On the complex behavior of disordered models in a field

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SISSA seminar, March 13th, 2018

Talk outline

- Large scale numerical simulations for finite dimensional spin glasses in a field [with L. Leuzzi, G. Parisi, J. Ruiz-Lorenzo and the Janus Collaboration]

- Analytic solutions for disordered models with external fields on random graphs [with F. Morone and G. Perugini]

Disordered models in a field have a
complex paramagnetic phase
Extracting the right critical behavior is not easy

Models definition

$$\mathcal{H}(\boldsymbol{s}) = -\sum_{(ij)\in E} J_{ij} s_i s_j - \sum_i H_i s_i \qquad s_i \in \{-1, 1\}$$

(Ising spins)

- Spin glass models in a field
  - random couplings $J_{ij} \in \{-1, 1\}$, $J_{ij} \sim \mathcal{N}(0, 1)$
  - constant field $H_i = H$
- Random field Ising models
  - ferromagnetic couplings $J_{ij} = J$
  - random field $H_i \sim \mathcal{N}(0, H^2)$

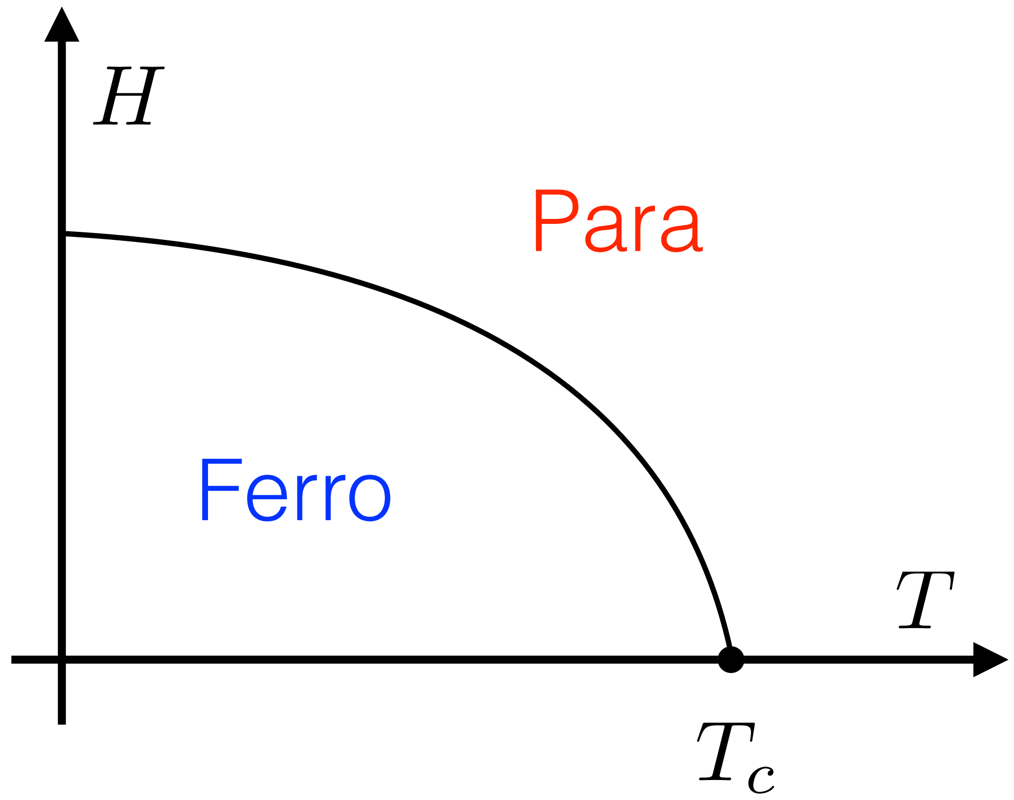
Models definition

$$\mathcal{H}(\boldsymbol{s}) = -\sum_{(ij)\in E} J_{ij} s_i s_j - \sum_i H_i s_i$$

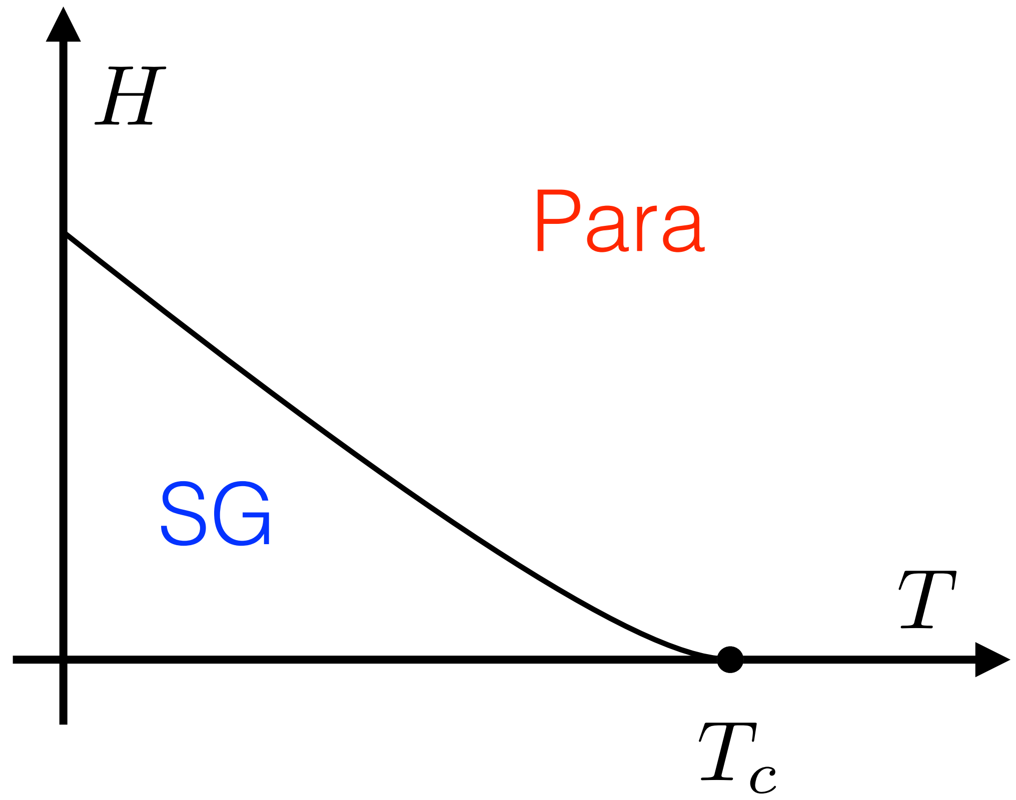
- Different topologies (edge set E)
  - Finite dimensional regular lattices (mainly d=3,4) with short range (i.e. nearest neighbor) interactions
  - d=1 chain with long range interactions (mimics any d)
  - sparse random graphs (with Poisson or regular degrees)
- All have finite mean degree and constant couplings

Qualitative phase diagram

RFIM

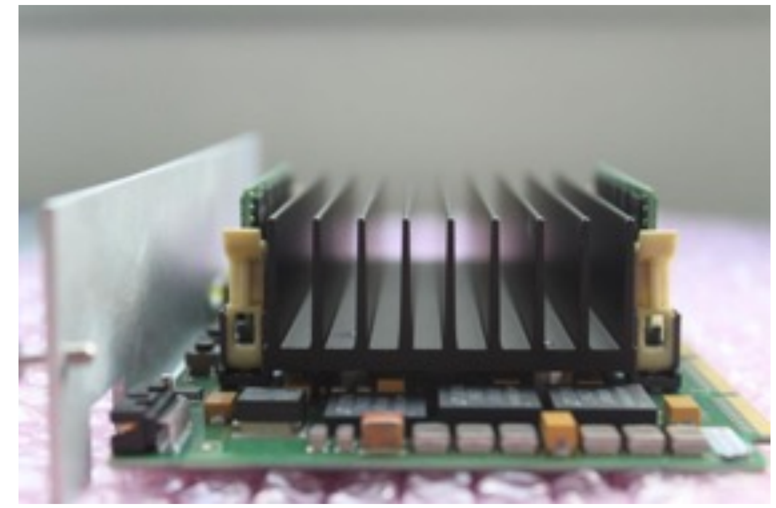


SG in field



Spin glasses in finite dimensions

Janus Collaboration
(Zaragoza, Madrid, Badajoz, Ferrara and Rome)



http://www.janus-computer.com/

- Reconfigurable FPGA-based special purpose computer to simulate finite-dimensional spin glasses (d=3,4 up to now)

- Thermodynamics
  Can thermalize tens of thousands of samples of sizes up to
  L=40 in d=3 [PRB 88 (2013) 224416]
  L=16 in d=4 [PNAS 109 (2012) 6452]

- Dynamics
  In d=3 systems of size L=160
  for times up to 10^{11} MCS [PNAS 114 (2017) 1838]

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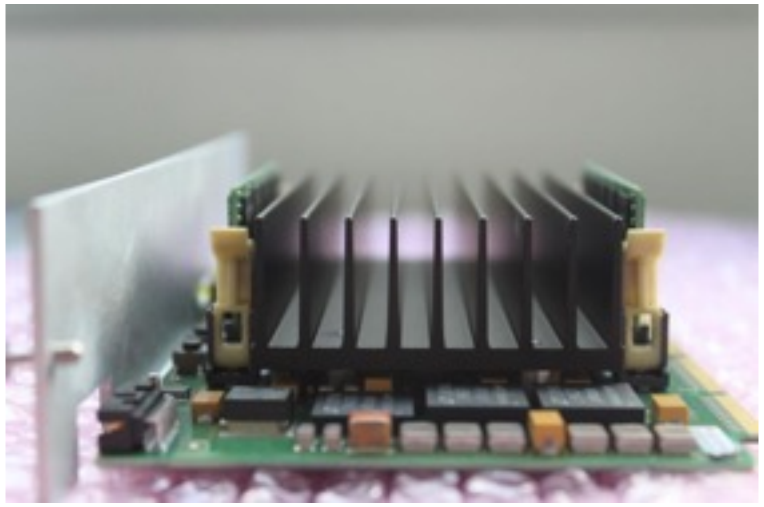

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- Dynamics
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  for times up to 10^{11} MCS [PNAS 114 (2017) 1838]

Approaching experimental time scales!!

Observables

- Spatial correlation function

$$G(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{x}} \overline{(\langle s_{\boldsymbol{x}} s_{\boldsymbol{x}+r}\rangle - \langle s_{\boldsymbol{x}}\rangle\langle s_{\boldsymbol{x}+r}\rangle)^2}$$ (replicon propagator)

- Fourier transform $\hat{G}(\boldsymbol{k}) = \mathrm{FT}[G(\boldsymbol{r})]$
  - Spin glass susceptibility $\chi_{\mathrm{SG}} = \hat{G}(\mathbf{0})$
  - Second-moment correlation length

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

Observables

- In the paramagnetic phase ($T > T_c$)

$$\lim_{L\to\infty} \xi(T,L) = \xi_{\mathrm{eq}}(T) \qquad \lim_{L\to\infty} \frac{\xi(T,L)}{L} = 0$$

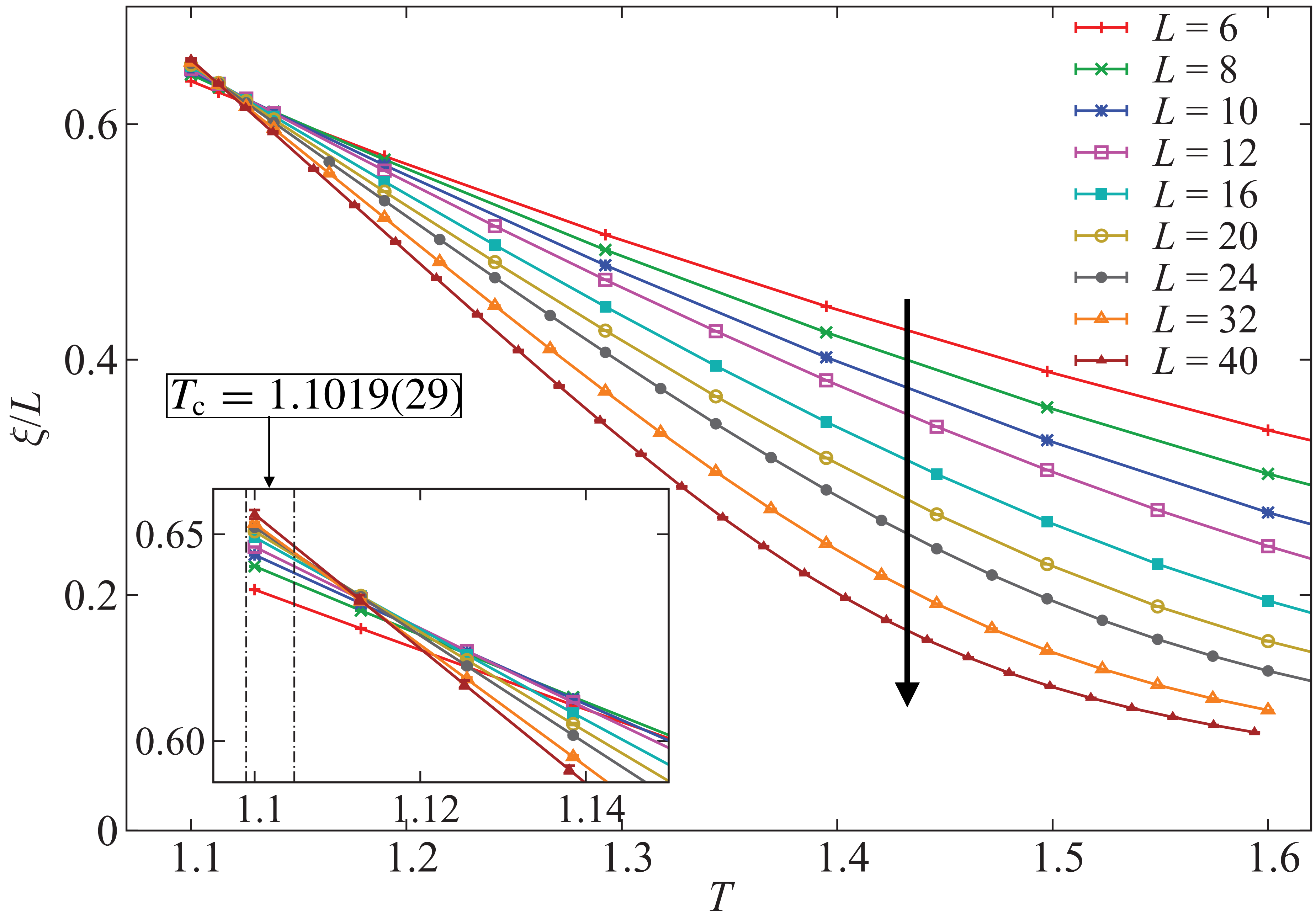
- At the critical point many scaling invariants

$$\frac{\xi(T_c,L)}{L}\ , \quad R_{12} = \frac{\hat{G}(\boldsymbol{k}_1)}{\hat{G}(\boldsymbol{k}_2)}\ , \quad \ldots$$

$$\boldsymbol{k}_1 = \left(\frac{2\pi}{L}, 0, 0\right) \quad \boldsymbol{k}_2 = \left(\frac{2\pi}{L}, \pm\frac{2\pi}{L}, 0\right)$$

d=3 spin glass (H=0)

[PRB 88 (2013) 224416]



