Is there a de Almeida-Thouless line in finite-dimensional spin glasses? (and why you should care)

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The Almeida-Thouless line

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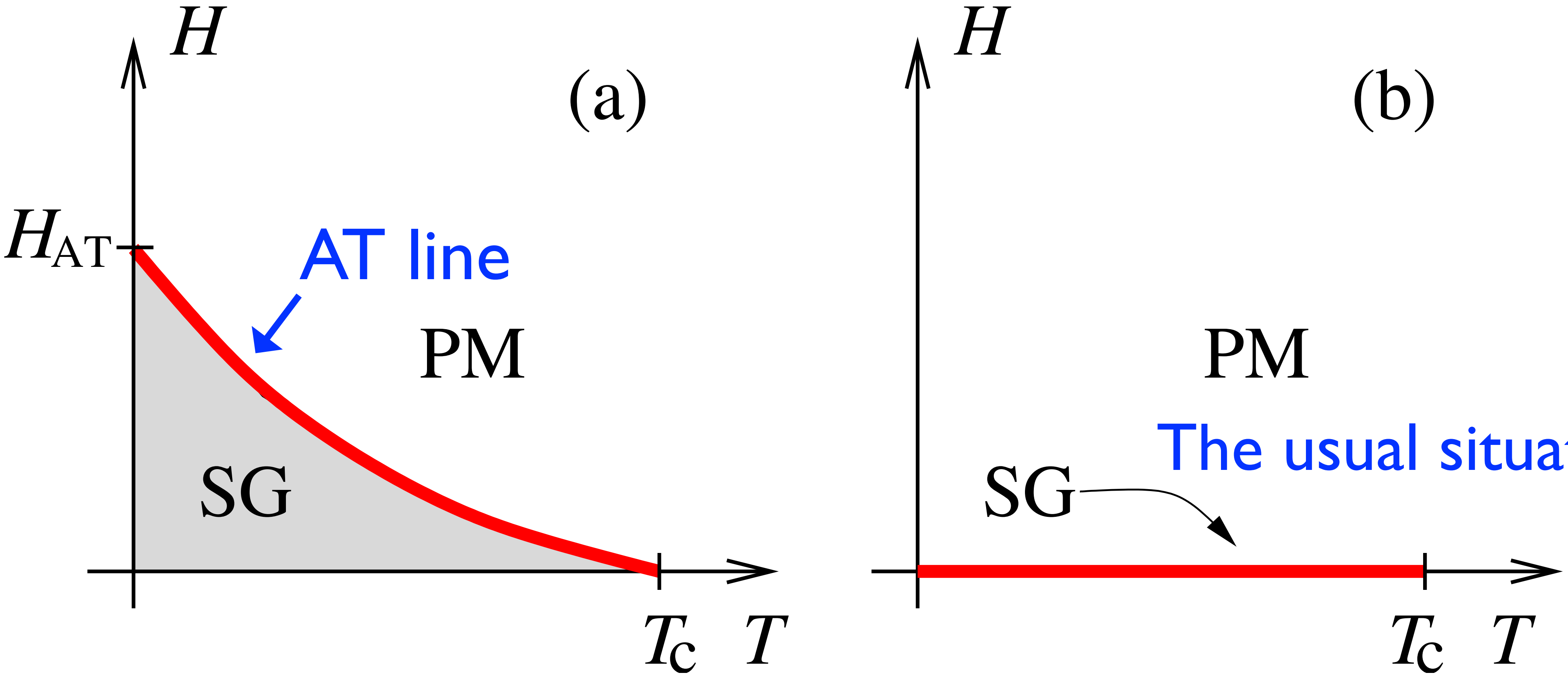


Does an AT line occur in real systems?

Overview

- Basic Introduction
  - What is a spin glass? Why are they important?
  - Why are Monte Carlo simulations hard for them?
- Are there phase transitions in spin glasses?
  - In zero field, the answer is clearly "yes" (e.g. Hasenbusch et al).
  - In a magnetic field the situation is less clear. In mean field theory there is a line of transitions in a field, the Almeida-Thouless (AT) line. Whether or not this actually occurs is of interest because
    - It is a transition without symmetry breaking and may be related to the putative "ideal glass transition" in structural glasses
    - The two phenomenological pictures of the spin glass state make opposite predictions for whether there is an AT line.

Spin glasses and structural glasses; are they related?

Supercooled liquid

Viscosity: Vogel-Fulcher law $\eta \propto \exp\left[\frac{A}{T - T_0}\right]$

Entropy difference between supercooled liquid and crystal

$$\Delta S \to 0 \text{ for } T \to T_K$$

where T_K is the Kauzmann temperature (the Kauzmann “paradox”)

Find $T_K \approx T_0$ (but system drops out of equilibrium at higher T so these are extrapolations.)

Is there an **“ideal glass transition”** at T_K?

Spin glasses and structural glasses

At mean field (MF) level:

Equations of "mode-coupling theory" of supercooled liquids are the same as the equations for the dynamics of a mean-field p-spin spin glass for $p > 2$.

Dynamic transition at T_d (which must disappear beyond MF)

Static transition at a lower temperature T_c.
Does T_c correspond to Kauzmann temperature T_K in a glass?

Spin glasses and structural glasses

Beyond mean field?

Moore and Yeo (2006) argue that the ideal glass transition corresponds to a spin glass transition in a magnetic field. Why? Argument involved, but perhaps related to the frozen density fluctuations below TK are (a) random (so spin-glass like) and (b) are not symmetric about zero (so like a spin model in a magnetic field).

According to Moore and Yeo

"The question, then, of whether there is a structural glass transition then turns to whether there is an AT line in the spin glass analogue."

Nature of the Spin Glass State?

Numerics and experiments clearly indicate that there is a spin glass transition in three dimensions in zero magnetic field.

But what is the nature of the spin glass state below T_c ?

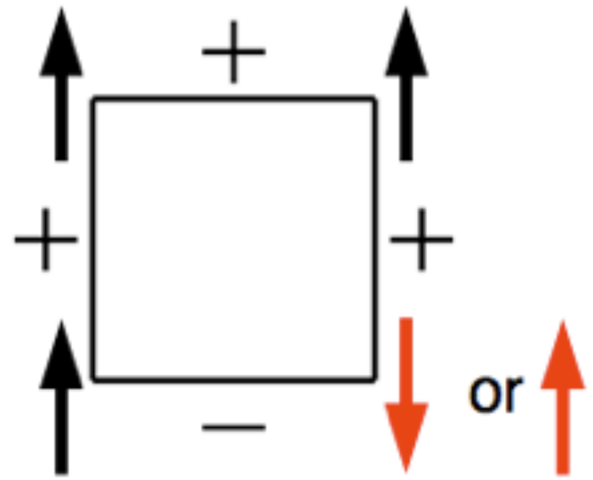
Two rival descriptions:

- "Replica Symmetry Breaking" (RSB) which is based on Parisi's solution of the spin glass mean field theory (MFT).
- "Droplet theory" of Fisher and Huse, Bray and Moore, McMillan.

Which, if either, is correct?
Here will focus on one aspect for which the two descriptions make opposite predictions and which should be checkable by simulations, namely whether or not there is a line of transitions in a magnetic field (AT line): RSB (YES), droplet theory (NO).

What is a spin glass?

