix the L-dependent critical temperature by means:

$$A(L, T_c(L)) = 0$$

A new observable R_{12}

- R_{12}:

$$R_{12} = \frac{\hat{G}(\boldsymbol{k}_1)}{\hat{G}(\boldsymbol{k}_2)},$$

  where $\boldsymbol{k}_1 = (2\pi/L, 0, 0, 0)$, $\boldsymbol{k}_2 = (2\pi/L, 2\pi/L, 0, 0)$ (and permutations)
- We have checked the behavior of this observable in the EA model in $D = 3$ and $D = 4$ ($h = 0$).
- And in the two dimensional (ordered) Ising model. We have been able to compute its value at criticality using Conformal Field Theory:

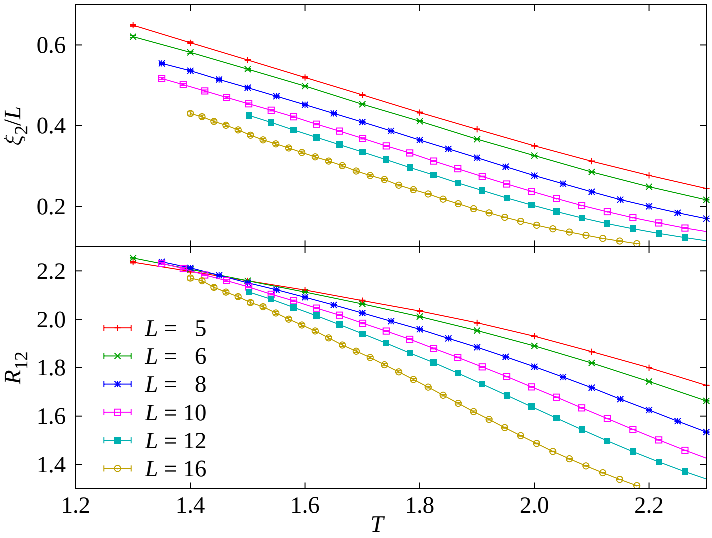
$$R_{12} = 1.694\ 024...$$

- In a paramagnetic phase, for large L: $R_{12} \to 1$.

$D = 4$ $(h \neq 0)$

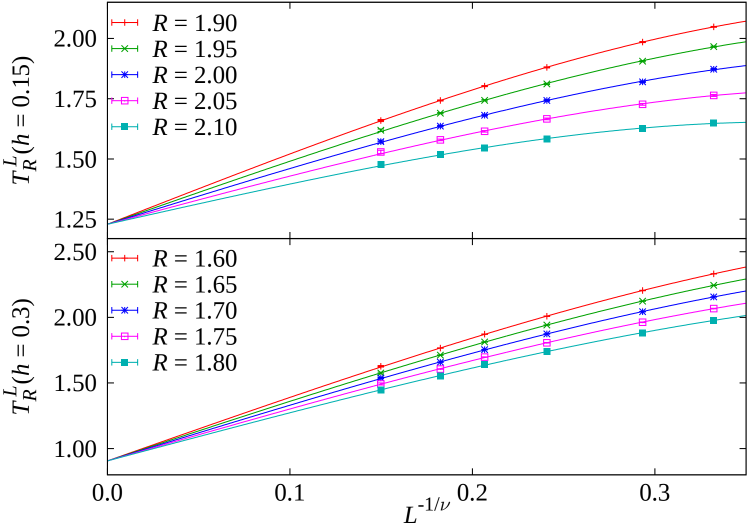
- We have simulated using the JANUS computer.
- $L = 5, 6, 8, 10, 12$ and 16.
- Three (uniform) magnetic Fields: $h = 0.075, 0.150$ and 0.3.
- Parallel Tempering in Temperature (e.g. 32 temperatures in $L = 16$)
- Single sample thermalization protocol.
- We avoid the mode $\boldsymbol{k} = 0$ in the analysis.