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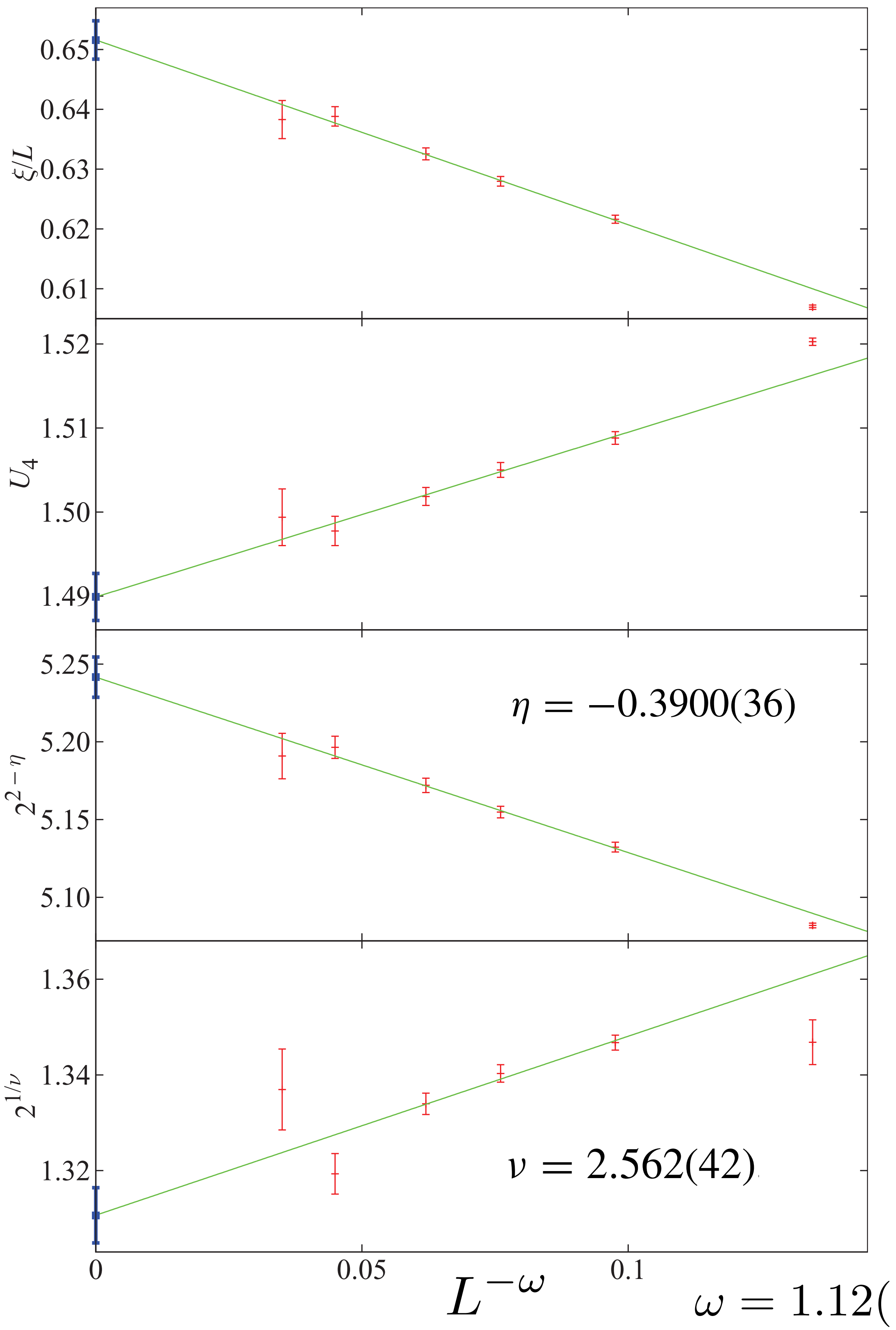
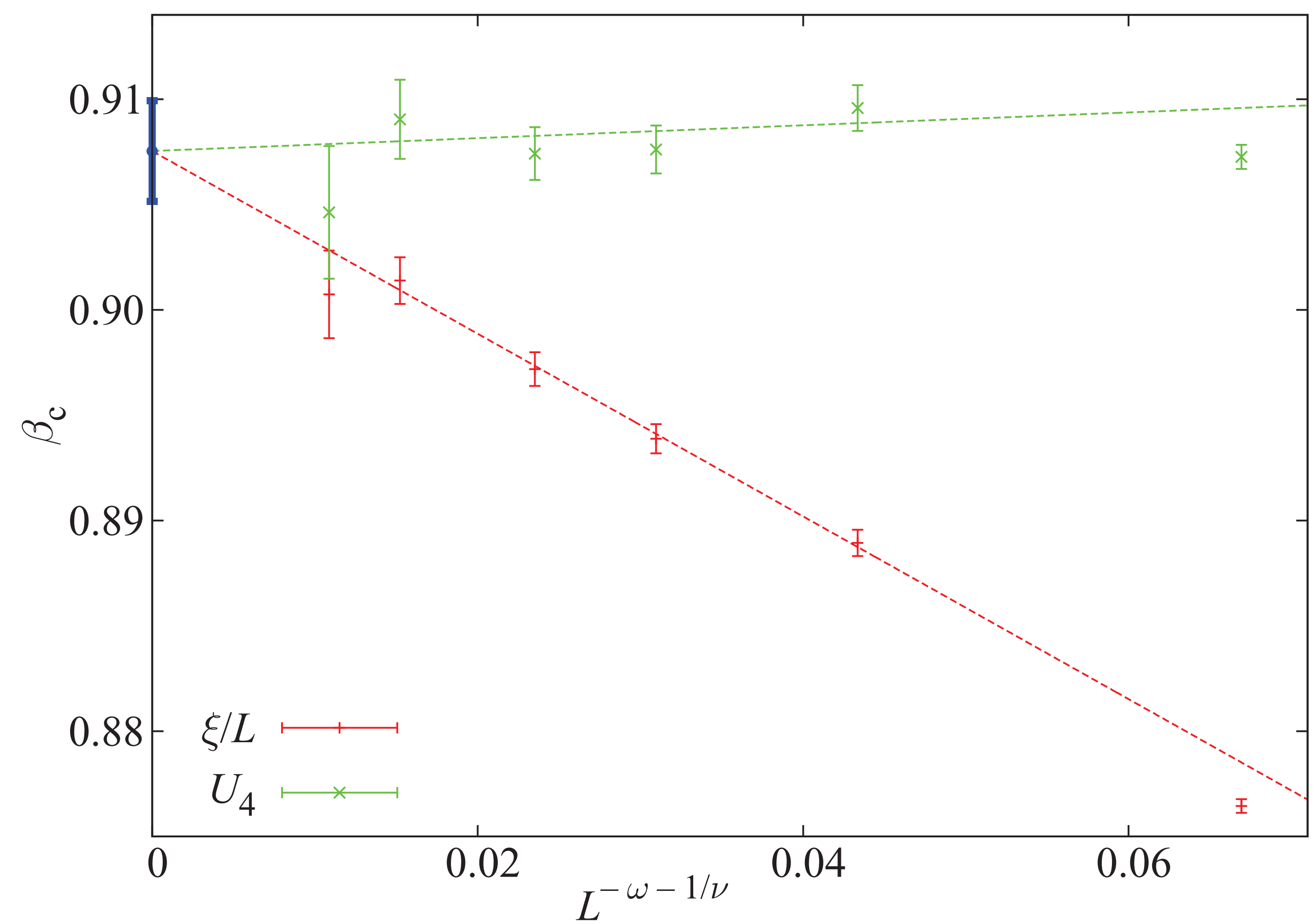


$\omega = 1.12(10)$

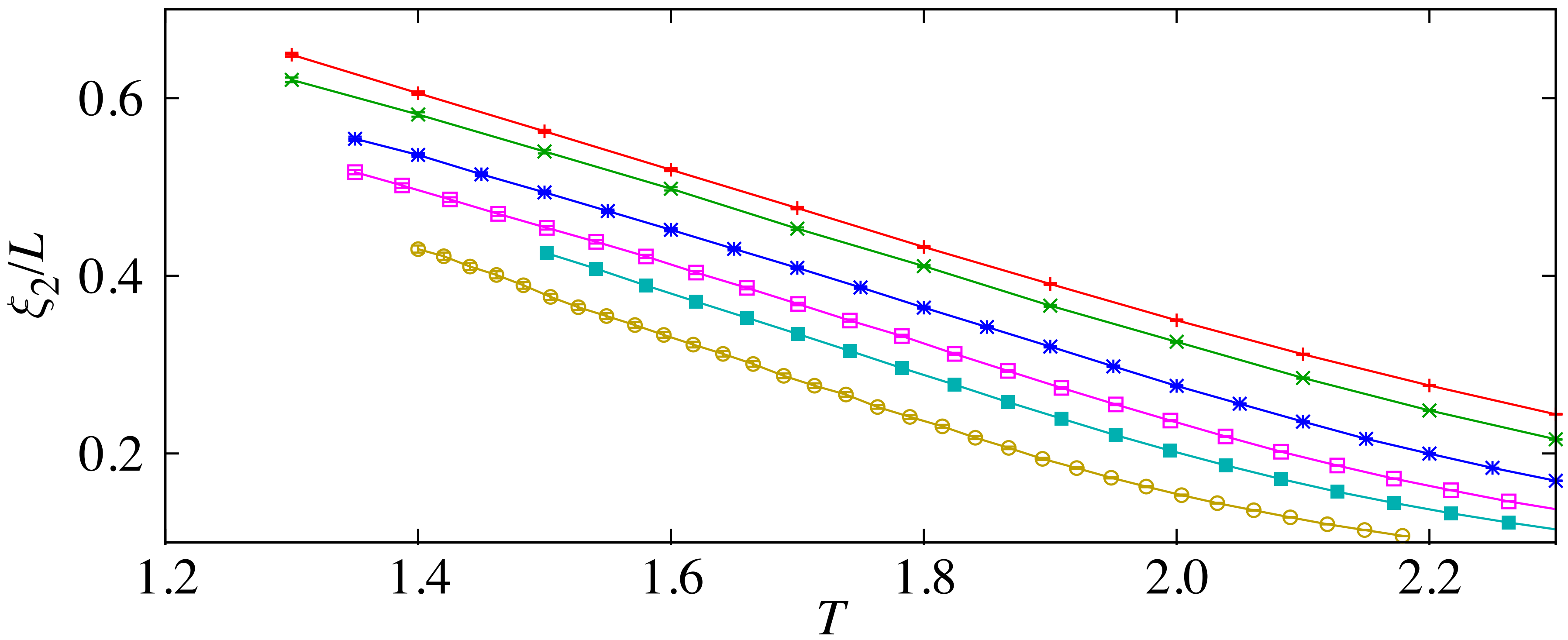
[PRB 88 (2013) 224416]

Corrections to scaling
are important



d=4 spin glass in field (H=0.15)

[PNAS 109 (2012) 6452]



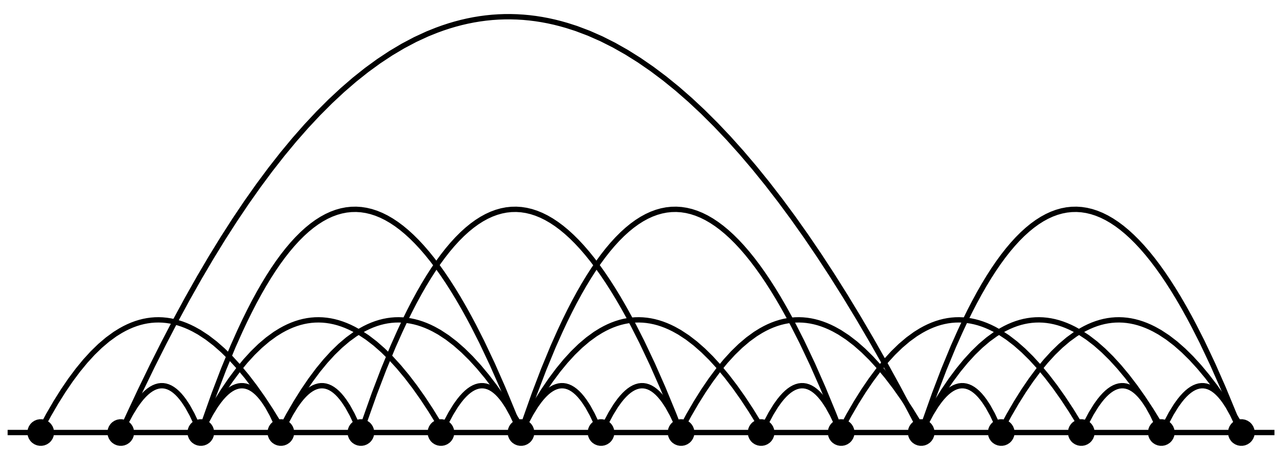
Evidence for lack of phase transition
in spin glasses with external field?!

Sparse d=1 long range model

[PRL 101 (2008) 107203]

$\mathbb{P}[J_{ij} \neq 0] \propto |i-j|^{-\rho}$

constant mean degree
and $J_{ij} = O(1)$



simulation times
are linear in N

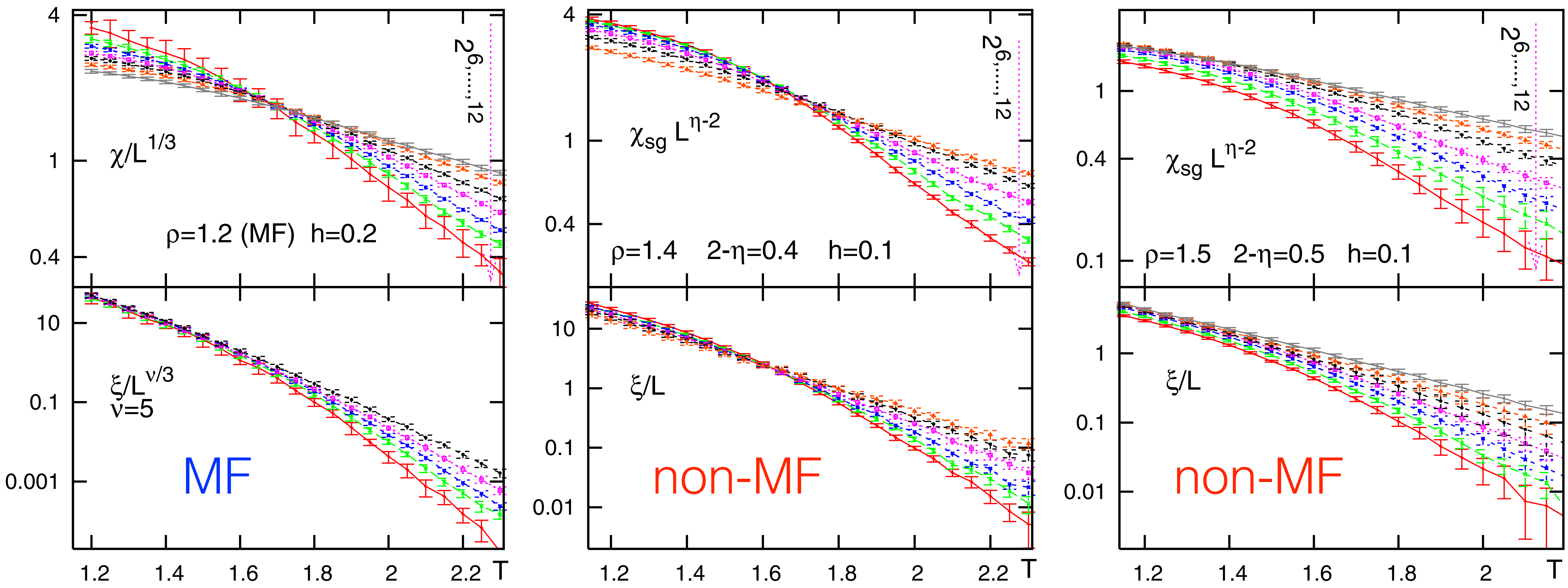
$$d_{\text{eff}} \simeq \frac{2}{\rho - 1}$$

MF non-MF no phase trans.