A system with disorder and frustration



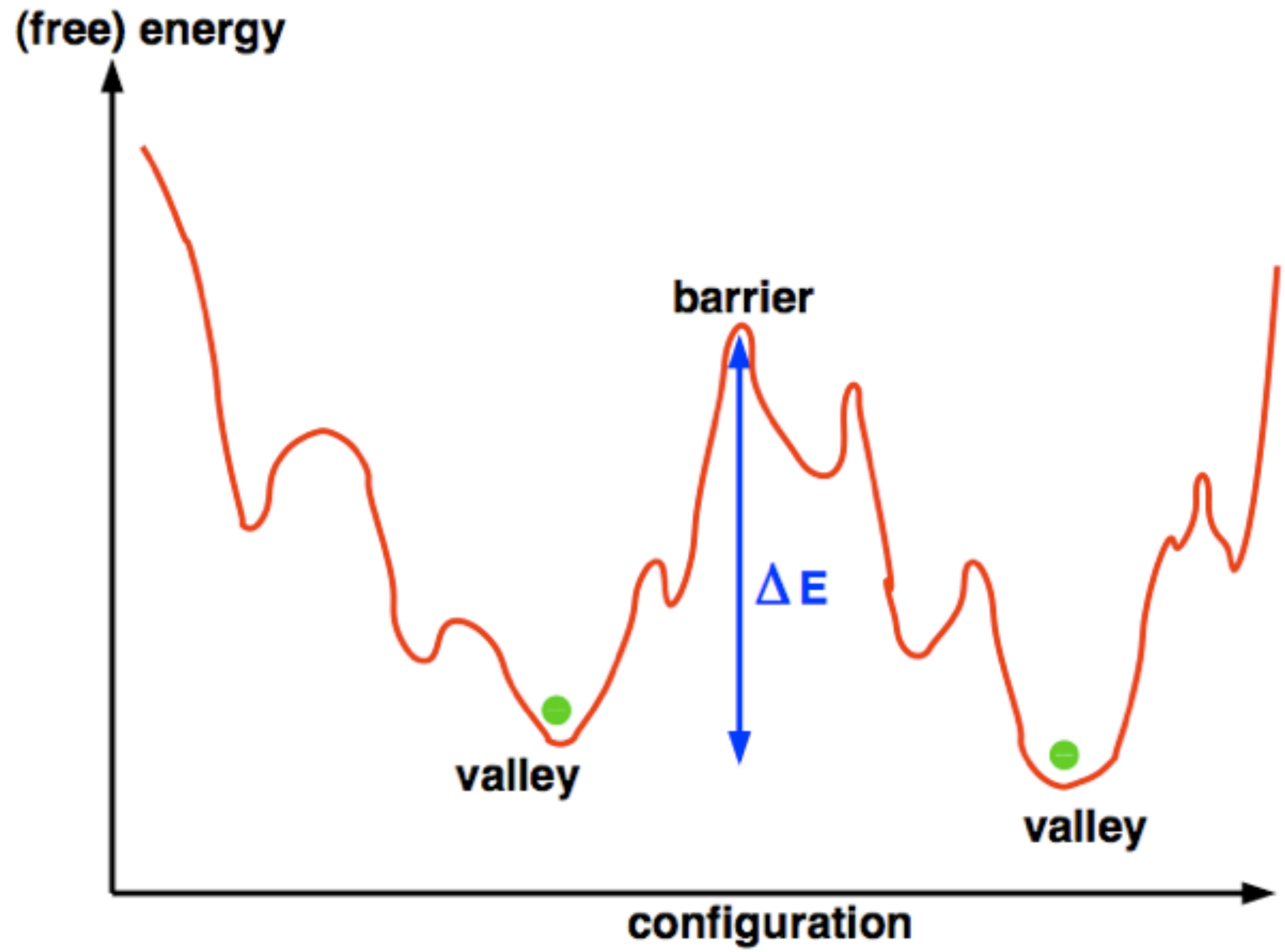
Most theory uses the simplest model with these ingredients: the Edwards-Anderson Model:

$$\boxed{\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}\, S_i S_j - \sum_i h_i\, S_i,} \qquad (S_i = \pm 1)$$

The J_{ij} are independent quenched random variables with a symmetric distribution (so no net preference for ferro- or antiferro-magnetism)

$$[J_{ij}]_{av} = 0, \qquad [J_{ij}^2]_{av} = J^2$$

Slow Dynamics



Slow dynamics The dynamics is very slow at low T. System not in equilibrium due to complicated energy landscape: system trapped in one "valley" for long times.

Many interesting experiments on non-equilibrium effects (aging).

Here concentrate on equilibrium phase transitions.

Spin Glass Systems

- The canonical spin glass:
  Dilute magnetic atoms, e.g. Mn in non-magnetic metal, e.g. Cu.
  RKKY interaction, sign oscillates with distance ⇒ frustration

- Important because relevant to other systems with complex energy landscape.
  - "Vortex glass" transition in high-Tc superconductors
  - Optimization problems
  - Protein folding
  - Error correcting codes
  - In a field, spin glasses may be related to structural glasses
  - ....

- Advantage of spin glasses:
  - very precise experiments (coupling to field)
  - "simple" models which can be easily simulated

Averaging in disordered systems

Two averages:

- Thermal average for a fixed (quenched) set of interactions. Done here by importance sampling Monte Carlo.

  $< \ \ldots\ldots \ >$

- Average over the disorder (i.e. quenched interactions). Do by repeating the simulation for many (typically several thousand) samples .

  $[\ \ldots\ldots\ ]_{av}$

Why is Monte Carlo hard (for SG)?

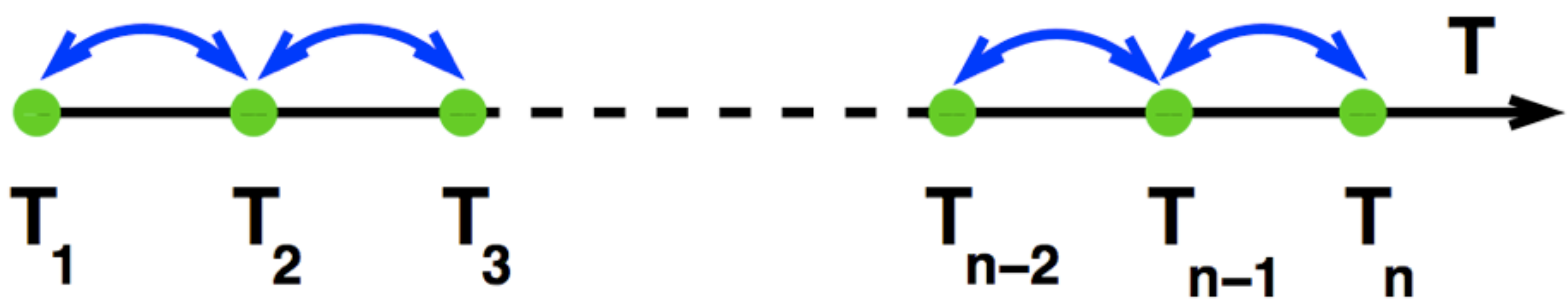
- Dynamics is very slow.
  System is trapped in valley separated by barriers.
  Use parallel tempering to speed things up.

- Need to repeat simulation for many samples
  but is trivially parallelizable.

Parallel Tempering

Problem: Very slow Monte Carlo dynamics at low-T;

System trapped in a valley. Needs more energy to overcome barriers. This is achieved by parallel tempering (Hukushima and Nemoto): simulate copies at many different temperatures:



Lowest T: system would be trapped:

Highest T: system has enough energy to fluctuate quickly over barriers.

Perform global moves in which spin configurations at neighboring temperatures are swapped.

Result: temperature of each copy performs a random walk between $\mathbf{T_1}$ and $\mathbf{T_n}$.

Advantage: Speeds up equilibration at low-T.

Correlation length

An important quantity is the bulk correlation length $\xi_{\rm bulk}$
This diverges like

$$\boxed{\xi_{\rm bulk} \propto (T - T_c)^{-\nu}}$$

What we actually calculate is the correlation length of the finite system, ξ_L. This can be defined from the wavevector dependent spin glass susceptibility, which for zero field, is defined by

$$\chi_{SG}(\mathbf{k}) = \frac{1}{N} \sum_{\langle i,j \rangle} \left[\langle S_i \, S_j \rangle^2 \right]_{av} \, e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$

using the (Ornstein-Zernicke form)

$$1/\chi_{SG}(\mathbf{k}) = 1/\chi_{SG}(0) \, \left(1 + \xi_L^2 k^2\right)$$

Using the two smallest wavevectors, k=0 and k=k_1=(2π/L)(1,0,0), gives

$$\xi_L = \frac{1}{k_1} \left(\frac{\chi_{SG}(0)}{\chi_{SG}(k_1)} - 1 \right)^{1/2}$$

Finite Size Scaling

Assumption: size dependence comes from the ratio L/ξ_{bulk} where

$$\xi_{\mathrm{bulk}} \sim (T - T_{SG})^{-\nu}$$

is the bulk correlation length.
In particular, the finite-size correlation length varies as

$$\boxed{\frac{\xi_L}{L} = X\left(L^{1/\nu}(T - T_{SG})\right),}$$

since ξ_L/L is $\boxed{\text{dimensionless}}$ (and so has no power of L multiplying the scaling function X).