$D = 4$ $(h = 0.15)$

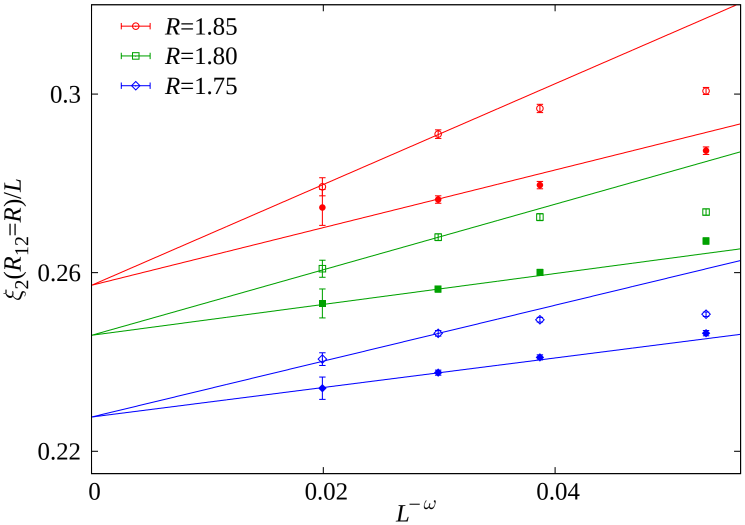


0.6
0.4
0.2
ξ_2/L
2.2
2.0
1.8
1.6
1.4
R_{12}
$L = 5$
$L = 6$
$L = 8$
$L = 10$
$L = 12$
$L = 16$
1.2
1.4
1.6
1.8
2.0
2.2
T

$D = 4$ $(h \neq 0)$: Critical exponents



$D = 4$ ($h \neq 0$): Corrections to scaling



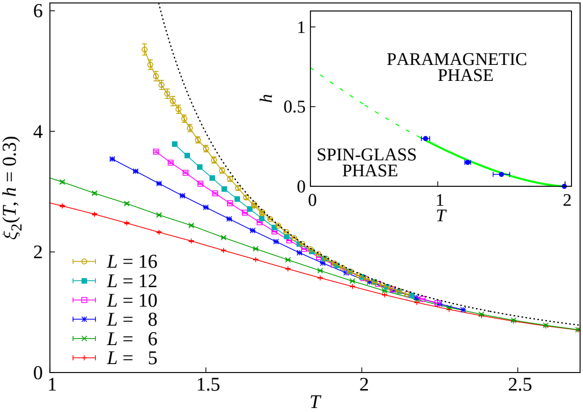
$D = 4$ $(h \neq 0)$: Critical exponents

Parameter	$h = 0.3$	$h = 0.15$	$h = 0.075$
$T_\mathrm{c}(h)$	0.906(40)[3]	1.229(30)[2]	1.50(7)
ν	1.46(7)[6]		—
η	−0.30(4)[1]		—
ω	1.43(37)		—

For reference $(h = 0)$:

$T_c^{(0)} = 2.03(3)$, $\nu^{(0)} = 1.025(15)$, $\eta^{(0)} = -0.275(25)$

$D = 4$ $(h \neq 0)$: Summary



Fisher-Sompolinsky relation: $h^2(T) \simeq A|T - T_c^{(0)}|^{\beta^{(0)}+\gamma^{(0)}}$

Dynamics $D = 3$ ($h \neq 0$)

- We have simulated using the JANUS computer.
- $L = 80$.
- Gaussian magnetic Fields (using Gauss-Hermite quadrature).
- Dynamical Studies (Fast and Slow annealing procedures):
  - Equilibrium dynamical studies in the high temperature region.
  - Out-of-equilibrium studies for the lower temperatures.