$\rho_{\text{U}} = 4/3$ ρ

d=1 long range SG model with field

[PRL 103 (2009) 267201]



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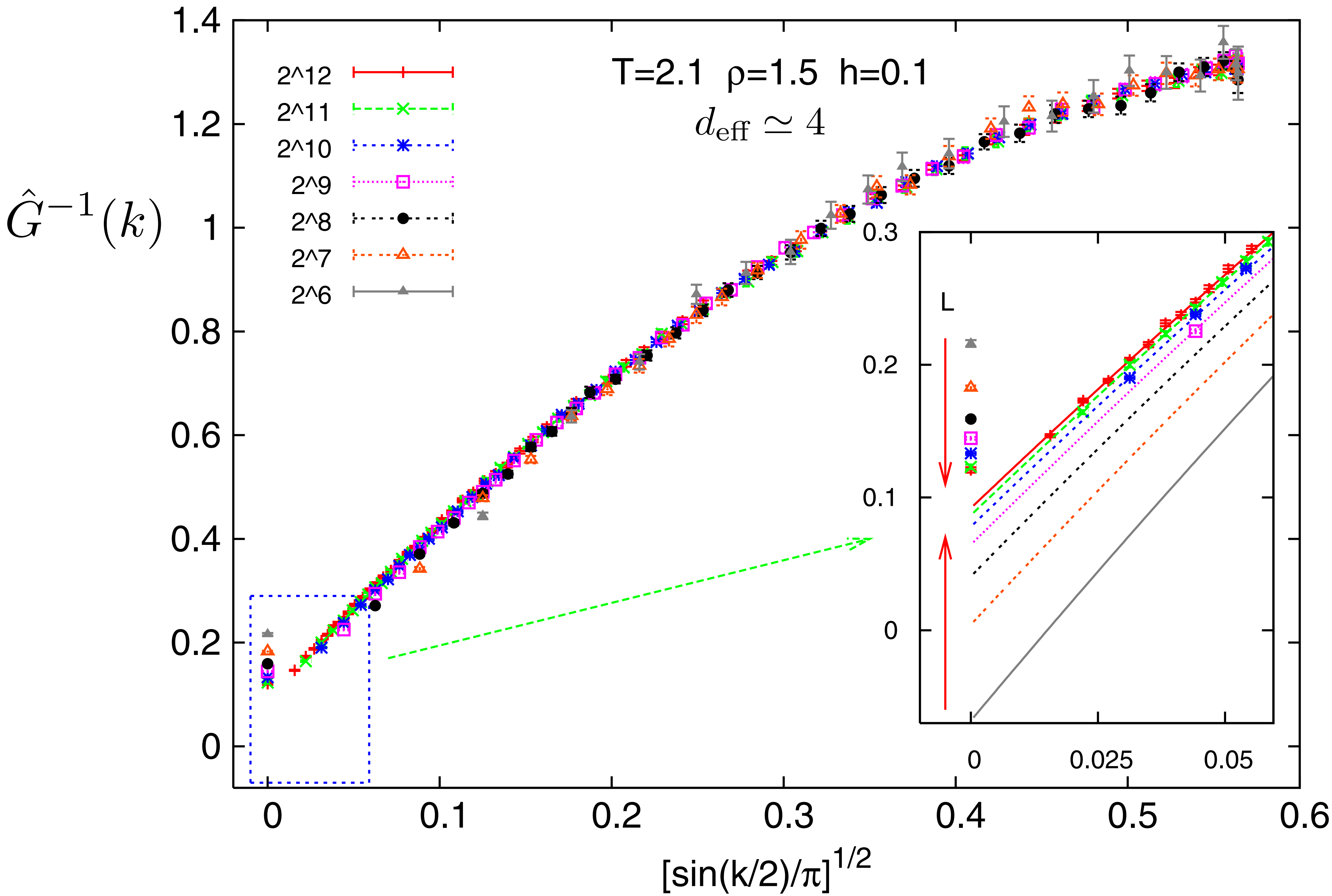

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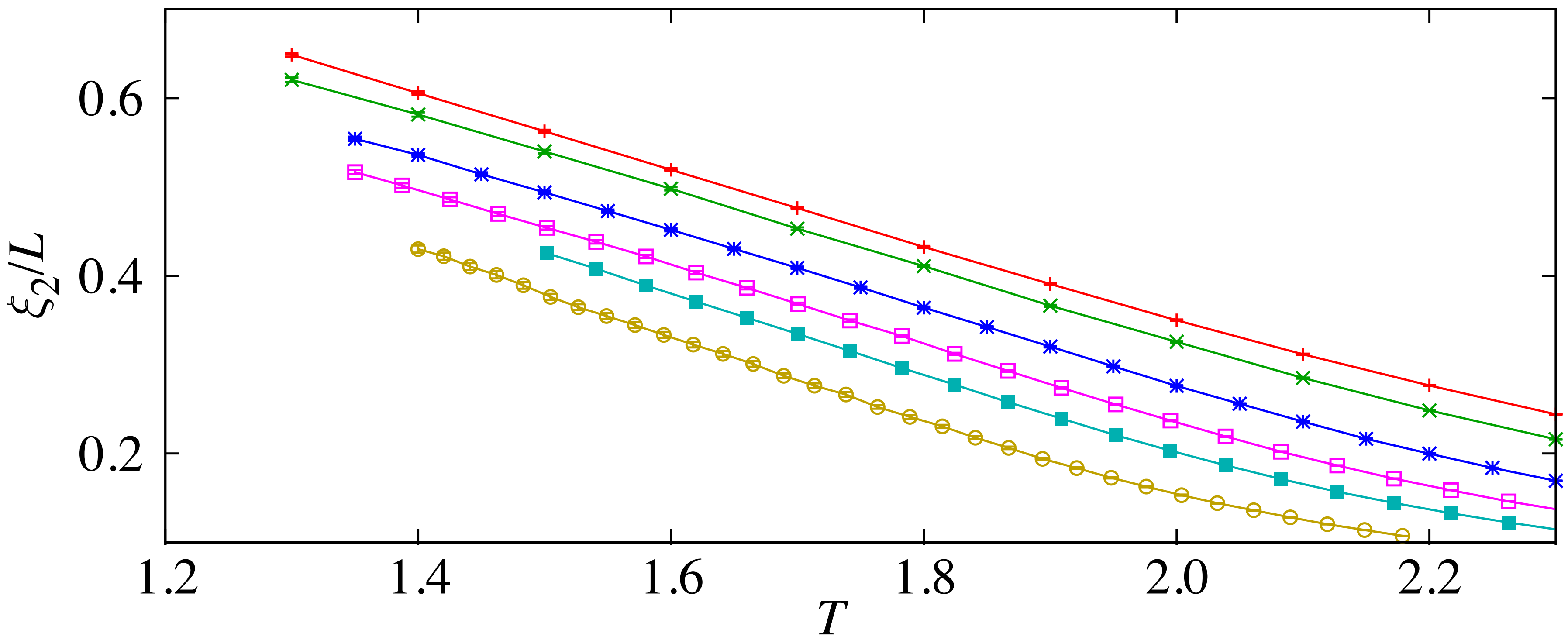

Evidence for lack of phase transition
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Not really!

d=4 spin glass in field (H=0.15)

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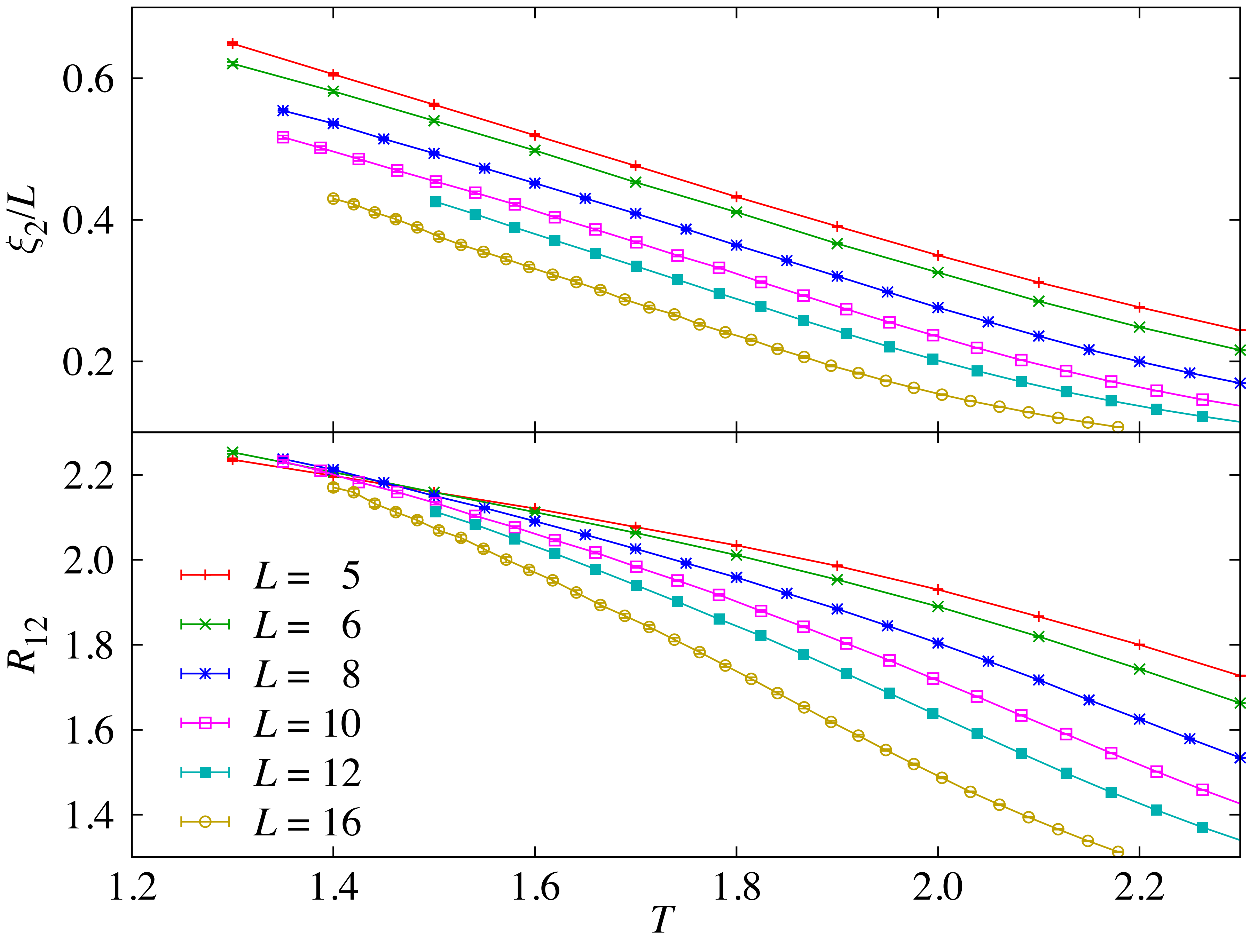
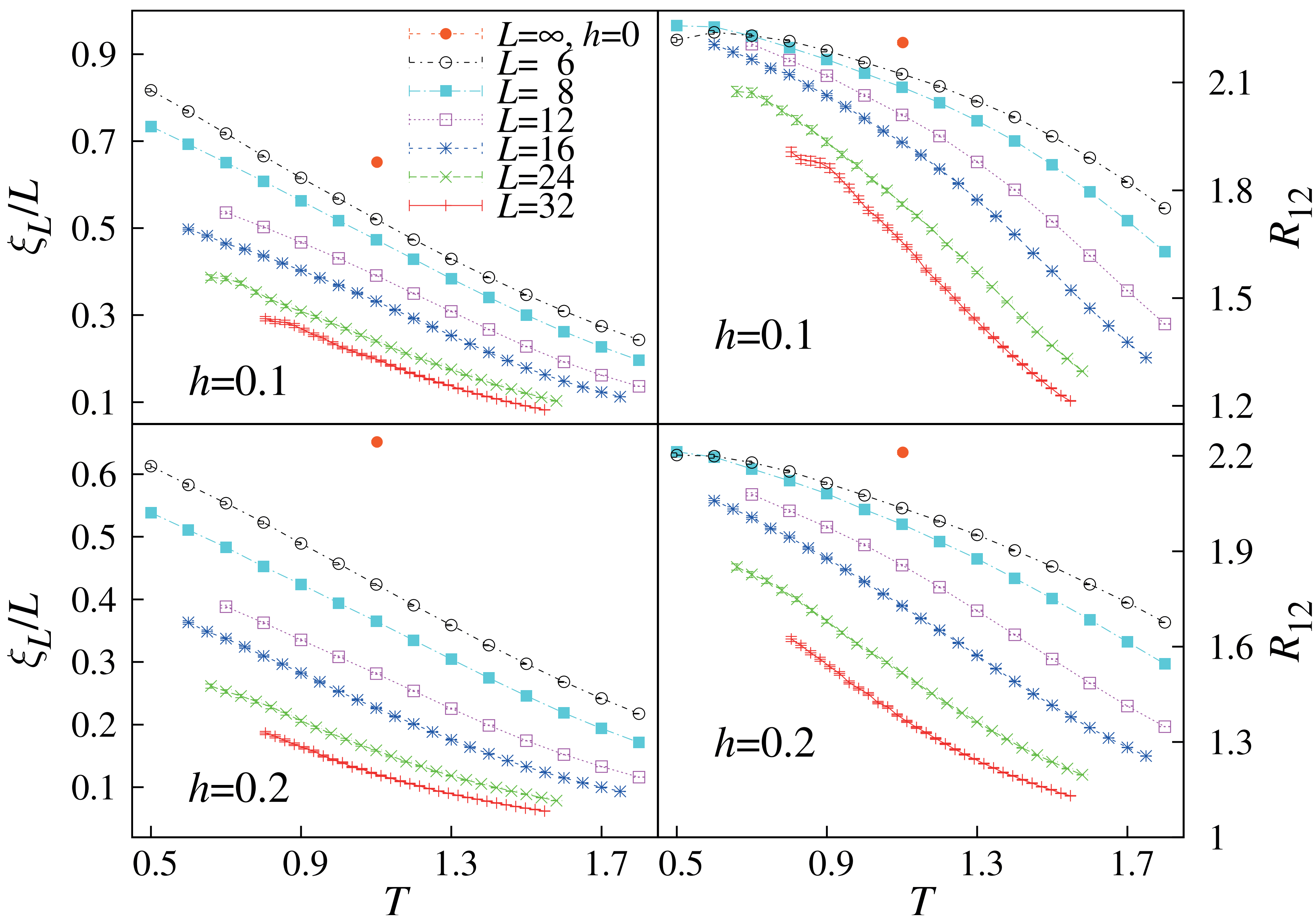
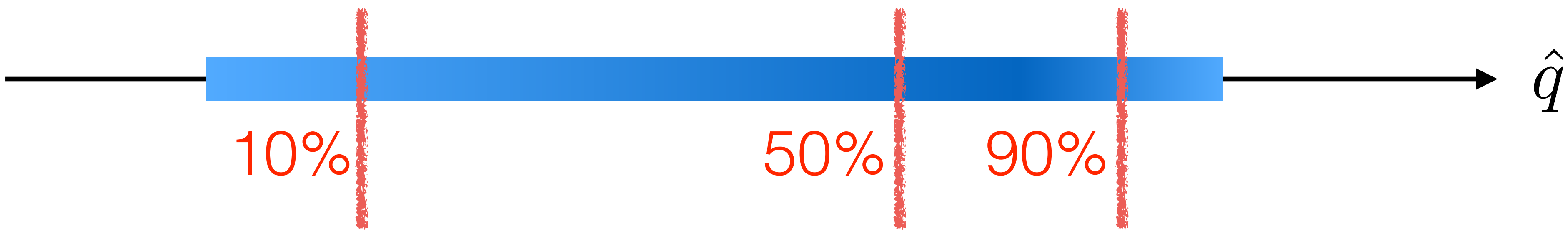


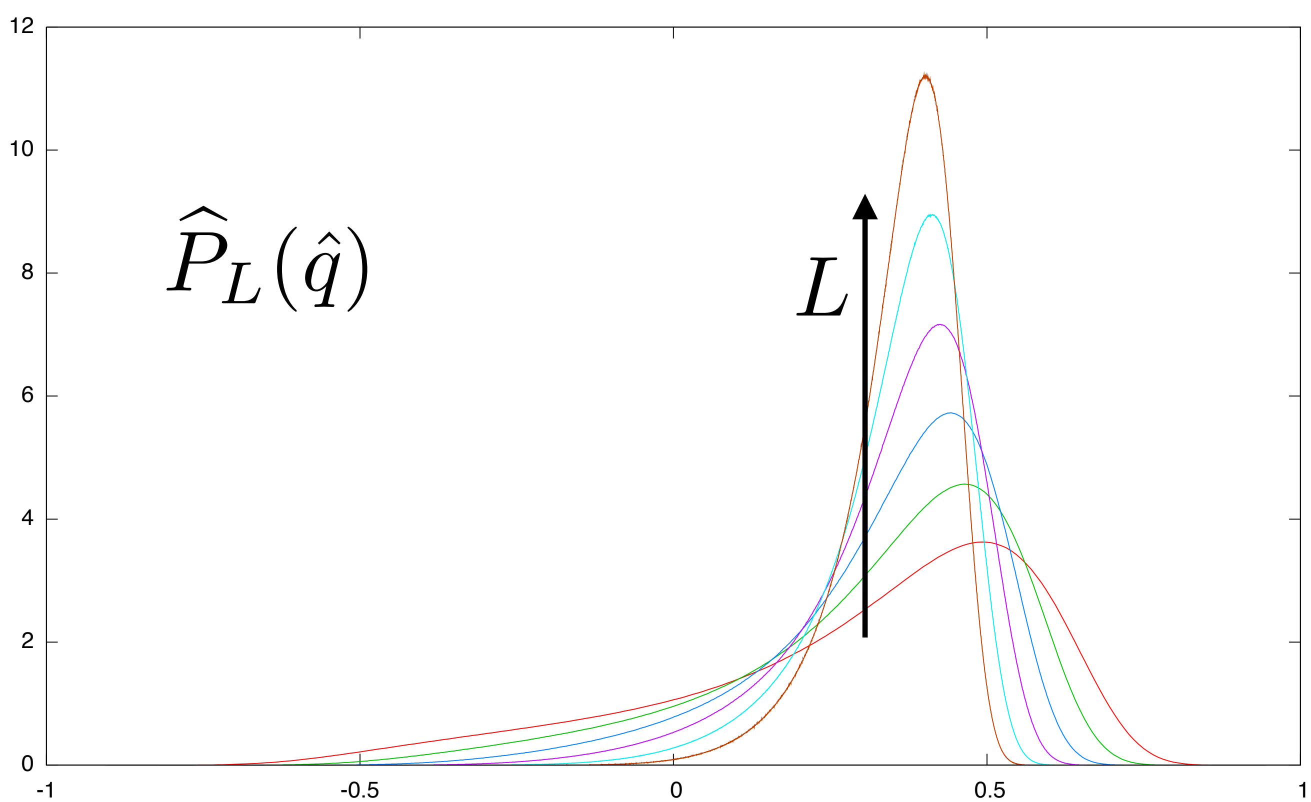
d=3 spin glass in field



An in-depth data analysis

Take all measurements and order them according to a conditioning variable $\hat{q}$