Hence data for ξ_L/L for different sizes should $\boxed{\text{intersect at } T_{SG} \text{ and splay out below } T_{SG}.}$

Let's first see how this works for the Ising SG . . . (still in zero field)

Results for Ising SG

FSS of the correlation length of the Ising SG

(from Katzgraber et al (2006))

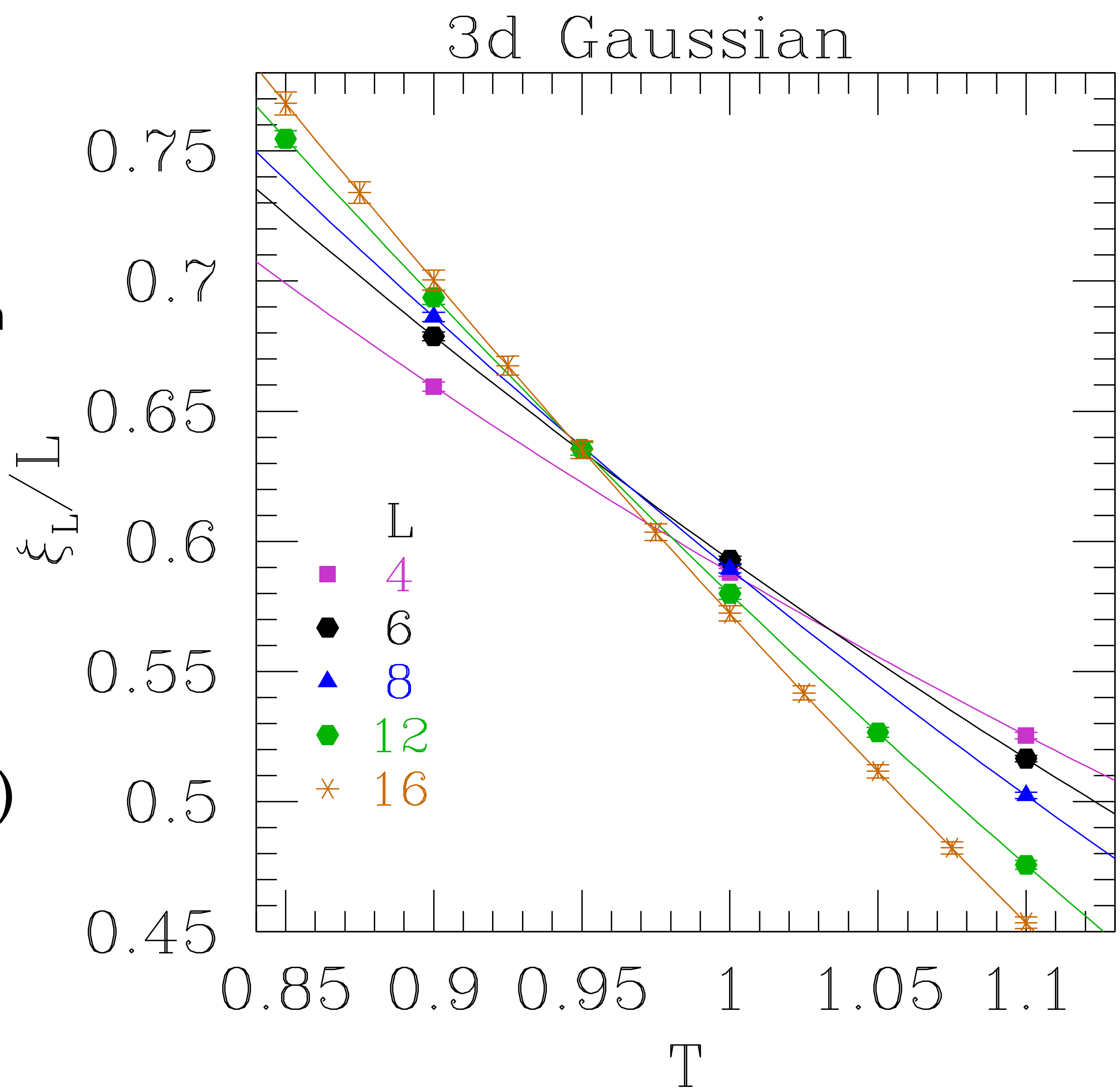
Correlation length determined from **k**-dependence of the FT of the spin-spin correlations $\langle S_i\, S_j \rangle^2$.

Method first used for SG by Ballesteros et al. but for the ± J distribution.

The clean intersections (corrections to FSS visible for L=4) imply

$T_{SG} \cong 0.96$

Previously, Marinari et al found $T_{SG} \cong 0.95 \pm 0.04$ by a different analysis.



Precise Results for Ising SG

To get precise results need to include **corrections** to FSS. e.g. the intersections are not precisely at a common temperature. Suppose sizes L and 2L intersect at $T^*(L)$, then

$$T^\star(L) = T_c + \frac{A}{L^{\omega + 1/\nu}}$$

where A is an amplitude and ω is the leading correction to scaling exponent.

Large scale simulations and VERY careful analysis of 3d Ising spin glass by Hasenbusch, Pelisetto and Vicari, arXiv:0809.3329, PRB, 78, 214205 (2008), identified the leading correction and hence get very accurate results for the parameters of the phase transition:

$$\begin{aligned} \nu &= 2.45(15), \\ \eta &= 0.375(10), \\ \omega &= 1.0(1), \\ T_c \equiv 1/\beta_c &= 1.109(11). \end{aligned}$$

$\Rightarrow$

There IS a (symmetry breaking) spin glass transition in zero field

Is there an Almeida-Thouless line?

In MFT (the exact solution of the infinite-range Sherrington-Kirkpatrick model) there's a transition in a field for an Ising spin glass the de Almeida Thouless (AT) line from a spin glass phase (divergent relaxation times, "replica symmetry breaking") to a paramagnetic phase (finite relaxation times, "replica symmetry").