Dynamics $D = 3$ $(h \neq 0)$

Observables:

- $q_{\boldsymbol{x}}(t) = \sigma_{\boldsymbol{x}}^{(1)}(t)\sigma_{\boldsymbol{x}}^{(2)}(t)$
- $q(t) = \frac{1}{V}\overline{\sum_{\boldsymbol{x}} q_{\boldsymbol{x}(t)}}$
- $E_{\mathrm{mag}}(t) = \frac{1}{V}\overline{\sum_{\boldsymbol{x}} h_{\boldsymbol{x}}\sigma_{\boldsymbol{x}}(t)}$
- $W(t) = 1 - TE_{\mathrm{mag}}(t)/H^2$
- $W = \overline{\langle q \rangle}$

- Droplet prediction: $W = q_{\mathrm{EA}}$ and $q(t) \to q_{\mathrm{EA}}$, so

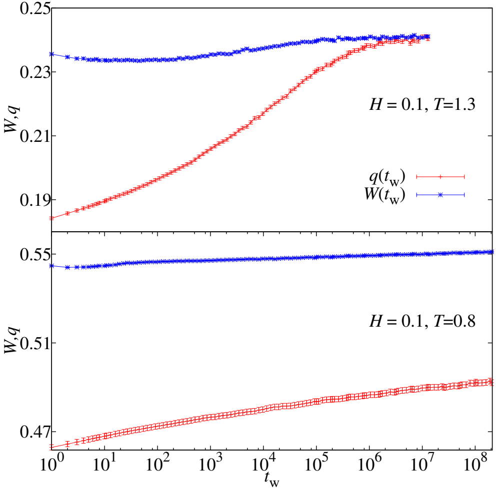
$$W - q \to 0$$

- RSB prediction, SG phase: $W = \overline{\langle q \rangle}$ and $q(t) \to q_{\mathrm{min}}$, so

$$q - W \to \overline{\langle q \rangle} - q_{\mathrm{min}} > 0$$

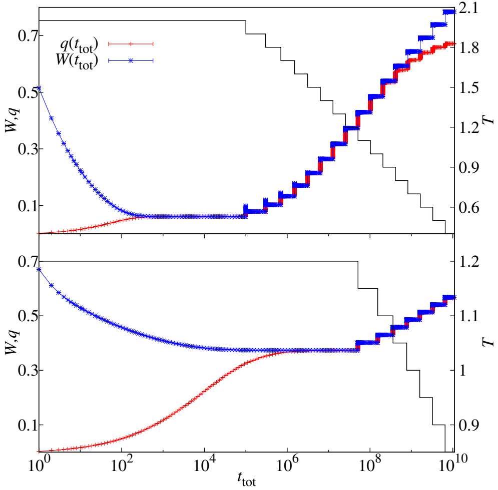
Dynamics $D = 3$ $(h \neq 0)$

Equilibrium and out-of-equilibrium regimes:

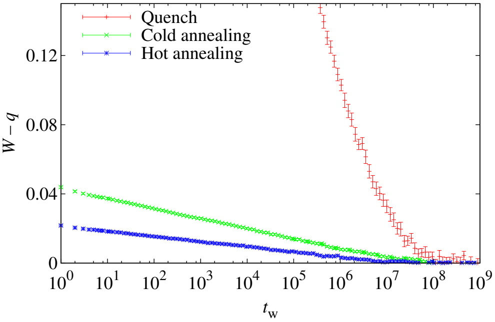


Dynamics $D = 3$ ($h \neq 0$)

Hot (high T region) and Cold annealing (low T region):



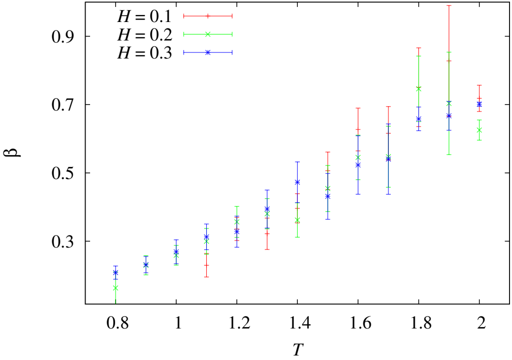
Dynamics $D = 3$ ($h \neq 0$): Comparison among the annealing protocols



Dynamics $D = 3$ $(h \neq 0)$

The equilibrium data (obtained at high T) follow a stretched exponential behavior:

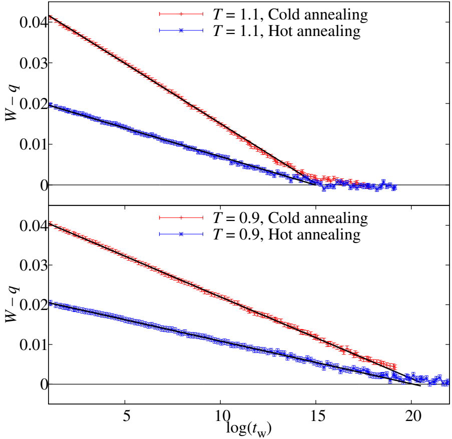
$$W - q = \frac{b}{t^x} \exp\left[-\left(t/\tau'\right)^{\beta}\right]$$



Caveat: Only for $\beta = 1$, τ' is a correlation time (τ).

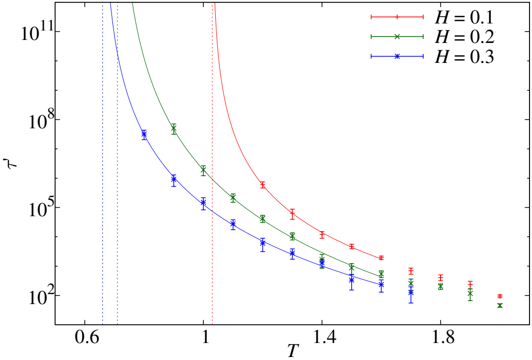
Dynamics $D = 3$ $(h \neq 0)$: A phenomenological approach for τ (τ'')

$$W(t_w) - q(t_w) \simeq A \left[1 - \frac{\log t_w}{\log \tau''} \right] \, , \; t_w < \tau''$$



Dynamics $D = 3$ ($h \neq 0$)

Analysis of τ':



On a Second Order Phase Transition:

$$\tau = \tau_0 (T - T_c)(H))^{-\nu z}$$

Dynamics $D = 3$ $(h \neq 0)$

Analysis of τ' and τ'':

- $H = 0.1$: $T_c^{\text{high}} = 1.03(7)$ and $z\nu = 4.8(1.1)$. $T_c^{\text{high}} = 0.98(3)$ and $z\nu = 7.2(5)$.
- $H = 0.2$: $T_c^{\text{high}} = 0.71(6)$ and $z\nu = 7.5(1.1)$. $T_c^{\text{high}} = 0.670(21)$ and $z\nu = 9.2(4)$.
- $H = 0.3$: $T_c^{\text{high}} = 0.66(5)$ and $z\nu = 6.2(9)$. $T_c^{\text{high}} = 0.614(17)$ and $z\nu = 8.4(4)$.

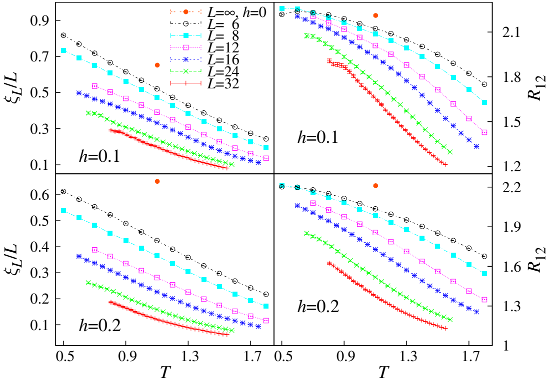
Remember $T_c(H = 0) = 1.109(10)$.

Dynamics $D = 3$ $(h \neq 0)$

Scenarios:

- RSB with a non zero magnetic field fixed point: critical dynamics for τ'.
- RSB with a zero magnetic field fixed point: activated dynamics for τ'.
- A dynamical transition at which "apparently" diverges τ' and then a thermodynamical phase transition (RSB?) (Mode Coupling Theory, supercooled liquids).
- A $T = 0$ phase transition.
- Our data do not follow the droplet predictions.