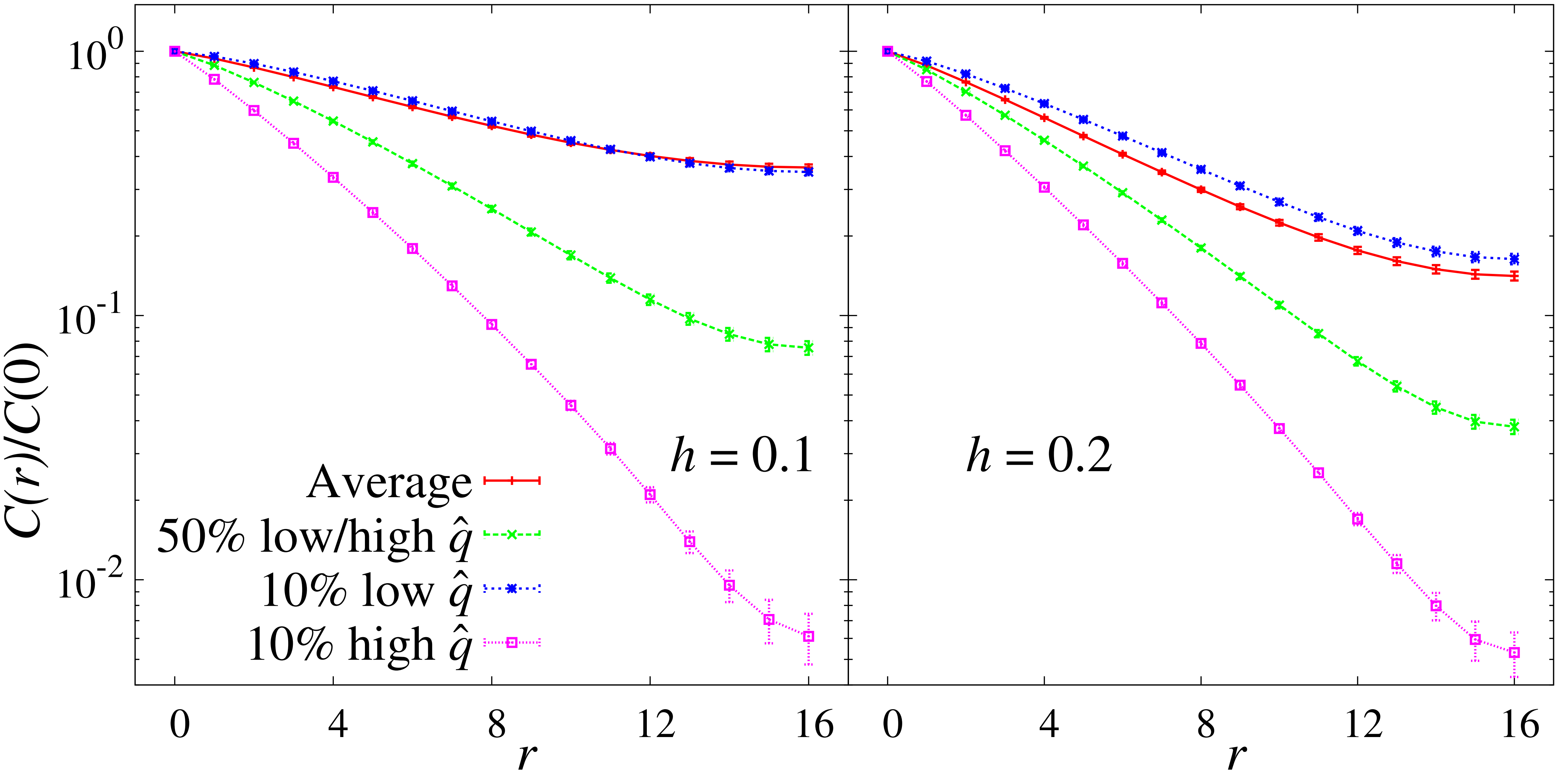
In the paramagnetic phase

$$\lim_{L\to\infty} \widehat{P}_L(\hat{q}) = \delta(\hat{q} - \hat{q}_0)$$

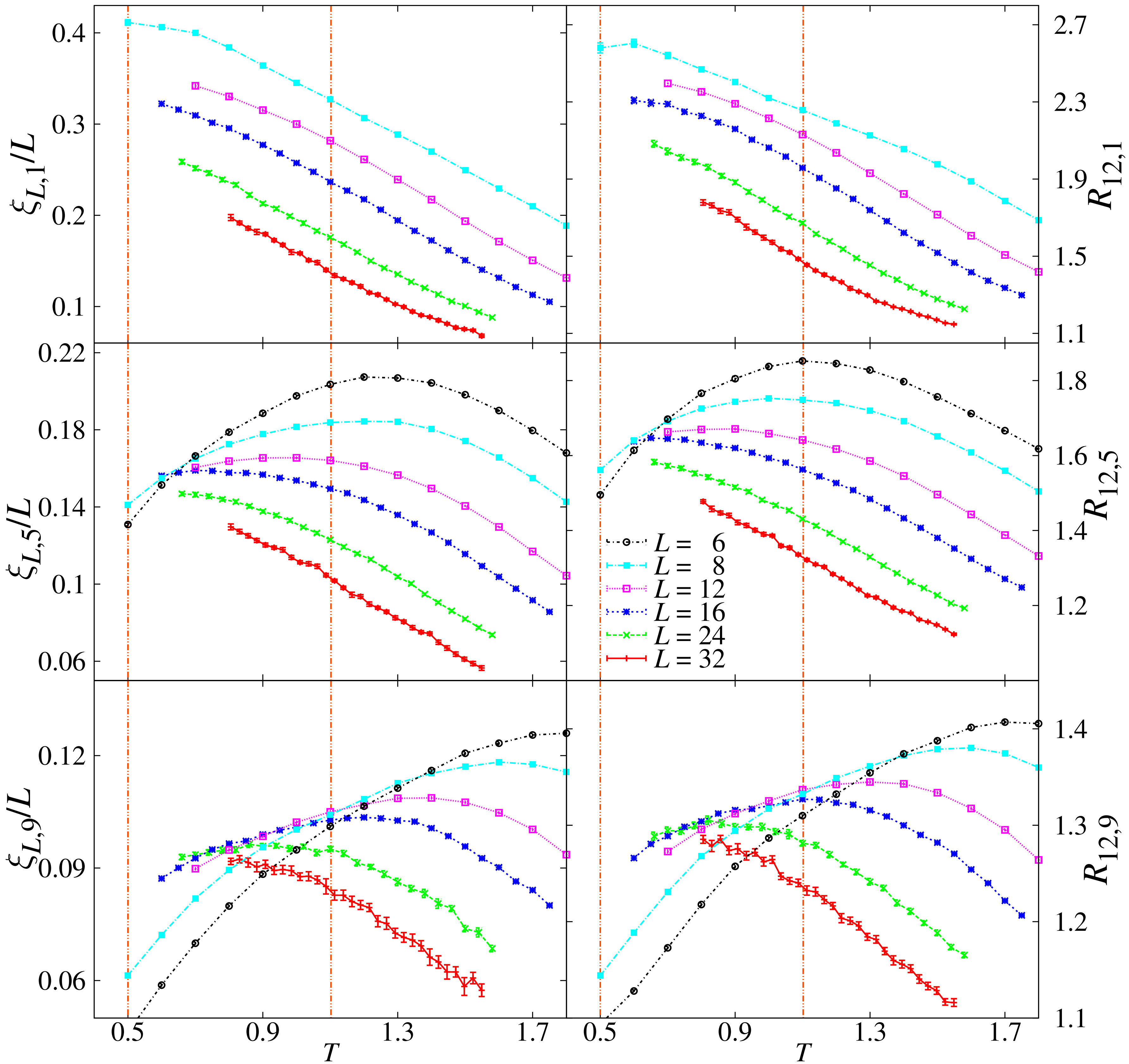
Analysis at different deciles should provide the same results in the limit $L \to \infty$

d=3 spin glass in field

Fluctuations in the paramagnetic phase are huge!



d=3 spin glass in field (H=0.2)



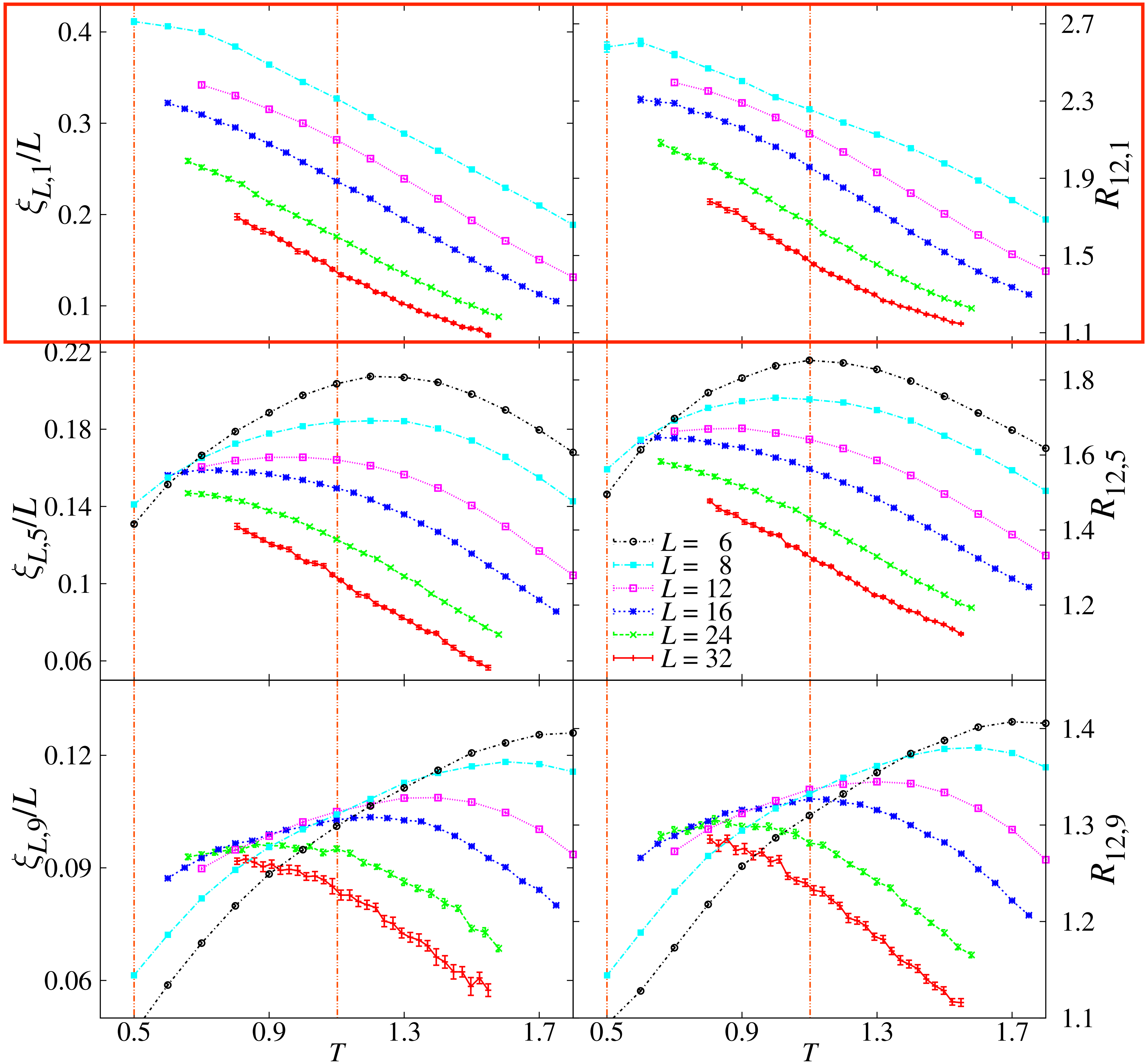
10%

50%

90%

d=3 spin glass in field (H=0.2)

Largely dominate average



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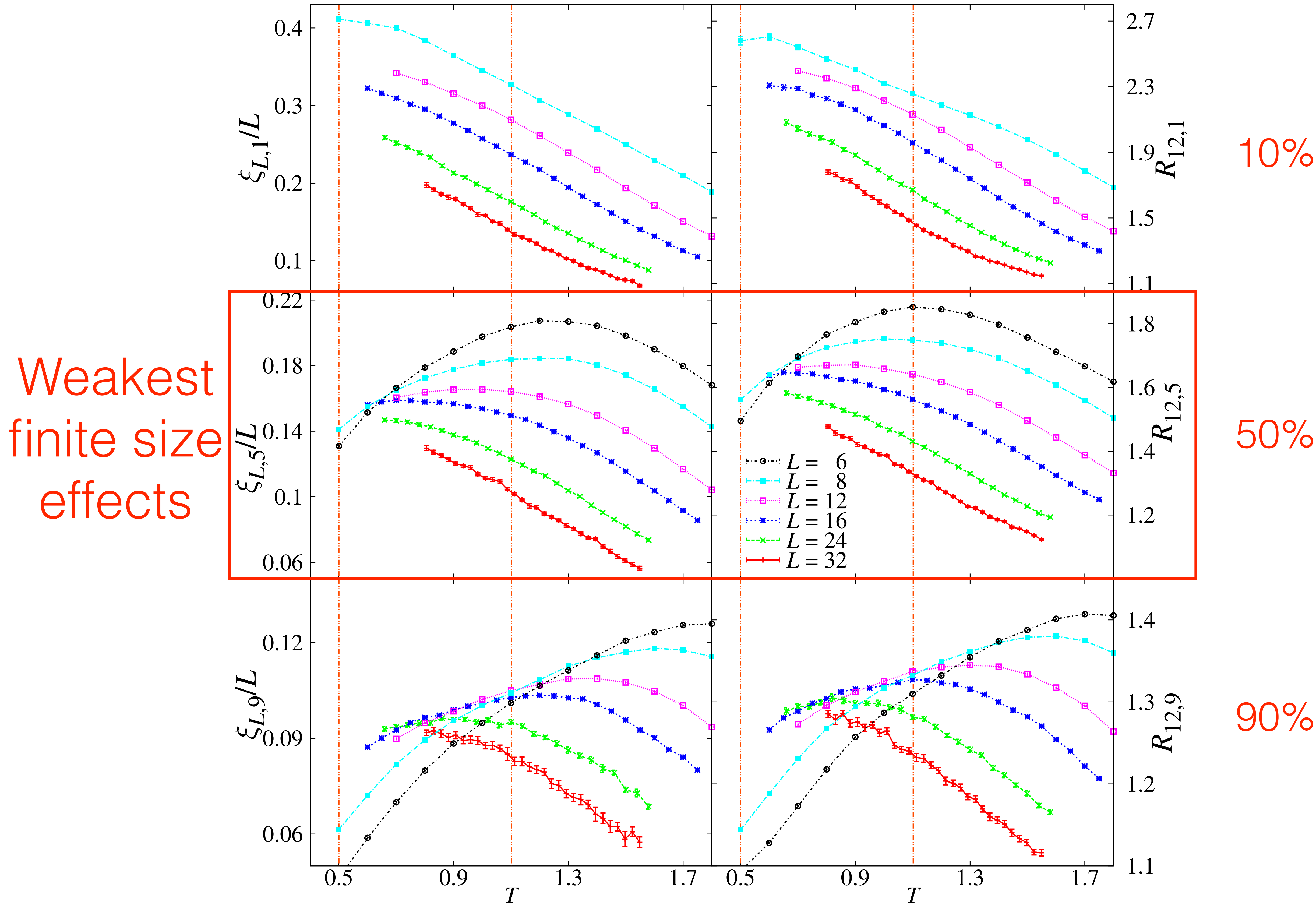
d=3 spin glass in field (H=0.2)



Conditioning on the overlap

- Consider 2 real replicas $\boldsymbol{\sigma}, \boldsymbol{\tau}$ with overlap

$$q = \boldsymbol{\sigma} \cdot \boldsymbol{\tau} = \frac{1}{N} \sum_i \sigma_i \tau_i$$