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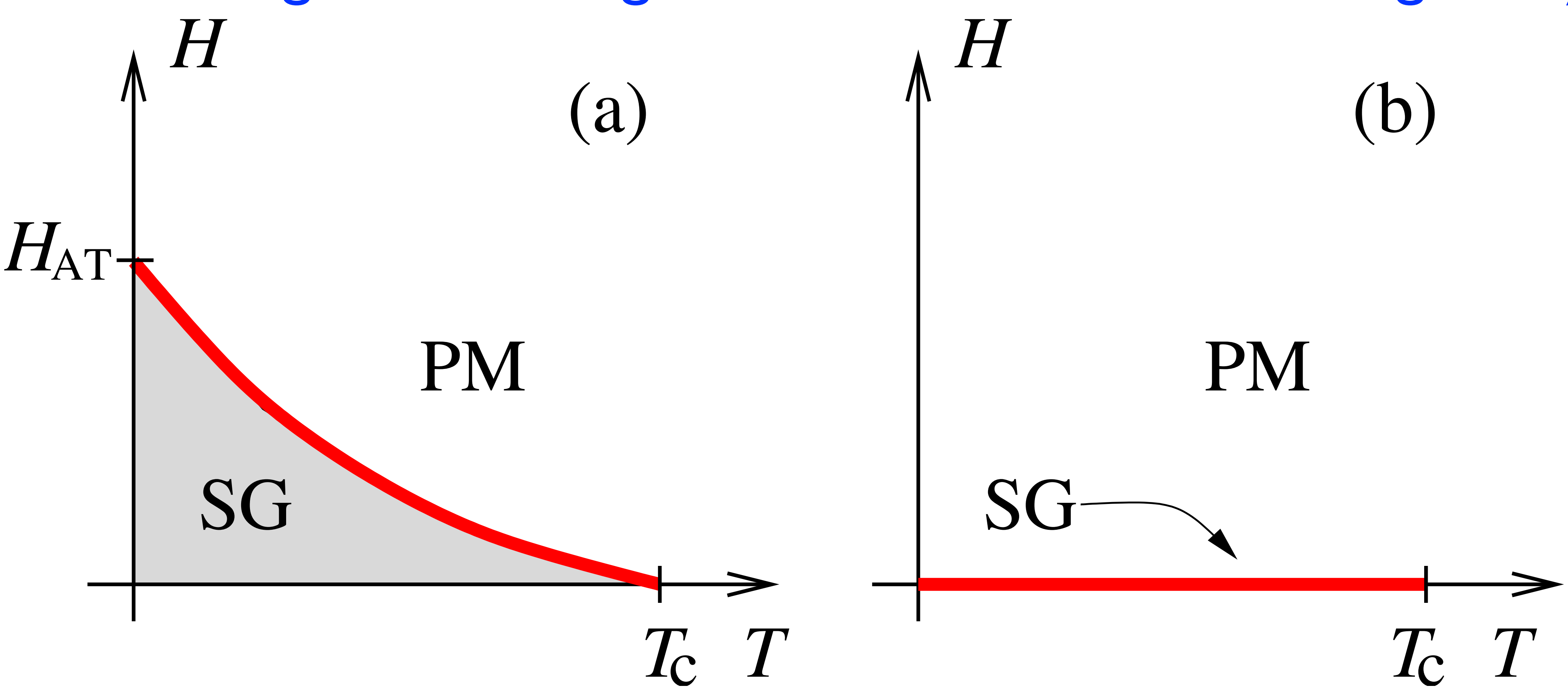


Does an AT line occur in real systems?

- "Replica Symmetry Breaking" picture: Yes, see (a)
- "Droplet" Picture: No, see (b)

How to detect the AT line

The quantity which diverges at the transition in a field is $\chi_{SG}(0)$ where

$$\chi_{SG}(\vec{k}) = \frac{1}{N} \sum_{\langle i,j \rangle} \left[\left(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \right)^2 \right]_{av} \exp[i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)]$$

i.e. ∝ square of connected correlation function.

Using "standard" finite-size scaling (FSS), Katzgraber and APY (d=3) and Parisi et al (d=4) do not find an AT line by this approach.

To study this question further, both groups have found it useful to get information from

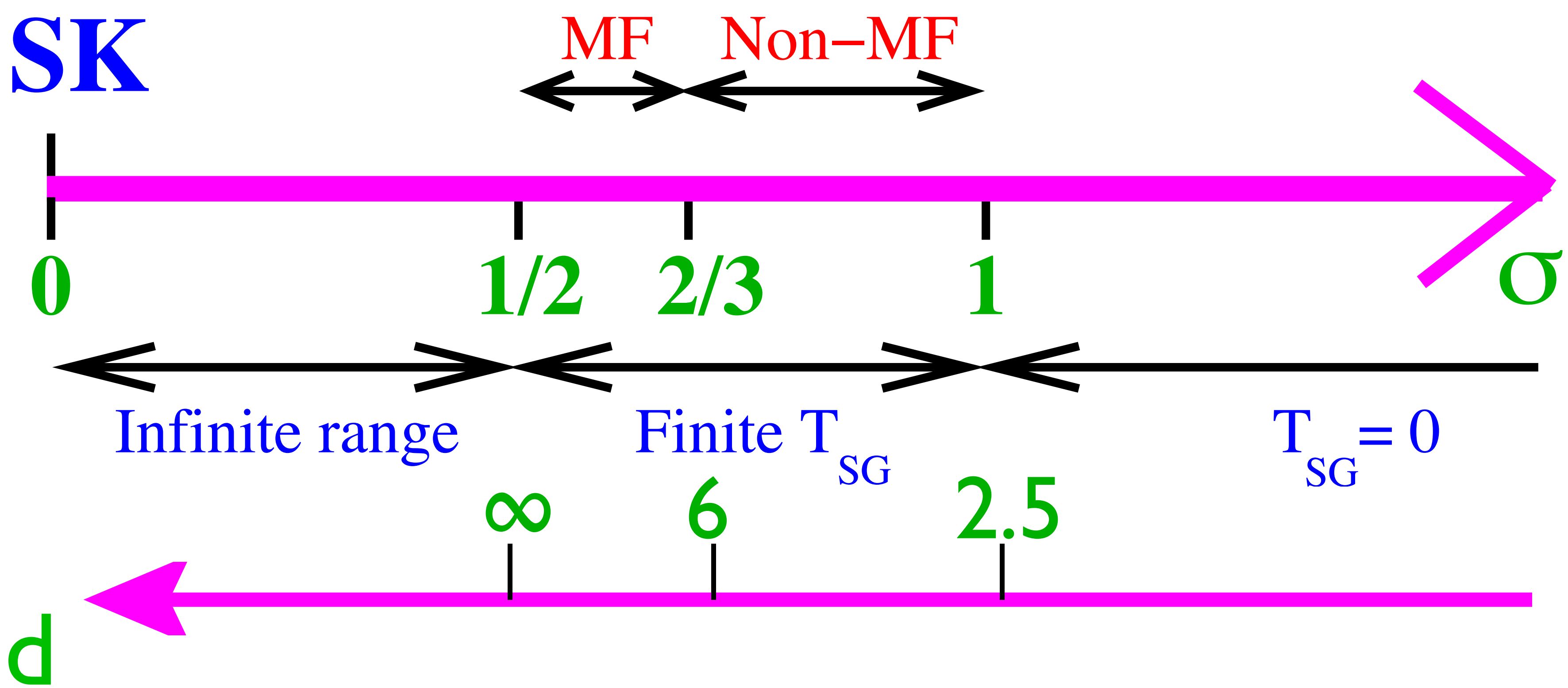
related models in one-dimension with long-range interactions

because one can study a large range of (linear) sizes and hence can do FSS for a range of dimensions d (including high-d).

1-d Models

We take 1-d models where $J_{ij} \sim 1/|r_i - r_j|^\sigma$

Increasing σ is like decreasing d:



For a given d there is a σ(d) for which the LR model in 1-d is a (rough) proxy for a SR model in d dimensions.

Advantages:

- Can study a wide range of d including high-d
- There are many values of L for FSS (and also of k)

The Model

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i H_i S_i$$

where

$$[J_{ij}]_{av} = 0, \qquad [J_{ij}^2] \propto 1/|r_i - r_j|^{2\sigma}$$

$$[H_i]_{av} = 0, \qquad [H_i^2] = H^2$$

Recent Results on LR model

To represent d = 3 and d = 4 we take

σ(3) = 0.896

σ(4) = 0.784

In standard finite-size scaling (FSS) we look for

Intersections of the scale-invariant quantities

ξ_L / L (correlation length, obtained from k=0 and 2π/L)