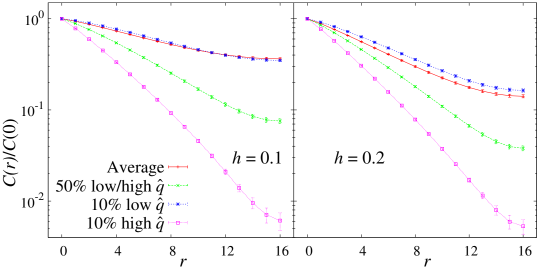
Spin Glass behavior in $D = 3$ ($h \neq 0$)?



No signal of a phase transition in the ξ_L/L and R_{12}-channels! [also see T. Jörg et al.]

The *fauna* of measurements $D = 3$ $(h \neq 0)$?

Study of the point-to-plane correlation function $C(r)$:



1. Average over all the data only describe the behavior of a small fraction of the data.
2. We develop an approach to classify the measurements in terms of a conditioning variate.

Conditioning variates.

- In the SK model, the negative overlap tail of $P(q)$ is due to a small number of samples [Parisi-Ricci-Tersenghi].
- Instead, in order to avoid bias and gain statistics, we work with measurements not with individual samples.
- For a Gaussian h, we need only two replicas to compute the replicon (and we have only one overlap).
  1. We can classify the measurements using q (as done alredy in the past, e.g. $G(r|q)$).
  2. However, we are simulating constant h, and we need four replicas and we can compute 6 different overlaps.

Conditioning variates.

The conditional expectation value is defined as the average of $\mathcal{O}$, restricted to the measurements i (out of the $\mathcal{N}_\mathrm{m} = N_\mathrm{t} N_\mathrm{samples}$ total measurements) that simultaneously yield $\mathcal{O}_i$ and $\hat{q}_i$ in a small interval around $\hat{q} = c$,

$$E(\mathcal{O}|\hat{q} = c) \;=\; \frac{E\left[\mathcal{O}_i \mathcal{X}_{\hat{q}=c}(\hat{q}_i)\right]}{E\left[\mathcal{X}_{\hat{q}=c}(\hat{q}_i)\right]} \,.$$

Where we have used the characteristic function

$$\mathcal{X}_c(\hat{q}_i) = \begin{cases} 1, & \text{if } |c - \hat{q}_i| < \epsilon \sim \frac{1}{\sqrt{V}} \\ 0, & \text{otherwise.} \end{cases}$$

$$E(\mathcal{O}) = \int \mathrm{d}\hat{q}\; E(\mathcal{O}|\hat{q}) P(\hat{q}) \quad , \quad P(\hat{q}) = E[\mathcal{X}_{\hat{q}}] \,,$$

where $P(\hat{q})$ is the probability distribution function of the conditioning variate.

Conditioning variates.

- We have simulated $N_{\rm samples}$ samples and taken N_t measurements on each sample: So we have $N_m = N_t N_{\rm samples}$ *total* measurements.
- On each measurements (out of N_m) we have computed 6 different overlaps (we are simulating 4 replicas!).
- We can sort the six overlaps as:

$$\left\{q^{(ab)}, q^{(ac)}, q^{(ad)}, q^{(bc)}, q^{(bd)}, q^{(cd)}\right\} \longrightarrow \{q_1 \leq q_2 \leq q_3 \leq q_4 \leq q_5 \leq q_6\}$$

- We can propose the following conditioning variates:

$$\hat{q} = \begin{cases} q_{\rm min} & = q_1 \qquad \text{(the minimum)} \\ q_{\rm max} & = q_6 \qquad \text{(the maximum)} \\ q_{\rm med} & = \frac{1}{2}(q_3 + q_4) \qquad \text{(the median)} \\ q_{\rm av} & = \frac{1}{6}(q_1 + q_2 + q_3 + q_4 + q_5 + q_6) \qquad \text{(the average)}\,. \end{cases}$$

- For Gaussian h, we have only one option, the usual overlap q.