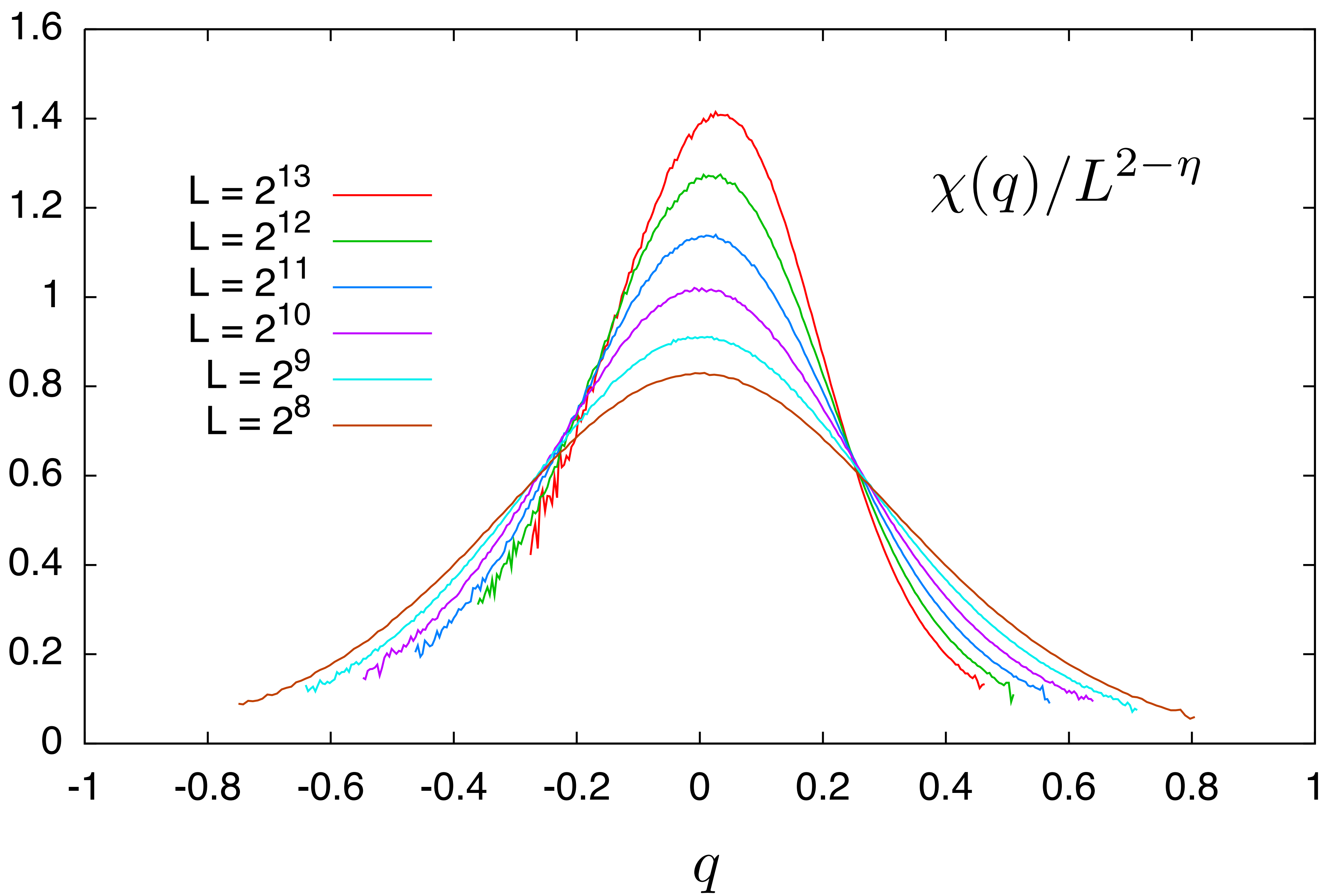
- Do the analysis conditioning on the overlap q

$$G(\boldsymbol{r}|q) \xrightarrow{\mathrm{FT}} \hat{G}(\boldsymbol{k}|q)$$

$$\hat{G}(\mathbf{0}|q) = q^2 \,, \qquad \chi(q) = \hat{G}(\boldsymbol{k}_1|q)$$

- The physical behavior strongly depends on the condition value, leading to phase transitions changing q

Phase transition for $T > T_c$ varying the distance among real replicas



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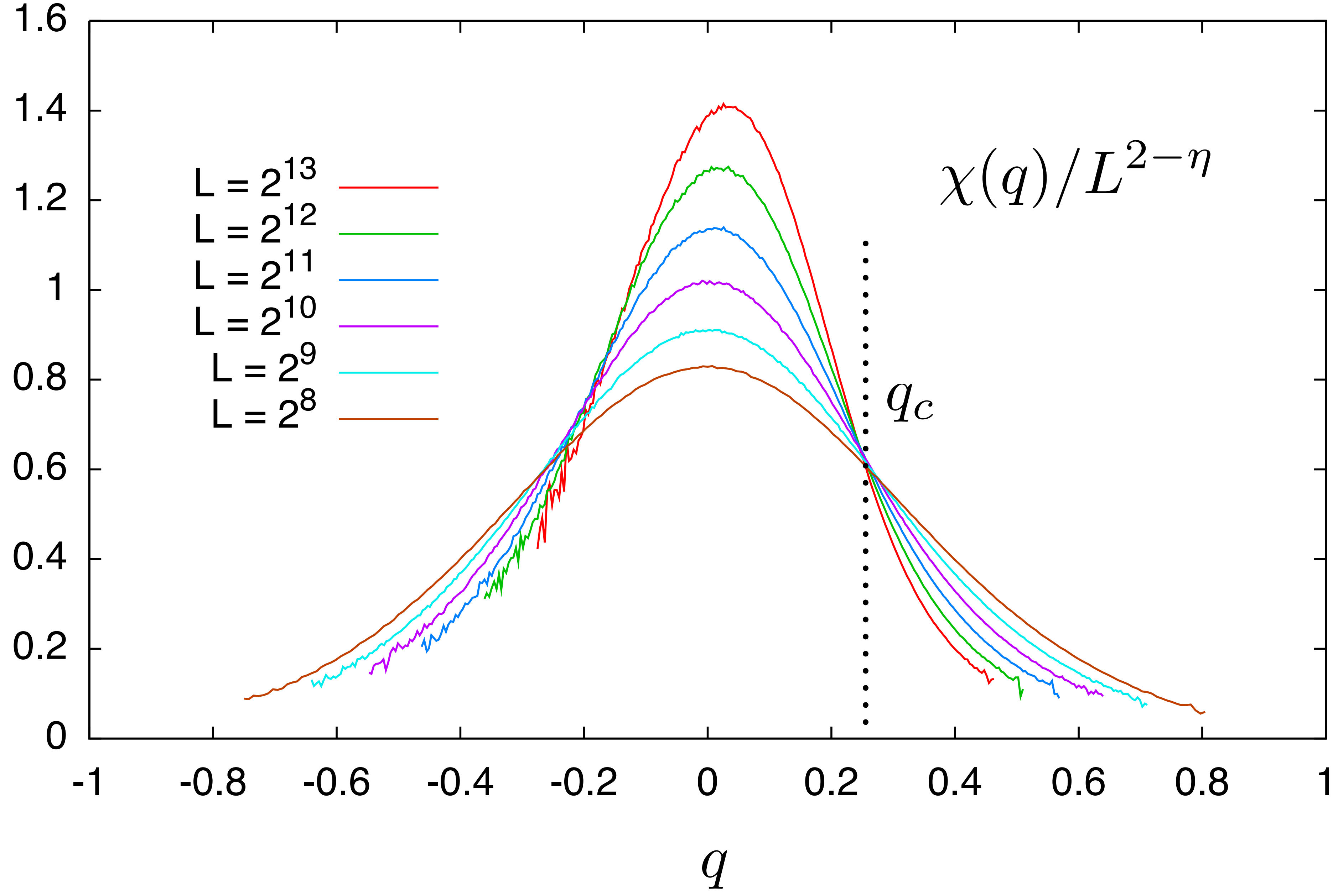
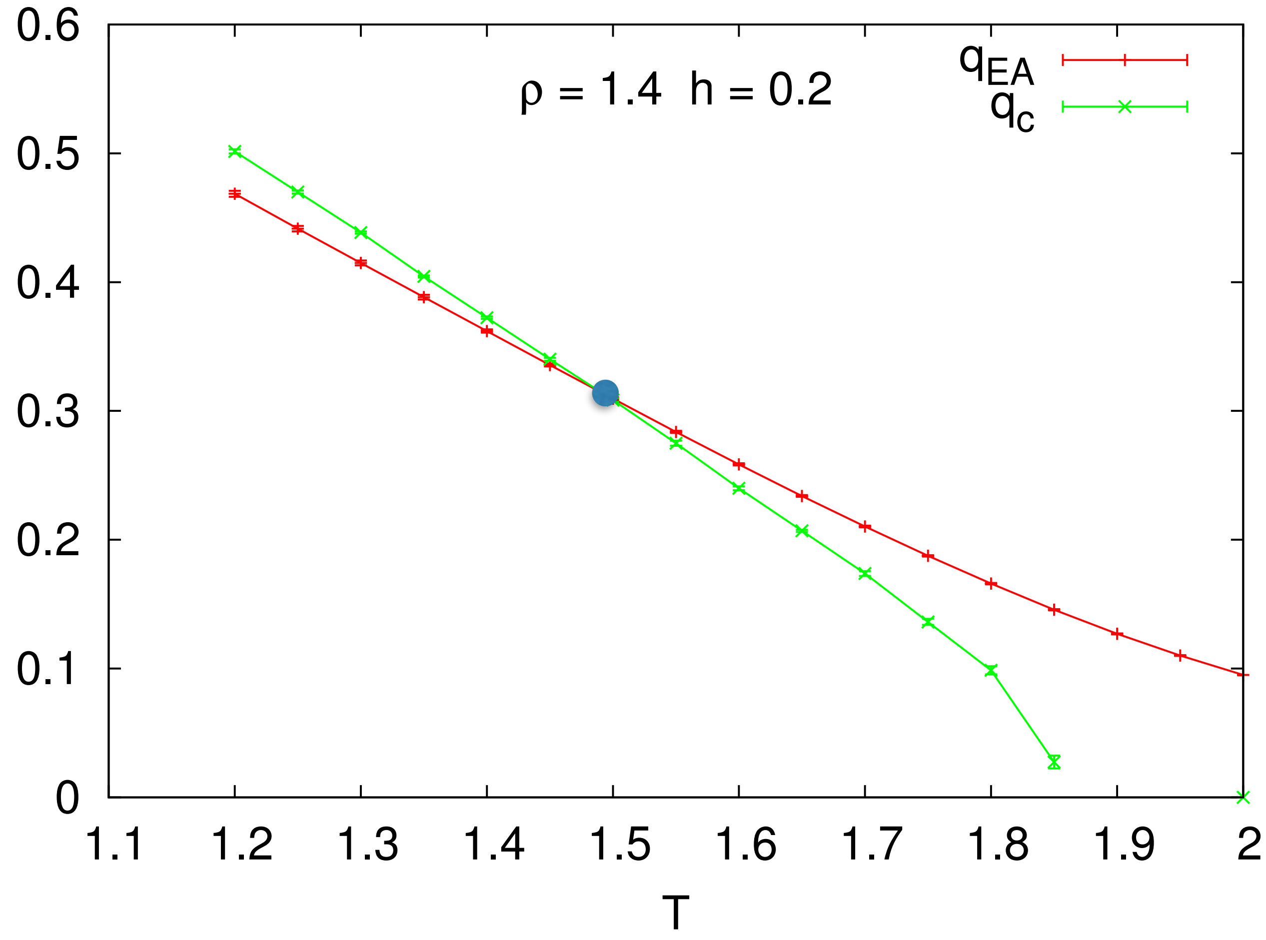


d=1 long range SG model

- Typical overlap q_{EA} : $\lim_{L \to \infty} P_L(q) = \delta(q - q_{\mathrm{EA}})$
- Thermodynamic phase transition if $q_{\mathrm{EA}} = q_c$



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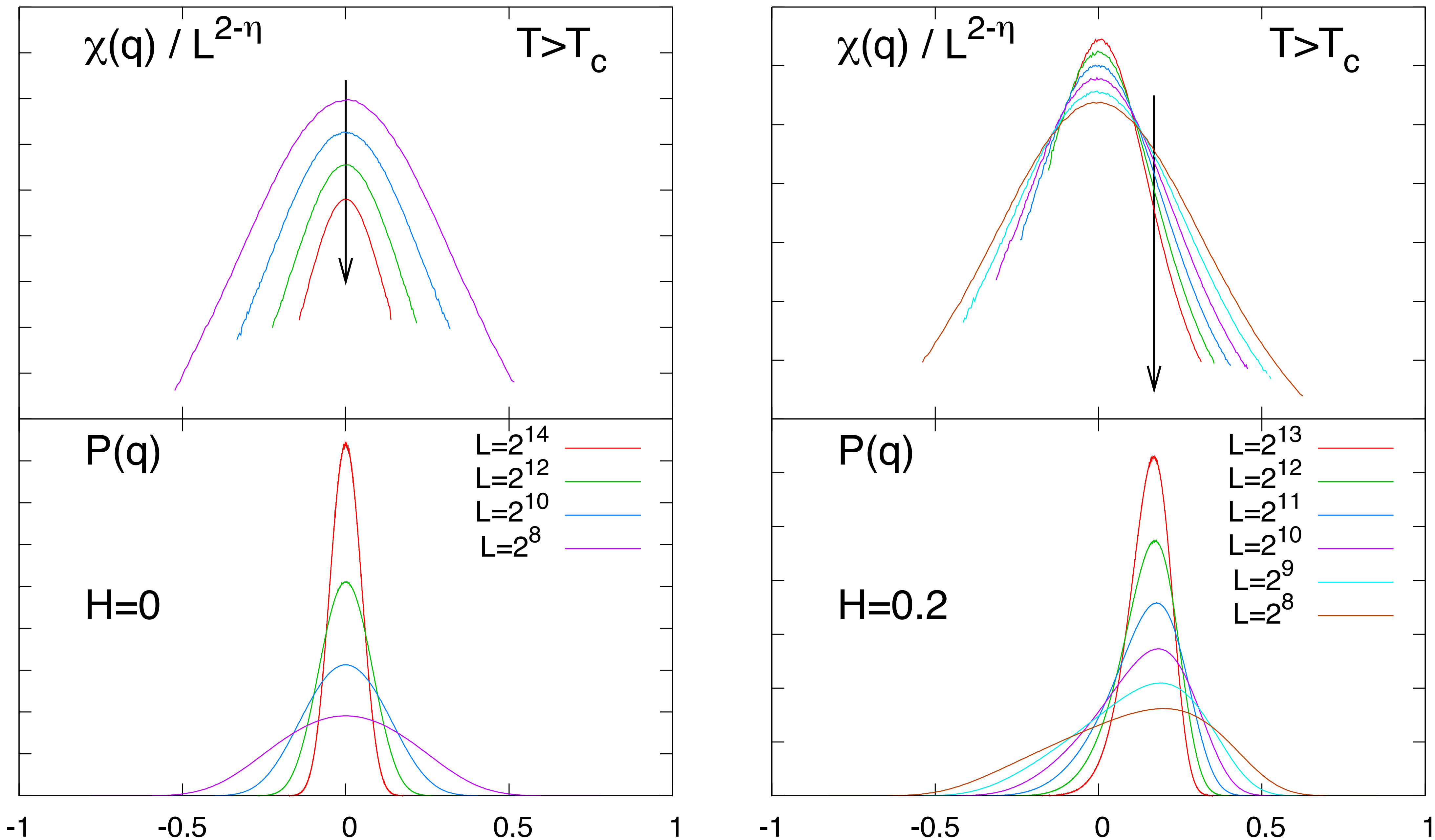


Evidences from numerical simulations of spin glass models

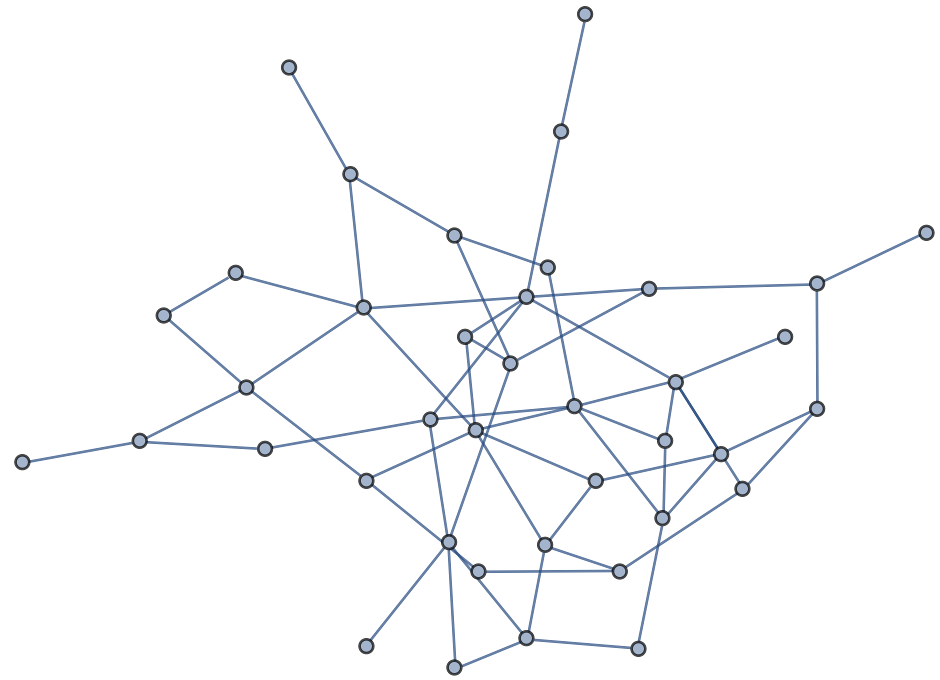
- Approaching the critical line from the paramagnetic phase (the spin glass phase is an even more complicated story…)
  - with scaling corrections the critical behavior at H=0 is under control
  - for H>0 fluctuations are huge and averages may be dominated by a minority of measurements
  - sub-dominant critical configurations are not so rare and must be taken into account carefully, maybe conditioning (even in the paramagnetic phase!)