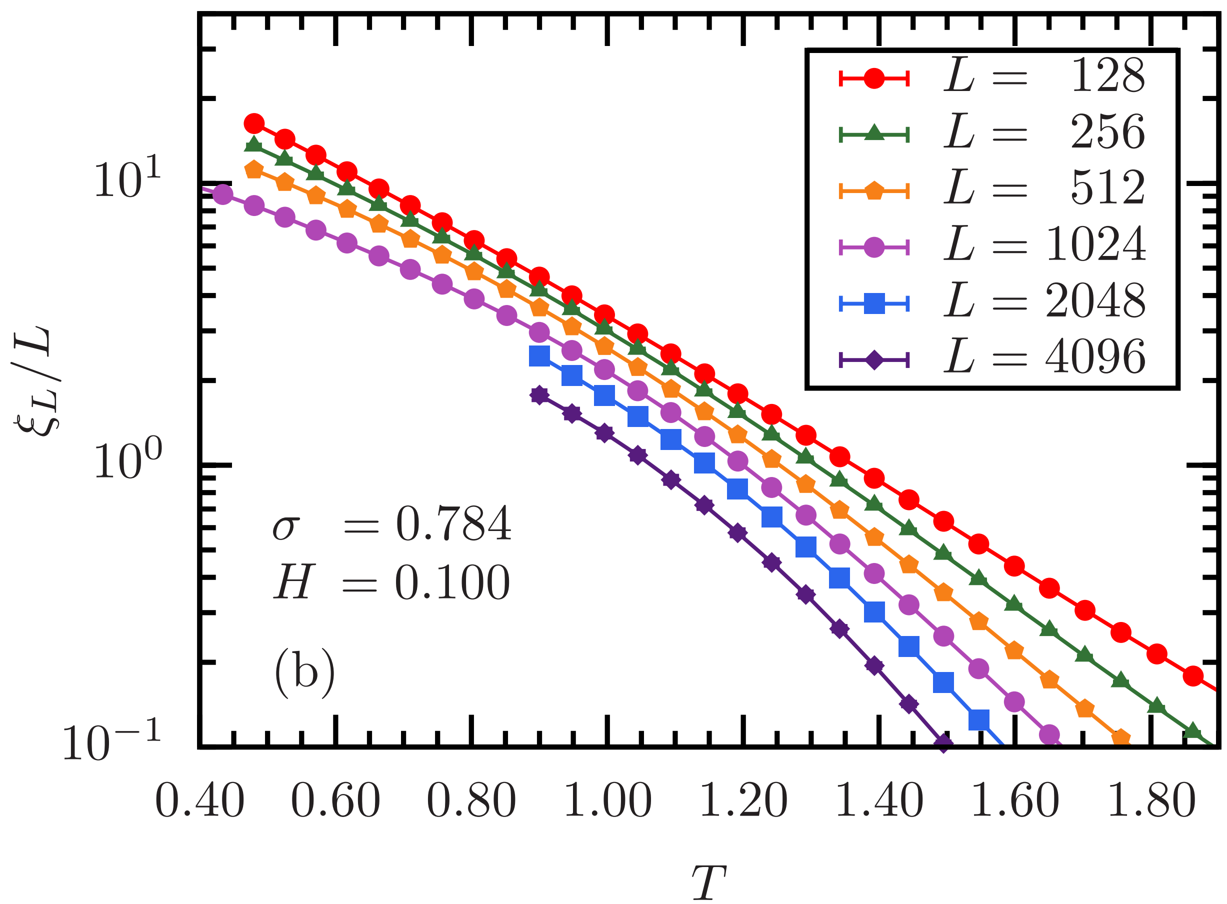
$\chi_{SG} / L^{2-\eta}$ $(2 - \eta = 2\sigma - 1 \text{ here})$ (η known exactly for LR)

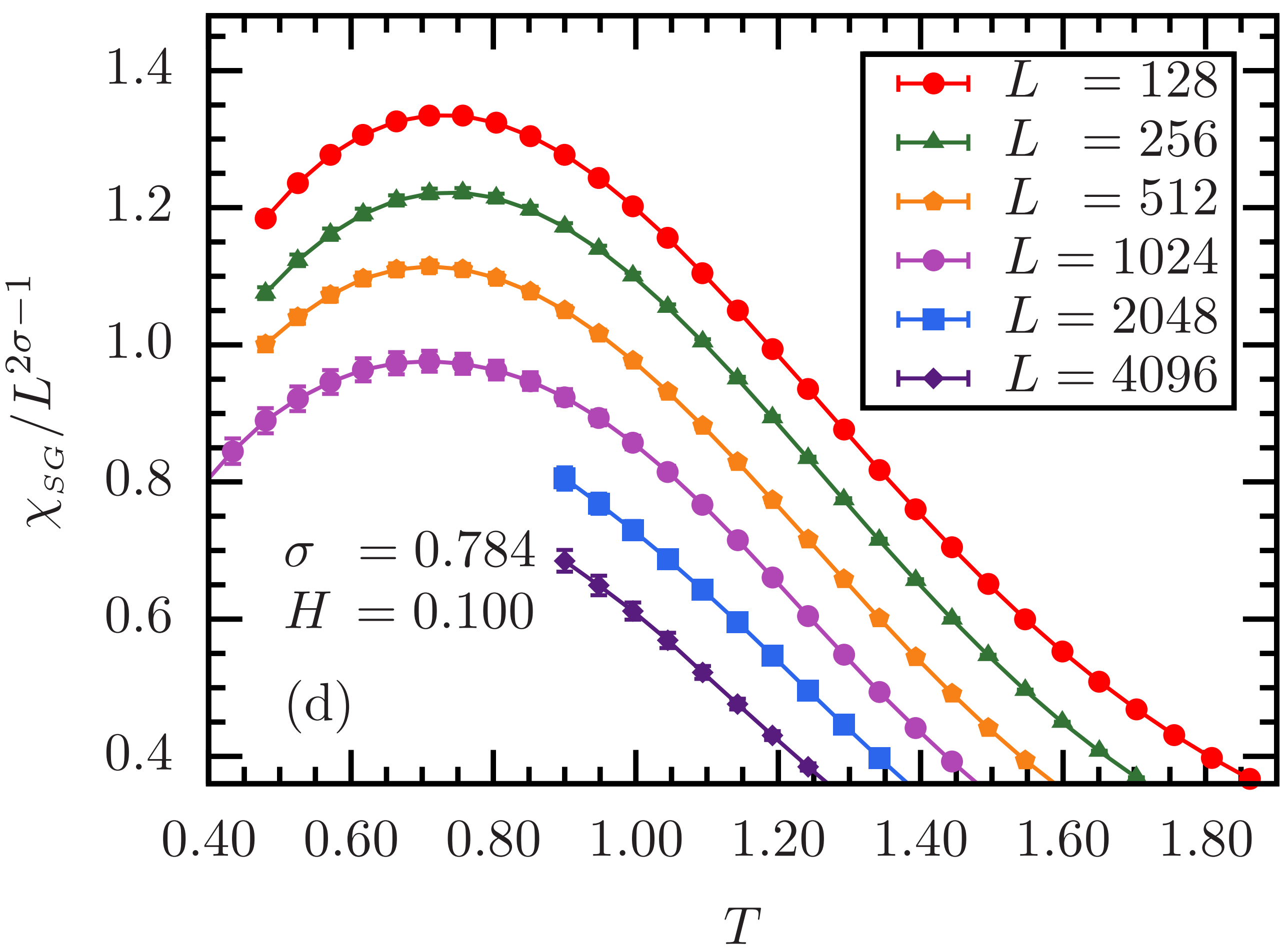
locate the transition, since, for a scale-invariant quantity X, the finite-size-scaling (FSS) form is

$$X(T, L) = \widetilde{X}\left(L^{1/\nu}(T - T_c) \right)$$

Hence data for scale-invariant quantities for different sizes intersect at T_c.