Selection of the Conditioning variate.

$$\mathrm{var}(\mathcal{O}) = c_1 + c_2,$$

where we defined

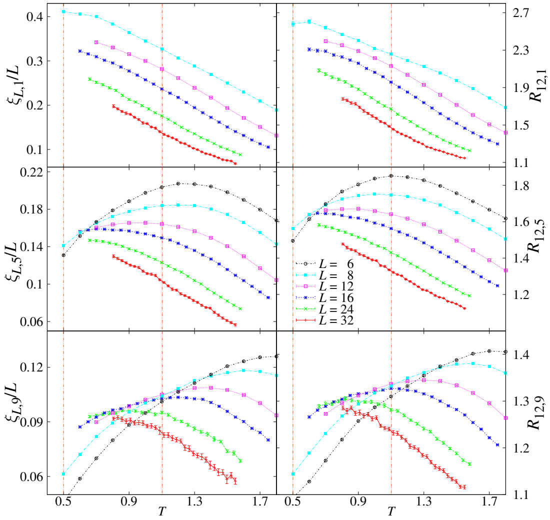
$$\begin{aligned} c_1 &\equiv \int_{-1}^{1} \mathrm{d}\hat{q}\, P(\hat{q}) \mathrm{var}(\mathcal{O}|\hat{q}) \quad , \qquad \mathrm{var}(\mathcal{O}|\hat{q}) = E([\mathcal{O} - E(\mathcal{O}|\hat{q})]^2 \mid \hat{q})\,, \\ c_2 &\equiv \int_{-1}^{1} \mathrm{d}\hat{q}\, P(\hat{q}) [E(\mathcal{O}) - E(\mathcal{O}|\hat{q})]^2\,. \end{aligned}$$

Remember: $c_1 + c_2$ is fixed!
A useful conditioning variate should have $c_2 \gg c_1$.

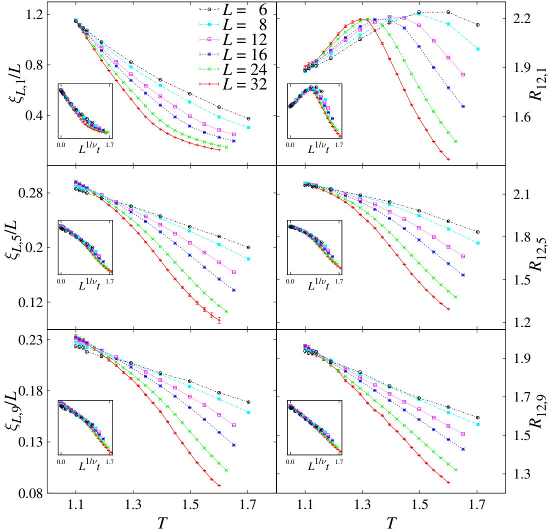
1. If $c_1 = 0$ the fluctuations of $\mathcal{O}$ would be explained solely by the fluctuations of $\hat{q}$: So c_2 is large.
2. Otherwise, if $c_2 = 0$, then $E(\mathcal{O}) = E(\mathcal{O}|\hat{q})$, and $\hat{q}$ is irrelevant!.

$\hat{q}$	c_1	c_2	c_2/c_1
q_{min}	399000 ± 37000	121000 ± 15000	0.30(6)
q_{max}	514000 ± 51000	6230 ± 690	0.012(3)
q_{med}	162000 ± 10000	358000 ± 45000	2.2(4)
q_{av}	328000 ± 26000	192000 ± 28000	0.6(1)

Quantile analysis in $D = 3$ ($h = 0.2$)



Test: Quantile analysis in $h = 0$



Conclusions

1. We have shown strong numerical evidences which support a dAT line below the upper critical dimension:
   - In $D = 4$ for the EA model.
2. However the situation in $D = 3$ dimensions is not yet clear:
   - Equilibrium dynamics (high T) shows a **diverging time at a finite temperature.**
   - Out of equilibrium dynamics (low T) can be explained with RSB.
   - Yet, another theoretical scenarios can explain the behavior of the numerical data.
   - Quantile analysis (equilibrium) shows traces of a phase transition.
   - But, will this picture (quantiles) survive for larger lattice sizes?
   - **Maybe Janus-II will be able to provide the solution!**