Disordered models on random graphs

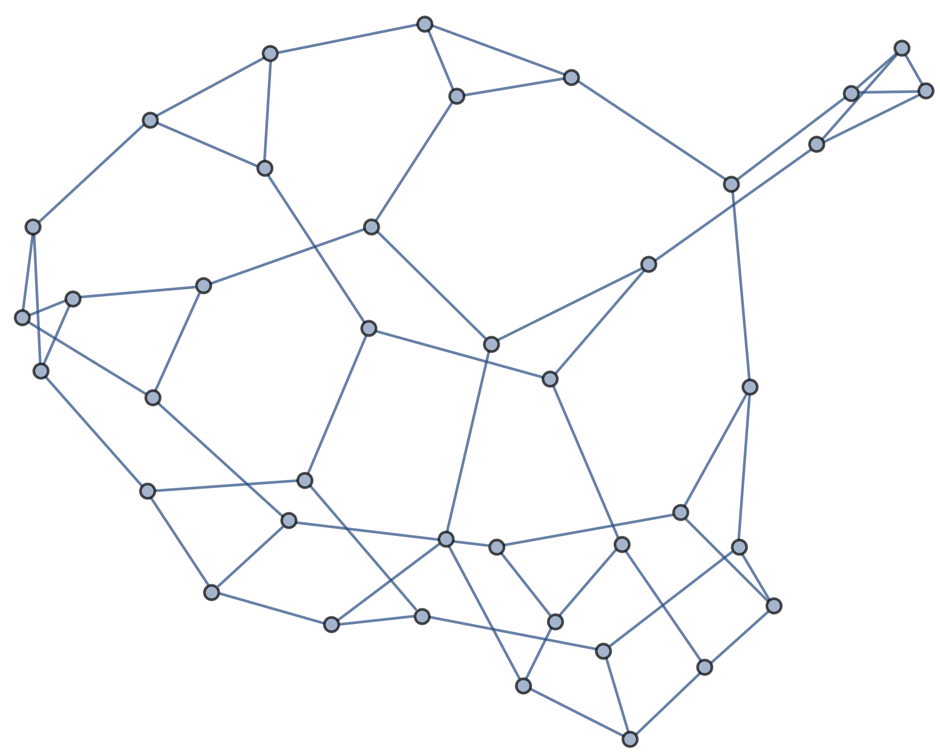
Random graphs

(with constant mean degree c)

- Poisson RG (Erdos-Renyi):
  N vertices
  M=cN/2 edges randomly chosen



- Regular RG:
  N vertices, each with c “legs”
  connect randomly the legs



- Locally tree-like
- Small loop are rare $O\left(\frac{1}{N}\right)$
- Typical loops are $O(\ln N)$

Random graphs

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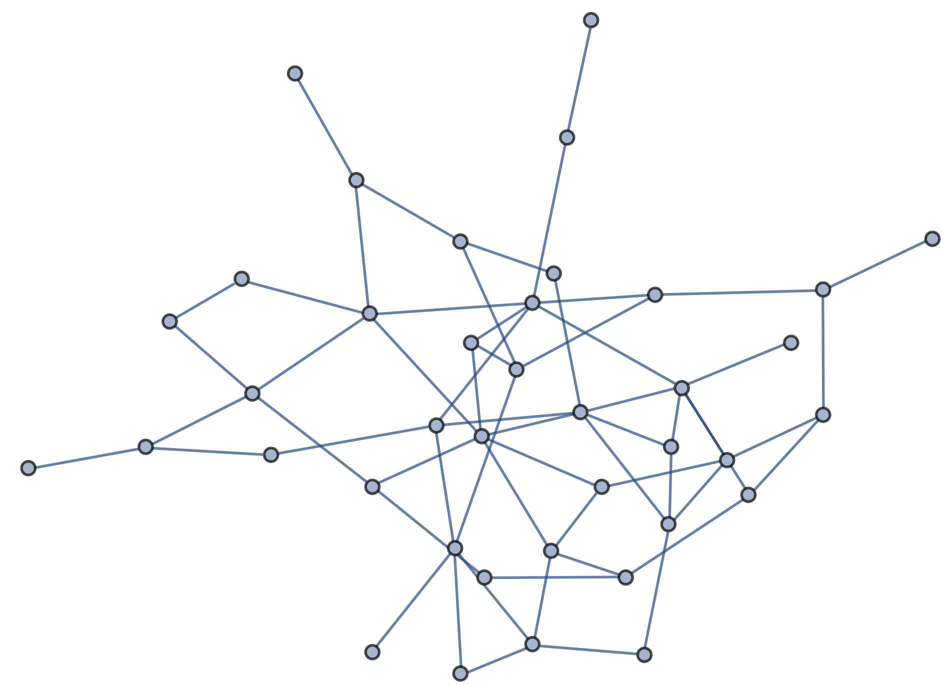

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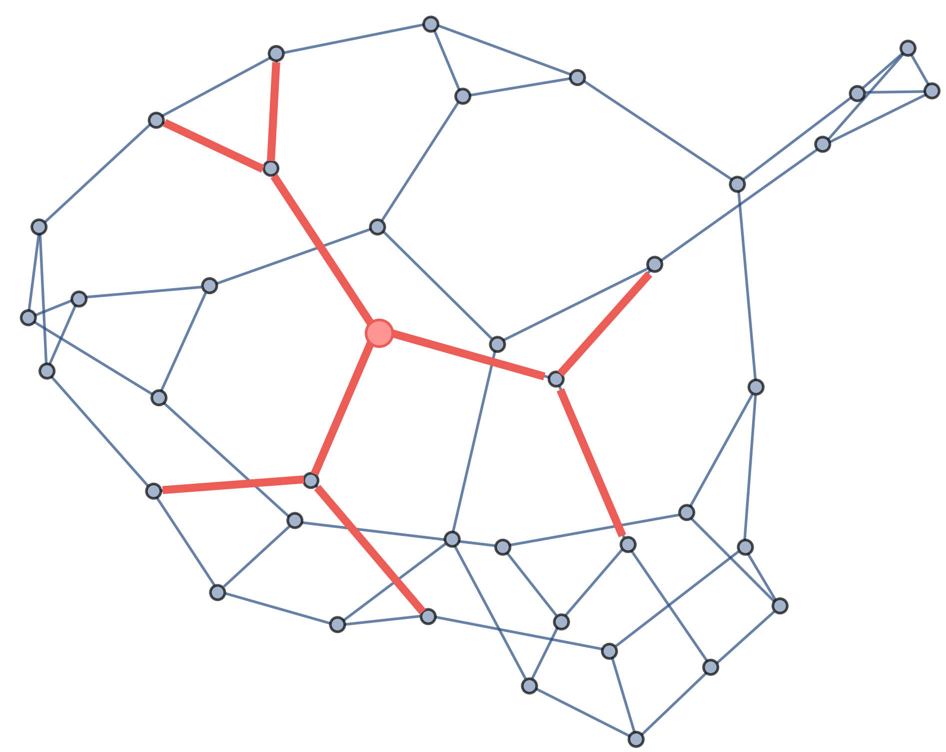

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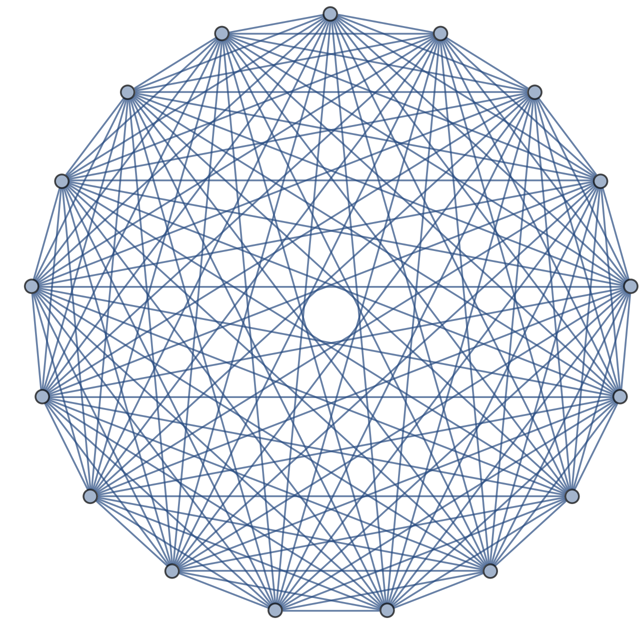
Why models on random graphs?

<u>Standard mean-field approximations have limitations</u>

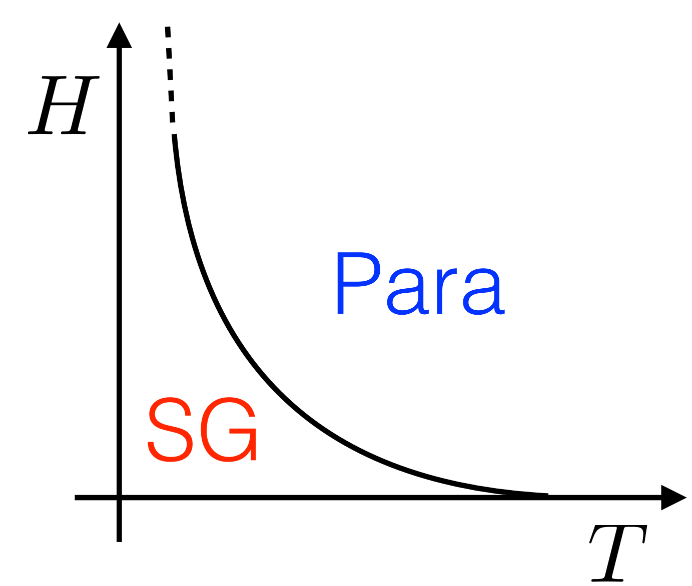
- Models on fully connected topologies



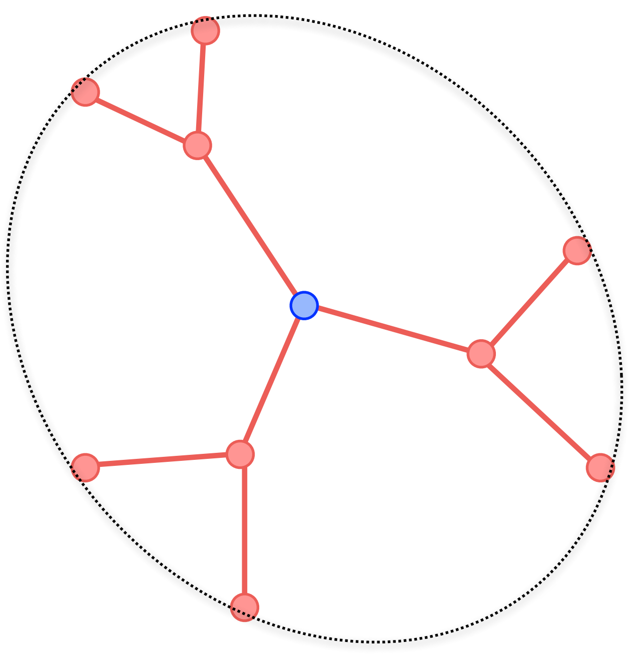
- Unphysical weak couplings:
  $J = O(1/N)$ in ferromagnets
  $J = O(1/\sqrt{N})$ in spin glasses

- Trivial geometry: no distance,
  no neighborhood, no correlation decay

- Some unphysical behavior:
  e.g. the critical line in the
  SK model diverges at T=0



How to solve models on random graphs



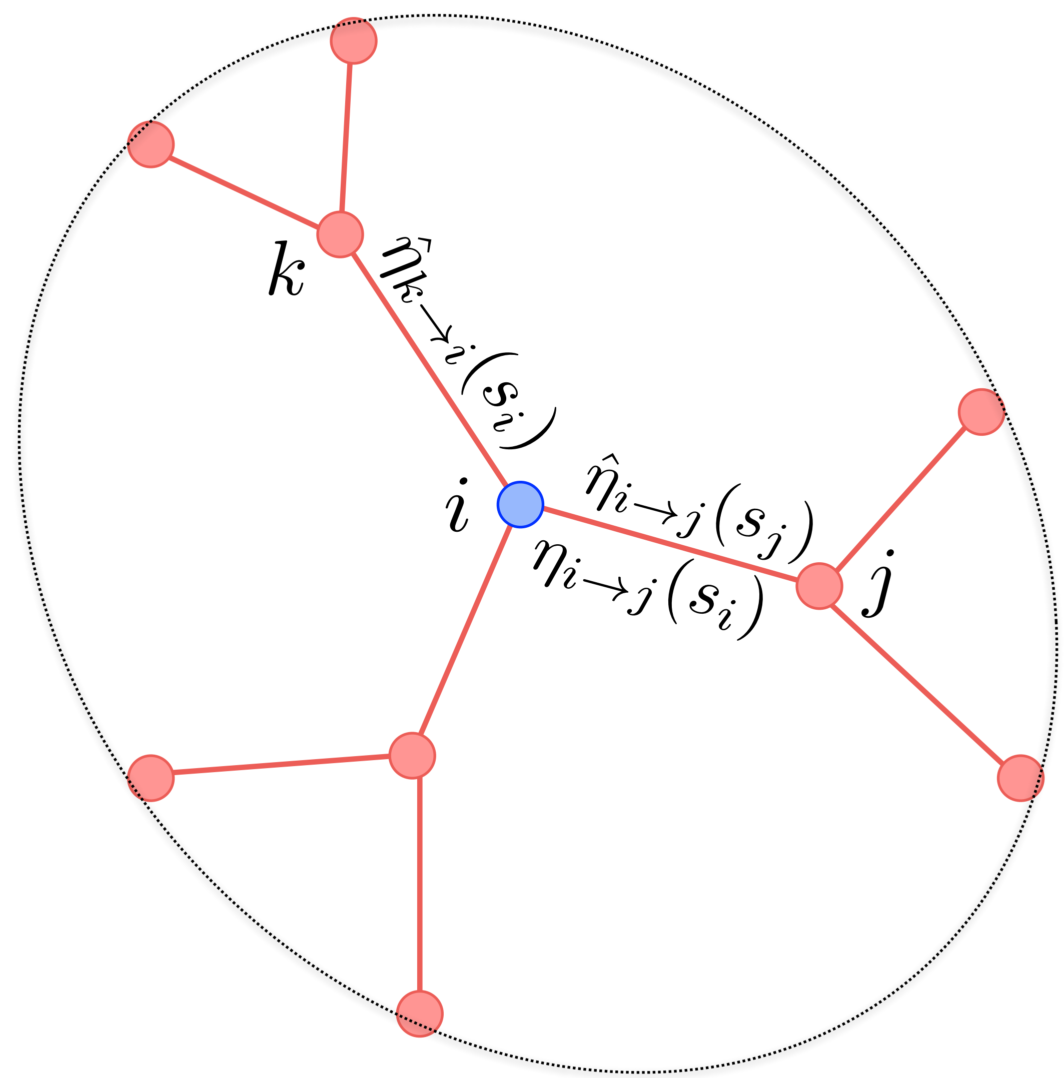
- In the large N limit a finite graph rooted on a randomly chosen vertex is a tree
- Assume correlations between the root vertex and boundary vertices are small (single state o replica symmetric ansatz)
- If connected correlations do not decay —> RSB
- To compute local marginals (e.g. on the root vertex) write recursion relations that hold on a tree and solve them on the actual graph