Standard FSS for σ(4) = 0.784

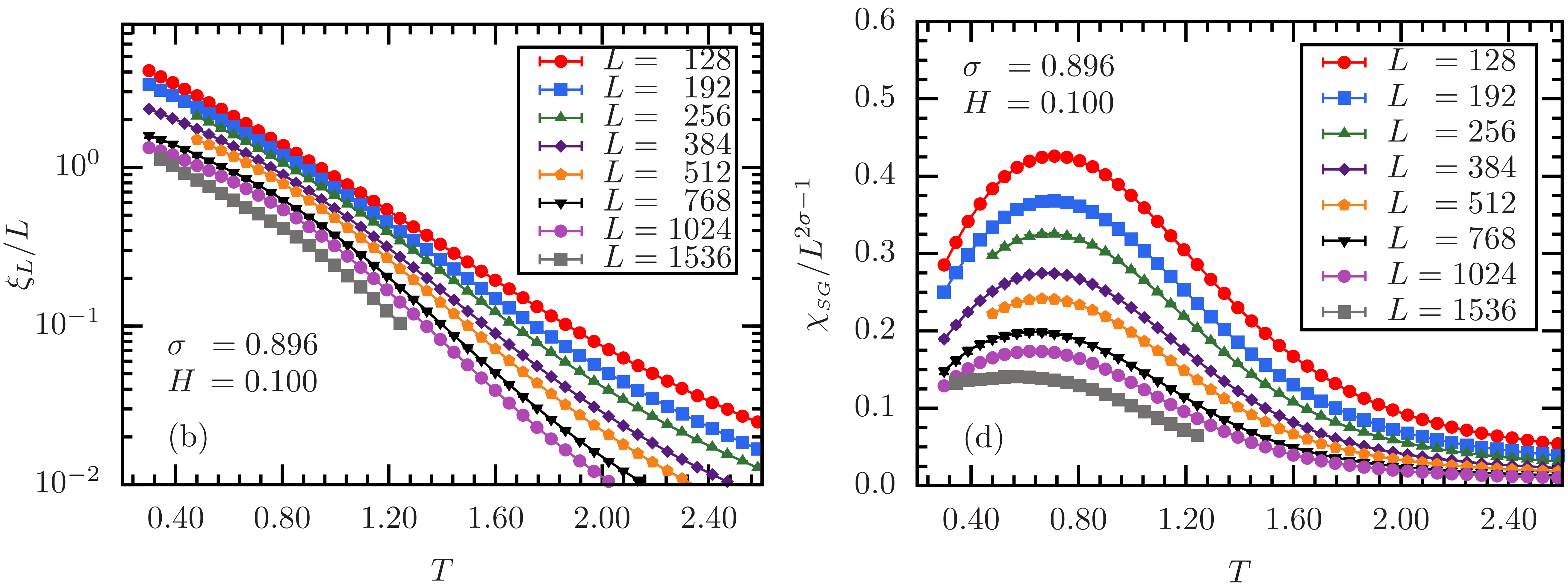




This model is a proxy for d=4.

No sign of intersections, i.e. implies no transition in a field

Standard FSS for σ(3) = 0.896



This model is a proxy for d=3.

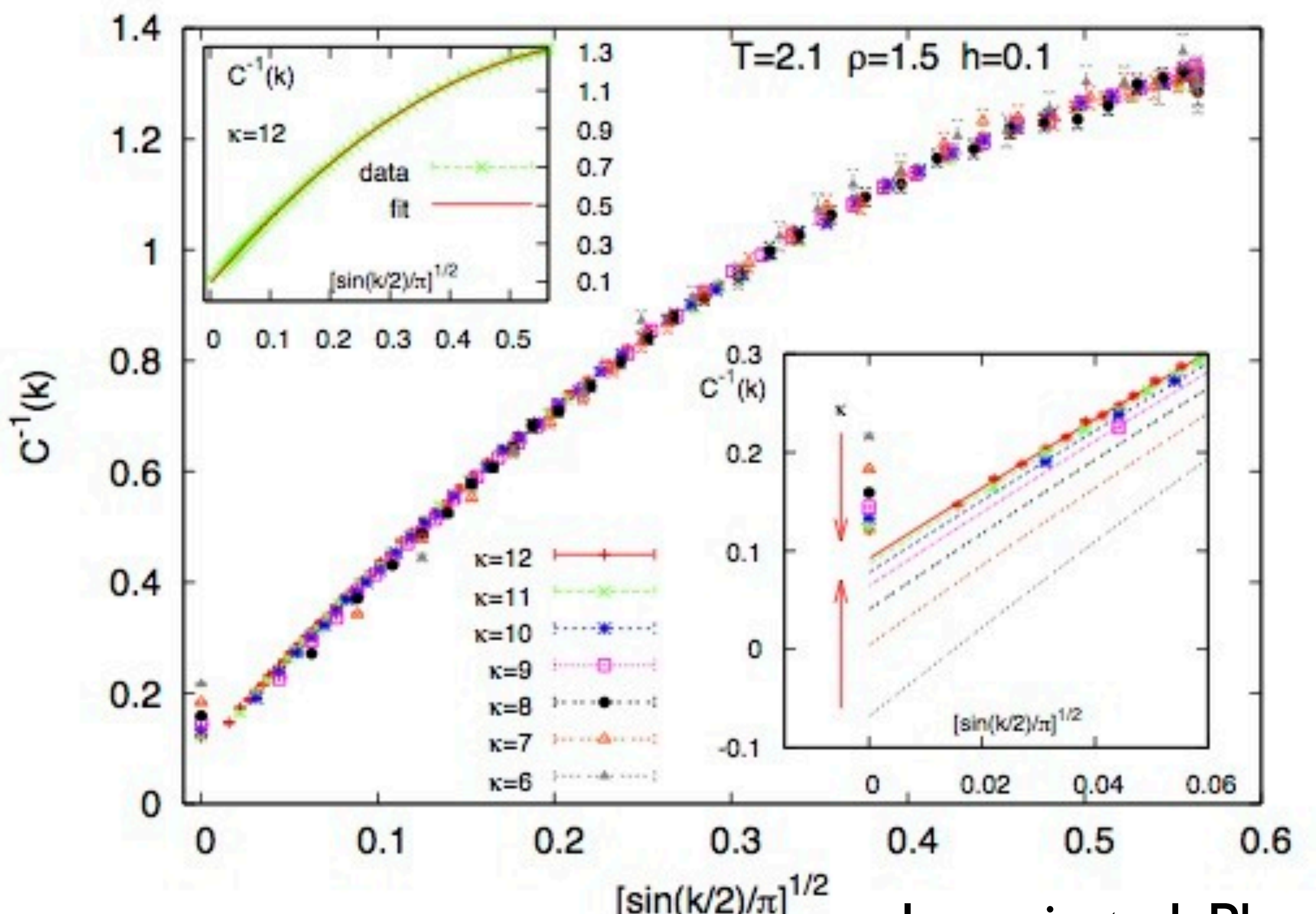
Again no sign of intersections, i.e. implies no transition in a field

"Non-Standard" FSS

Previous analysis used k=0 fluctuations. Leuzzi, Parisi, Ricci-Tersenghi, Ruiz-Lorenzo, [PRL, **103**, 267201 (2009)] claim, one should avoid k = 0 data because it has large corrections to FSS.

Ornstein-Zernicke form:

$$\chi_{SG}^{-1}(k) = \chi_{SG}^{-1}(0) + Ak^y + \cdots \quad \text{where} \quad \begin{cases} y = 2 & \text{short-range,} \\ y = 2\sigma - 1 & \text{long-range,} \end{cases}$$