How to solve models on random graphs

- Recursion relations close on cavity marginals
  $\eta_{i\to j}(s_i)$: marginal on s_i if edge (ij) is removed
  $\hat{\eta}_{k\to i}(s_i)$: marginal on s_i if all edges around s_i are removed but (ik)

$$\eta_{i\to j}(s_i) \propto e^{\beta H_i s_i} \prod_{k\in\partial i\setminus j} \hat{\eta}_{k\to i}(s_i)$$

$$\hat{\eta}_{i\to j}(s_j) \propto \sum_{s_i} e^{\beta J_{ij} s_i s_j} \eta_{i\to j}(s_i)$$

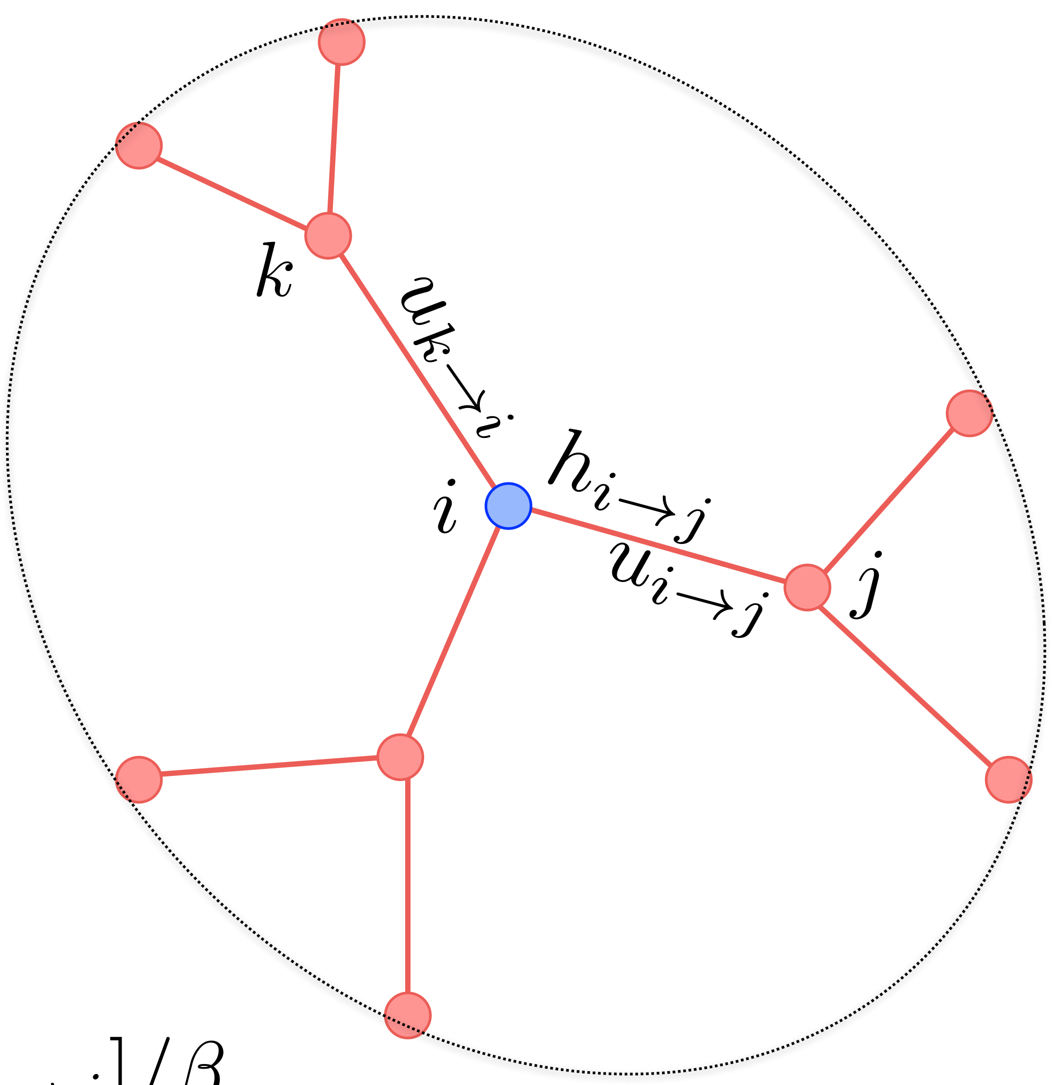


- Cavity marginals can be seen as <u>messages</u> passing along the edges and carrying local information to global level

How to solve models on random graphs

- For Ising models, marginals can be represented by a single scalar number (e.g. the magnetization)

$$\hat{\eta}_{k\to i}(s_i) \propto \exp(\beta \boxed{u_{k\to i}} s_i)$$
$$\eta_{i\to j}(s_i) \propto \exp(\beta \boxed{h_{i\to j}} s_i)$$



- Equations to be solved are 4 x the number of edges

$$h_{i\to j} = H_i + \sum_{k\in\partial i\setminus j} u_{k\to i}$$

$$u_{i\to j} = \hat{u}_\beta(J_{ij}, h_{i\to j}) =$$
$$= \mathrm{atanh}[\tanh(\beta J_{ij}) \tanh(\beta h_{i\to j}]/\beta$$

Belief Propagation

- Iterative solution

$$h_{i\to j}^{(t+1)} = H_i + \sum_{k\in\partial i\setminus j} u_{k\to i}^{(t)}$$

$$u_{i\to j}^{(t+1)} = \hat{u}_\beta\left(J_{ij}, h_{i\to j}^{(t+1)}\right)$$

Belief Propagation

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damping (friction)
helps convergence

Belief Propagation

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damping (friction) helps convergence

- BP fixed point messages give local marginals

$$m_i = \langle s_i \rangle = \tanh\left(H_i + \sum_{k\in\partial i} u_{k\to i}^{\star}\right)$$

$$c_{ij} = \langle s_i s_j \rangle = \frac{\tanh(\beta J_{ij}) + \tanh(\beta h_{i\to j})\tanh(\beta h_{j\to i})}{1+\tanh(\beta J_{ij})\tanh(\beta h_{i\to j})\tanh(\beta h_{j\to i})}$$

- Can be run on a given graph, while cavity method is for the ensemble average in the thermodynamic limit

Bethe states and BP fixed points

- Bethe approximation (at least locally) $$P(\boldsymbol{s}) = \frac{e^{-\beta \mathcal{H}(\boldsymbol{s})}}{Z} \approx \prod_i b_i(s_i) \prod_{(ij)\in E} \frac{b_{ij}(s_i, s_j)}{b_i(s_i) b_j(s_j)}$$

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Bethe state

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Bethe state

$$\begin{tikzcd}
\text{BP fixed points} \arrow[rr, leftrightarrow] \arrow[dr, leftrightarrow] & & \text{Bethe states} \arrow[dl, leftrightarrow] \\
& \begin{array}{c}\text{minima of} \\ \text{Bethe free-energy}\end{array} &
\end{tikzcd}$$

Limits of the RS ansatz

- Bethe approximation (at least locally) $$P(\boldsymbol{s}) = \frac{e^{-\beta \mathcal{H}(\boldsymbol{s})}}{Z} \approx \prod_i b_i(s_i) \prod_{(ij)\in E} \frac{b_{ij}(s_i, s_j)}{b_i(s_i) b_j(s_j)}$$

- Many equivalent ways to become critical

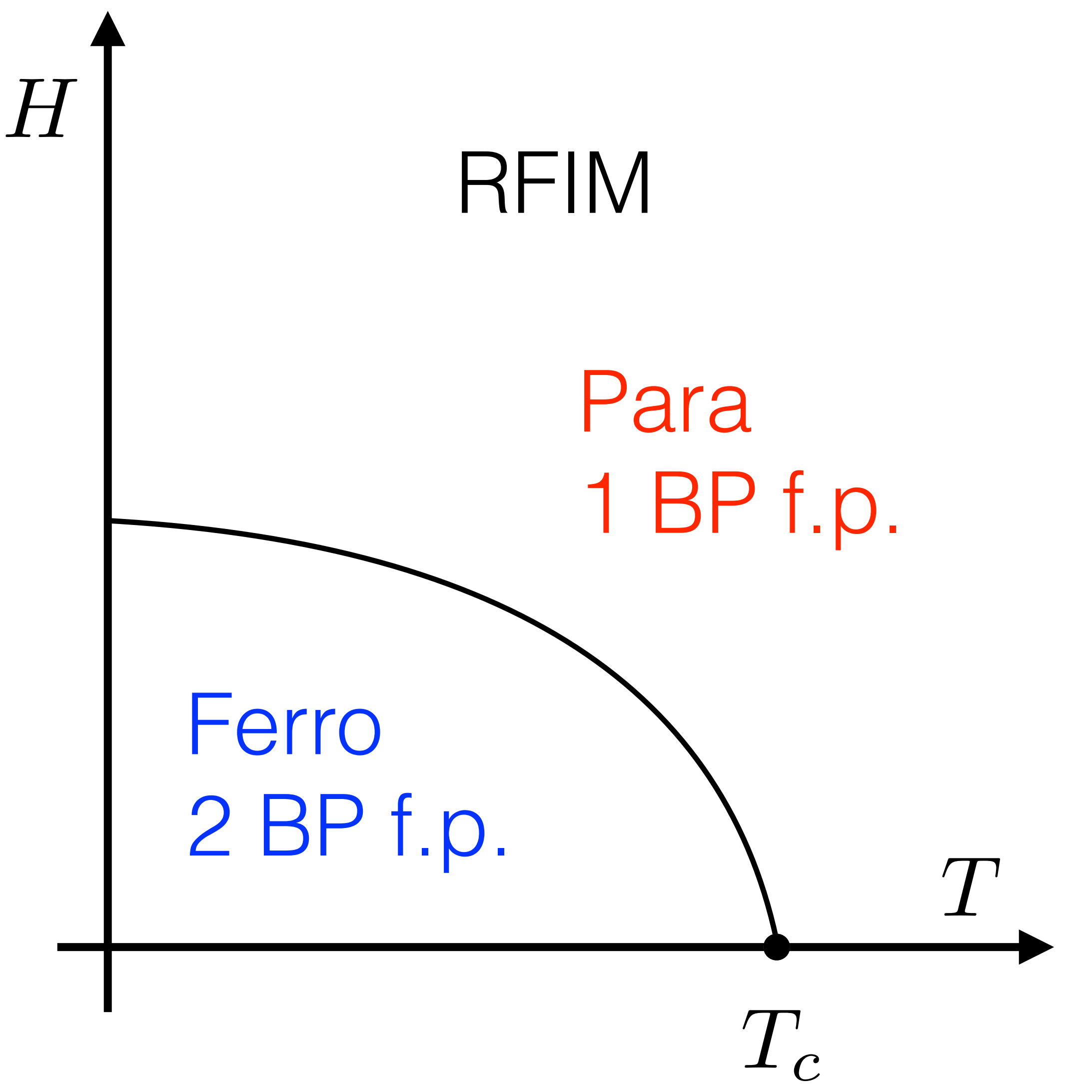
  - Susceptibility diverges

  - Hessian of the Bethe free-energy becomes singular

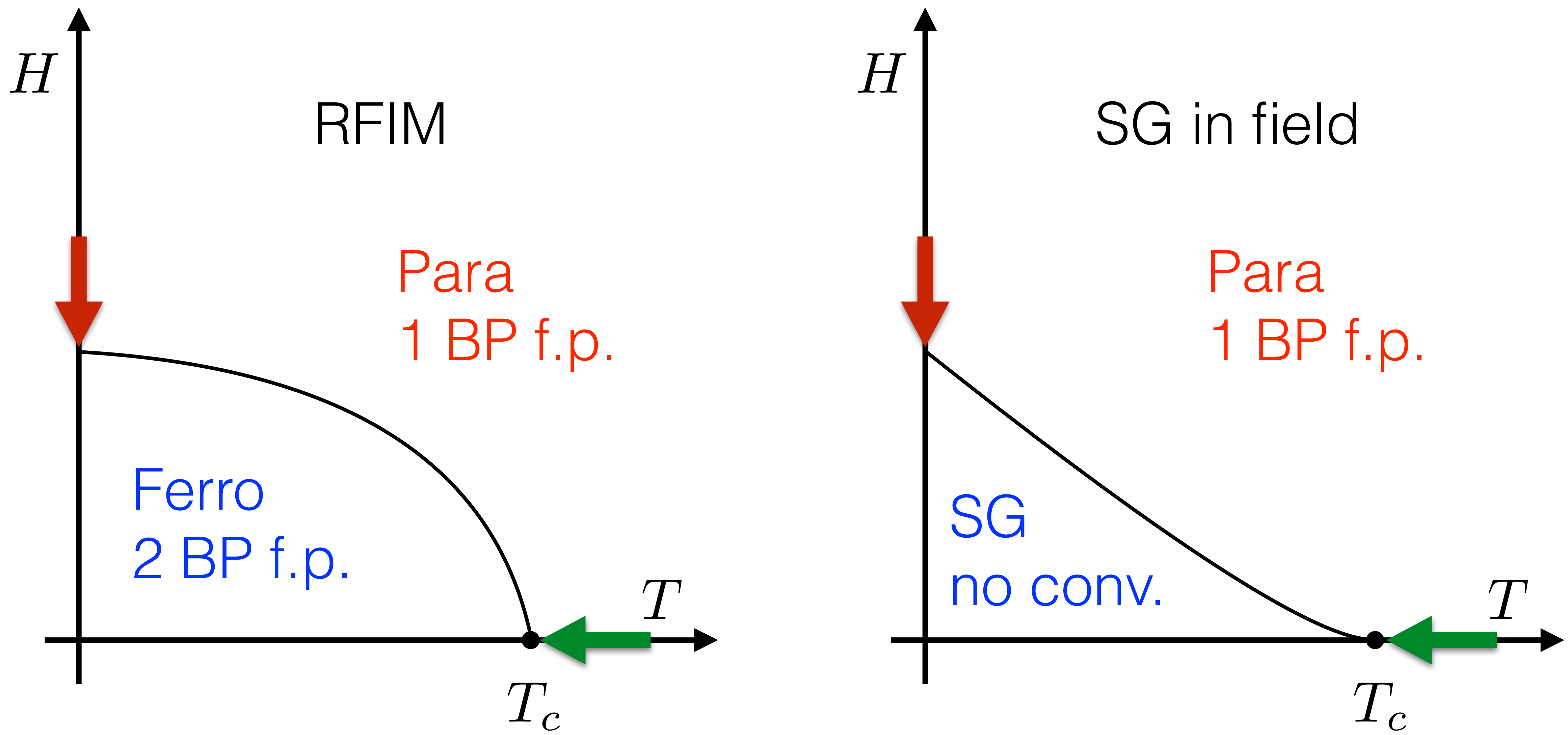
  - BP fixed point becomes unstable

  Phase transition on a given sample!
  Algorithmic vs thermodynamic phase transitions

Common belief expectations

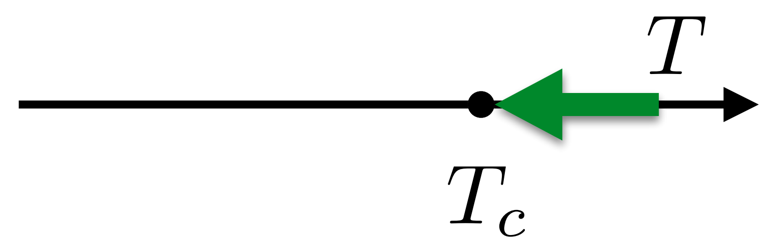


Approaching the critical line



Approaching the critical line

- Without field (H=0)



- Compute correlations on a tree branch

$$C(r) = \langle s_0 s_r \rangle = \prod_{i=0}^{r-1} \tanh(\beta J_{i,i+1})$$

- Sum over all branches (e.g. on a c-RRG)

$$\chi_F = \sum_i \langle s_0 s_i \rangle = \sum_r c(c-1)^{r-1} C(r) \propto \frac{1}{1-(c-1)\tanh(\beta)}$$

$$\chi_{SG} = \sum_i \langle s_0 s_i \rangle^2 = \sum_r c(c-1)^{r-1} C(r)^2 \propto \frac{1}{1-(c-1)\tanh^2(\beta)}$$

Approaching the critical line

- Without field (H=0) correlations are similar on all branches
- At the critical condition $(c-1)\tanh(\beta) = 1$ or $(c-1)\tanh^2(\beta) = 1$
  - Paramagnetic susceptibility diverges
  - Hessian at the paramagnetic state becomes singular
  - Paramagnetic BP fixed point $u^\star = h^\star = 0$ becomes unstable