We see that

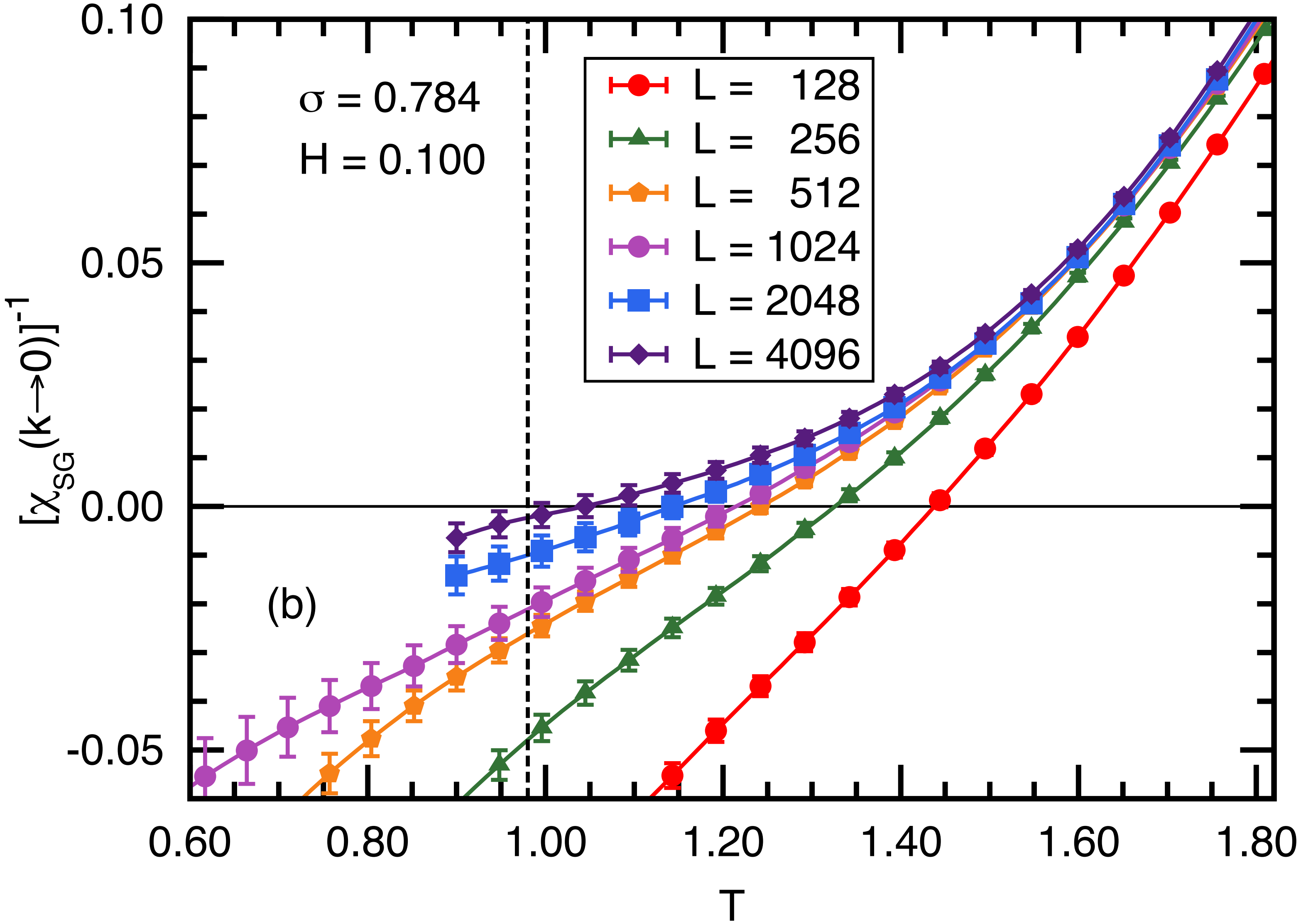
$$\chi_{SG}^{-1}(k \to 0) \neq \chi_{SG}^{-1}(0)$$

Suggestion:
look at $\chi_{SG}^{-1}(k \to 0)$

Leuzzi et al, Phys. Rev. Lett. 103, 267201 (2009)

"Non-Standard" FSS II

Example of (our) data for σ(4) = 0.784:
This model is a proxy for d=4.



$\chi_{SG}^{-1}(k \to 0)$ vanishes at

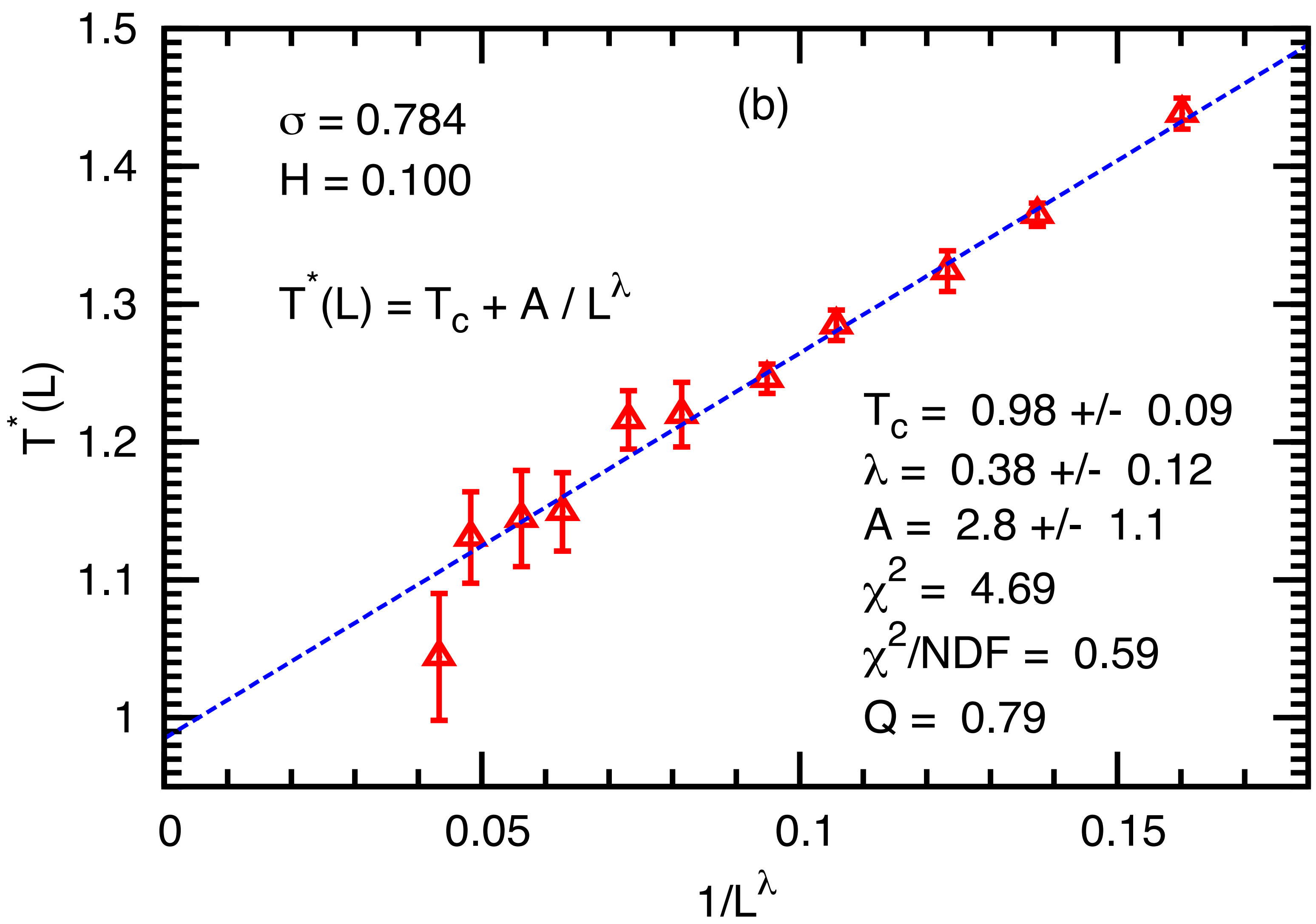
T = T*(L)

Fit T*(L) to

$$T^\star(L) = T_c + \frac{A}{L^\lambda}$$

"Non-Standard" FSS III

$T^*(L)$ for (our) data for $\sigma(4) = 0.784$:
This model is a proxy for d=4.



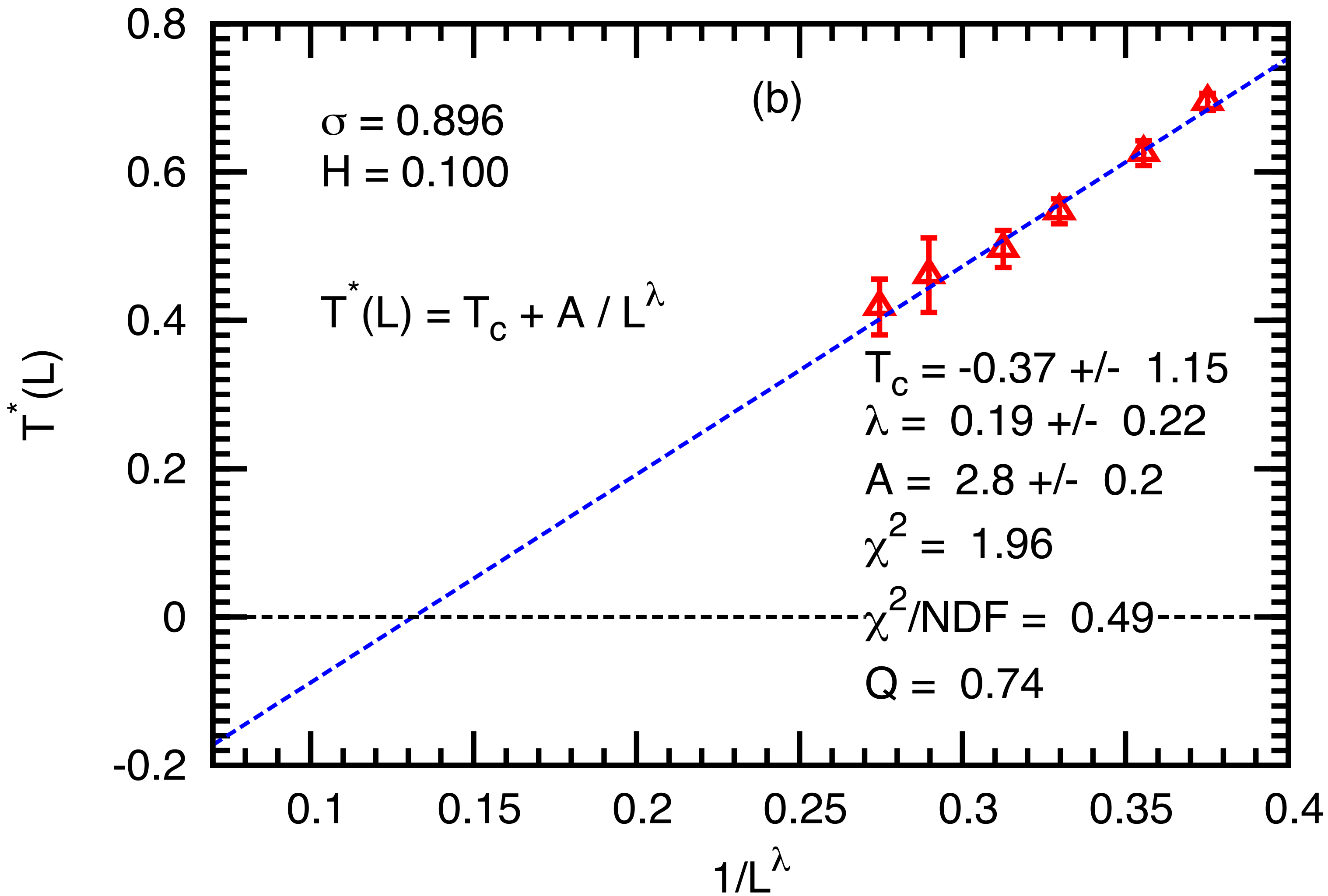
$$T^\star(L) = T_c + \frac{A}{L^\lambda}$$

The fit is good and gives a non-zero T_c. This is also the result of Leuzzi et al. Contradiction with "standard" FSS. Explanation?

"Non-Standard" FSS IV

$T^*(L)$ for (our) data for $\sigma(3) = 0.894$:
This model is a proxy for d=3.

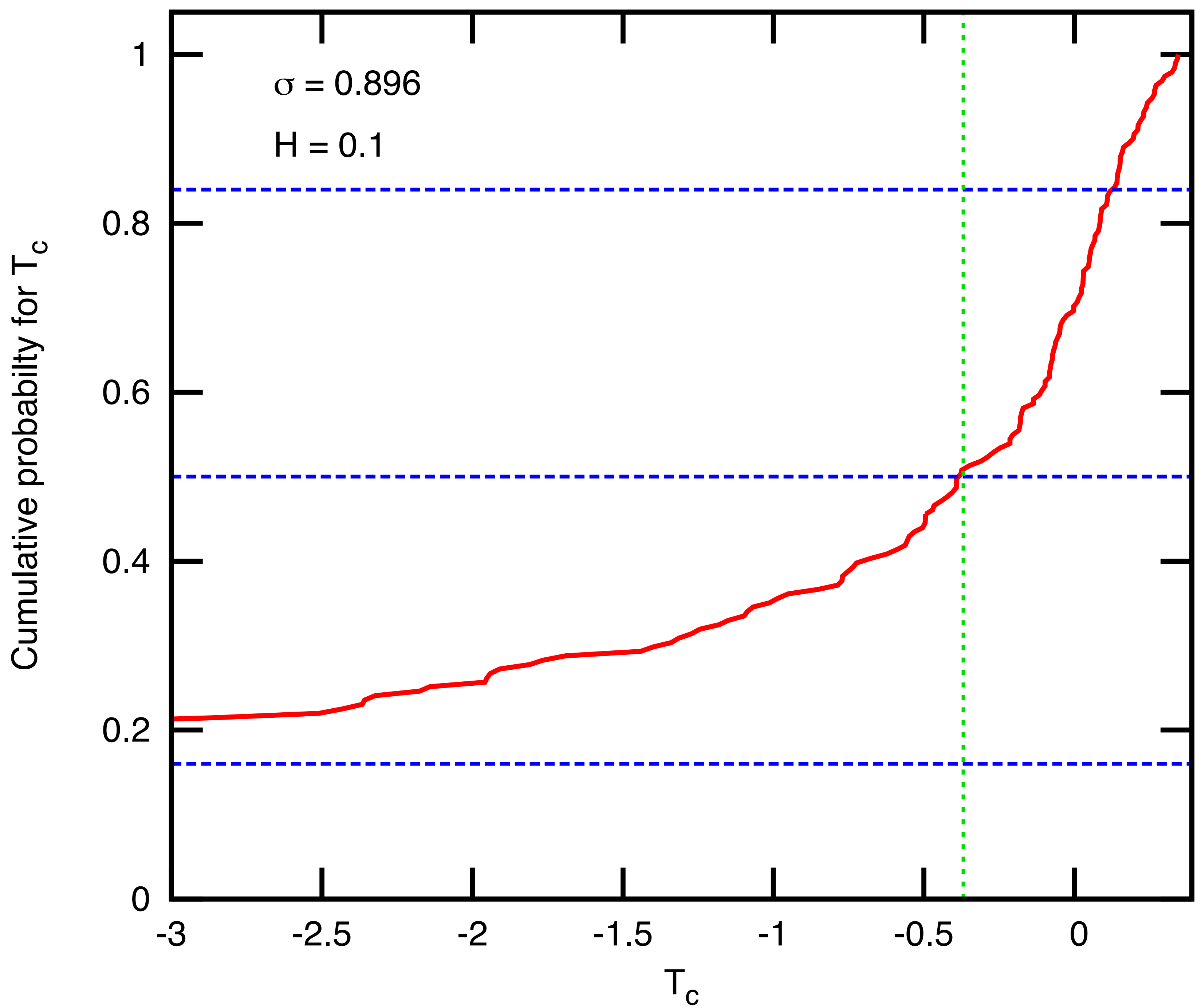
$$T^\star(L) = T_c + \frac{A}{L^\lambda}$$



Seems consistent with Tc = 0, but error bars ridiculously large. Do a more detailed analysis using bootstrap.

"Non-Standard" FSS V

(Our) T_c data for $\sigma(3) = 0.894$, analyzed with bootstrap.
This model is a proxy for d=3.



Fitted each bootstrap dataset.
Confidence limit taken: cumulative probability between 16% and 84%.
Gives $T_c < 0.13$.
Only 30% of bootstraps give $T_c > 0$.
Hence, compatible with $T_c = 0$ (the "standard" FSS result).

Conclusions

- For $\sigma(4)$, (proxy for 4d) there is an apparent contradiction:
  "standard" FSS gives no AT line
  "non-standard" FSS gives an AT line
  One or other of the analyses must be using data which is not in the asymptotic scaling regime.
  Which one, "standard" or "non-standard"?
  For the future: How can we reduce corrections to FSS?
- For $\sigma(3)$ (proxy for 3d):
  "standard" FSS gives no AT line
  "nonstandard" FSS data has a large scatter but is compatible with no AT line.
  Hence probably no contradiction, and **no AT Line**, and probably no ideal glass transition.

Danke schön