On the critical line in a field

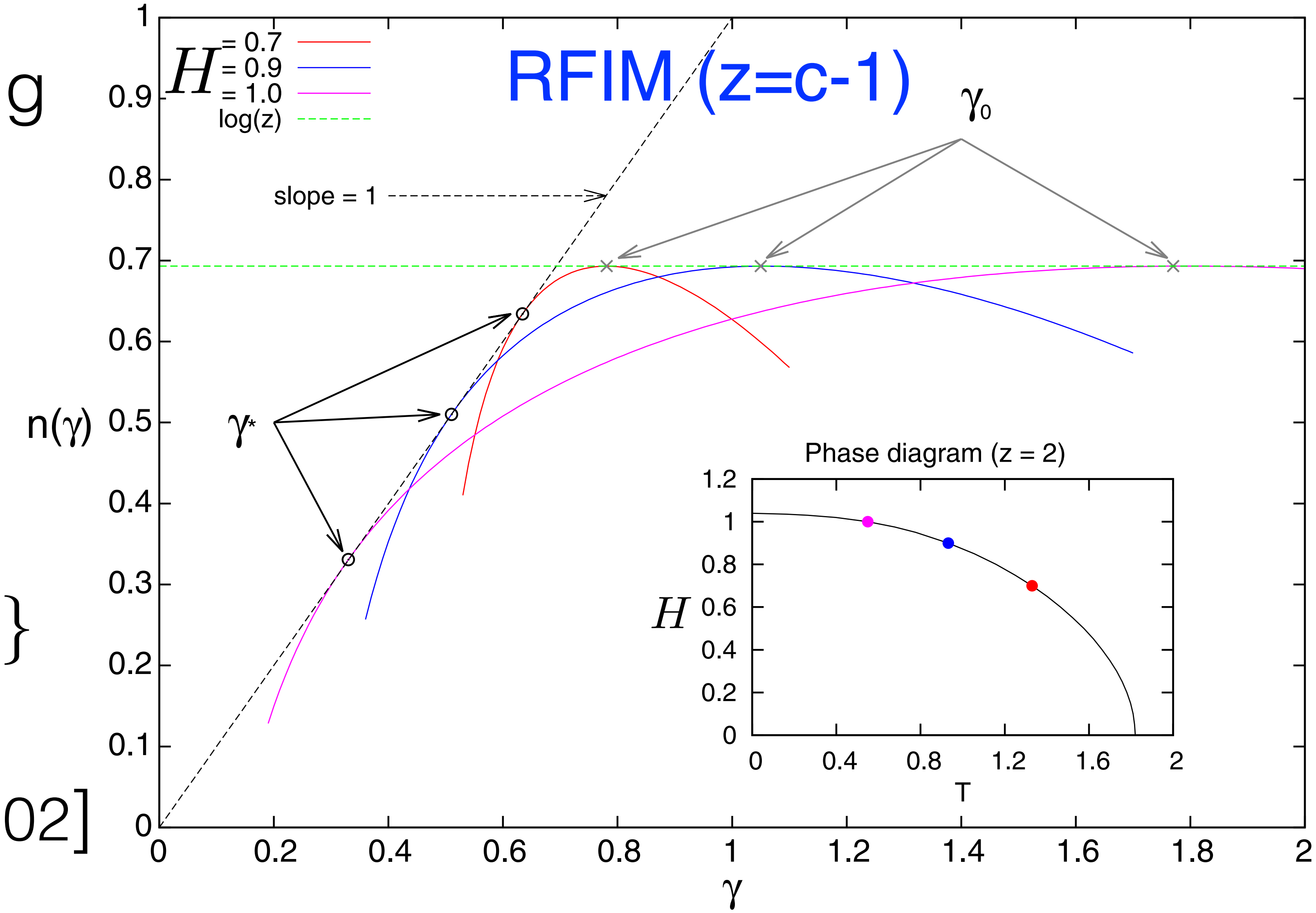
- With field (H>0) correlations strongly depend on the disorder along the branch (fields and couplings)

- Critical behavior dominated by a minority decaying slower than typical ones

- At T=0 extreme heterogeneity

$$C(r \gg 1) \in \{0, 1\}$$

$$\# \left[C(r) \simeq e^{-\gamma r} \right] \propto e^{n(\gamma) r}$$



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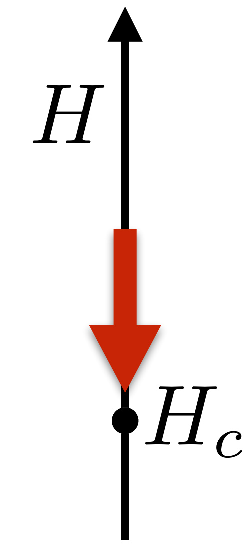
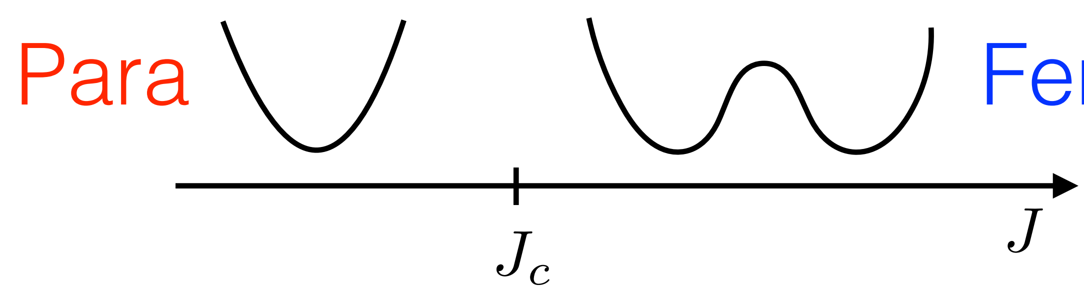
Approaching the critical line at T=0



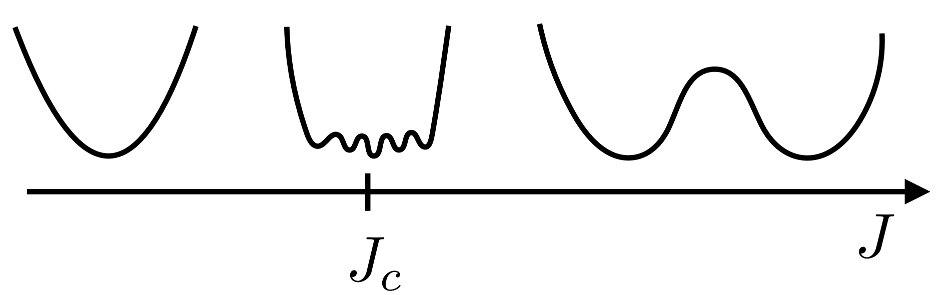
- Very heterogeneous paramagnetic phase!
  What are the consequences on the criticality?

- RFIM at T=0: decreasing H <—> increasing J

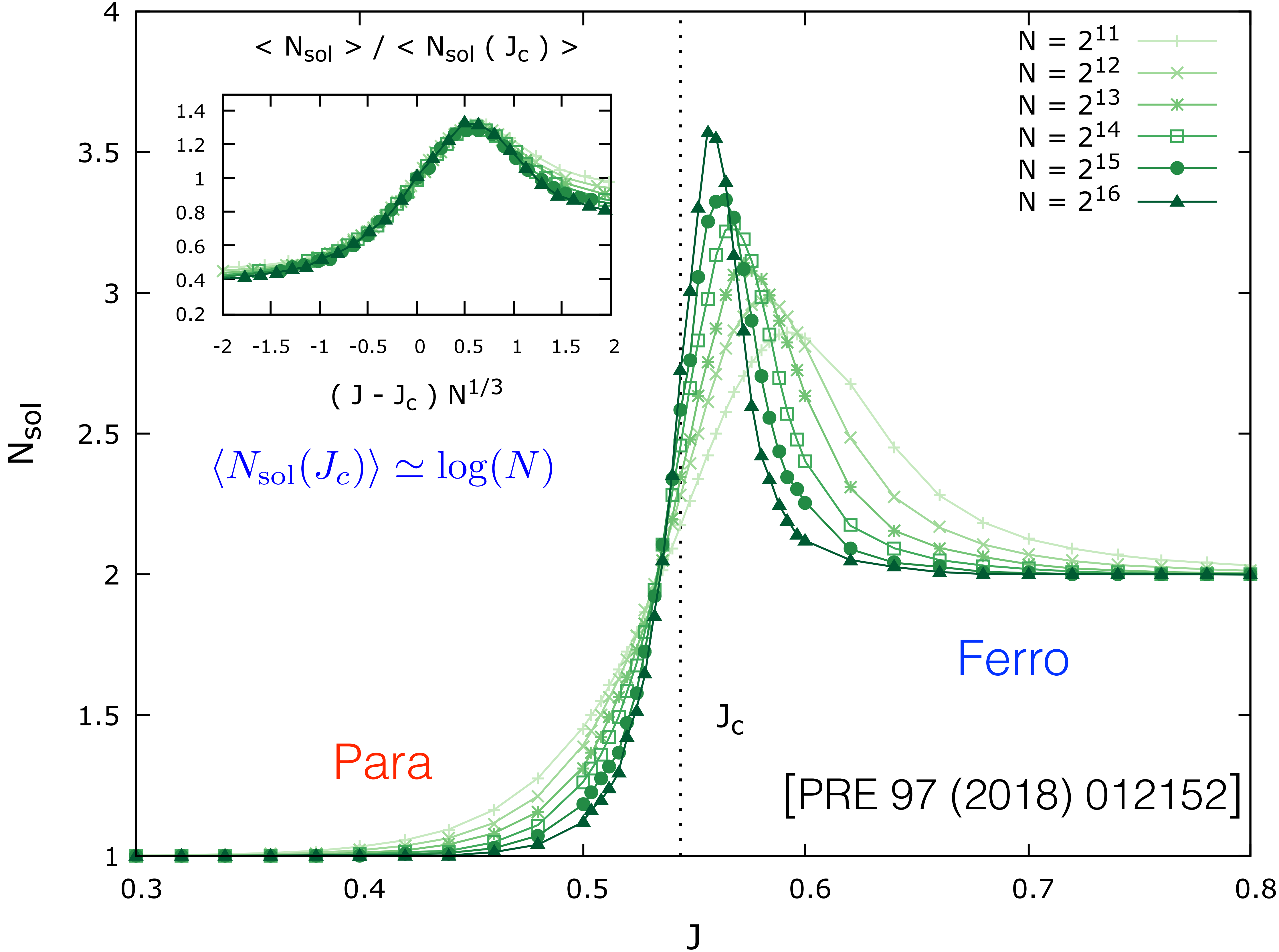
- Standard scenario at a 2nd order phase transition



- Should we modify it to something rougher?



Number of BP fixed points in the RFIM

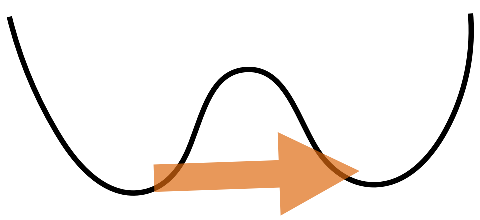


Structure of Bethe states (RFIM at J_c)

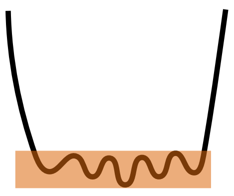
- 3 kind of samples (at J_c each kind appears with a <u>constant probability</u> in the large N limit)

  - Paramagnetic —> 1 BP fixed point

  - Ferromagnetic —> 2 BP fixed points
    $d_H \sim N \quad \Delta E \sim N^{1/2}$



  - <u>Critical</u> —> 2 or more BP fixed points
    lowest energy excitation has
    $d_H \sim N^{1/2} \quad \Delta E \sim N^{-\omega} \quad \omega \approx 0.25$



practically degenerate!

Structure of Bethe states (RFIM at J_c)

- The limits $N \to \infty, \beta \to \infty$ do not commute

- Choosing $\beta(N) \sim N^\zeta$ $(\zeta < \omega)$ the partition function

$$\sum_{\alpha \in \{\text{BP f.p.}\}} e^{-\beta(N) E_\alpha}$$

  is not dominated by the ground state!!

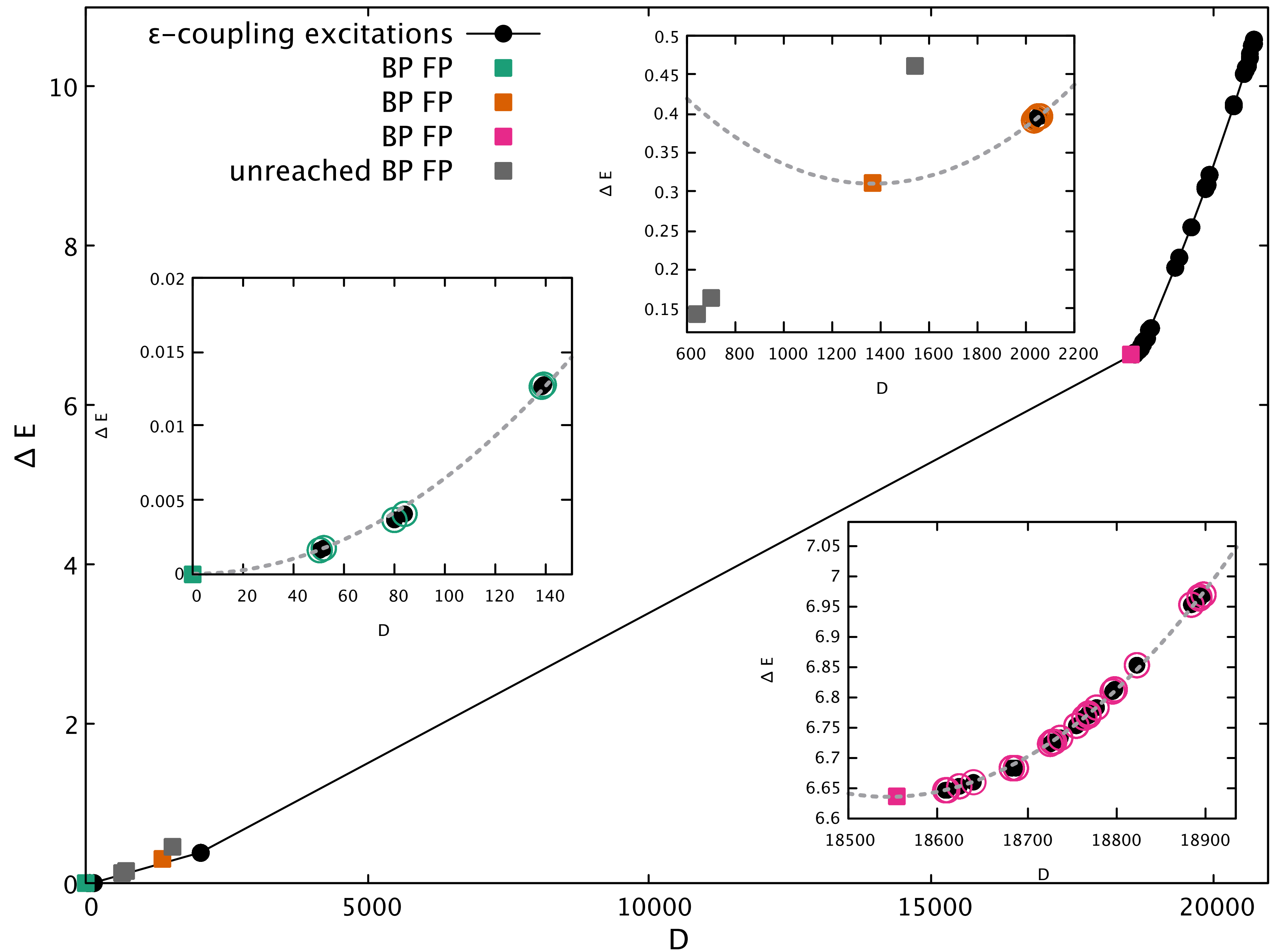
- Computing the ground state is enough to understand the critical behavior of the RFIM?

- Can we sample critical excitations efficiently via ground state computations?

Structure of Bethe states (RFIM at J_c)

Searching for low-energy excited states via the ε-coupling method

$$\mathcal{H}_\varepsilon(\boldsymbol{s}) = \mathcal{H}(\boldsymbol{s}) + \varepsilon\, \boldsymbol{s} \cdot \boldsymbol{s}_0$$



Evidences from analytic solutions on random graphs

- Approaching the critical line from the paramagnetic phase with H>0:

  - fluctuations in correlation functions are severe and averages are dominated by a minority

  - number of Bethe states is larger than expected (in SG models even more than in the RFIM) and diverges at the critical point

  - the ground state is probably not enough for describing fully the low temperature physics (a sort of weak RSB?)

  - criticality is driven by changes in the relative weights between Bethe states rather than a single state becoming critical

Thank you!