

Phase Transition in Spin Glasses

A.P. Young



UNIVERSITY OF CALIFORNIA

SANTA CRUZ

**Invited talk at “Monte Carlo Algorithms in Statistical Physics”,
University of Melbourne, July 26, 2010**

Collaborators:

H. Katzgraber, D. Larson, L.W. Lee, J. Pixley, V. Martin-Mayor, L. Fernandez, S. Perez-Gaviro, A. Tarancon

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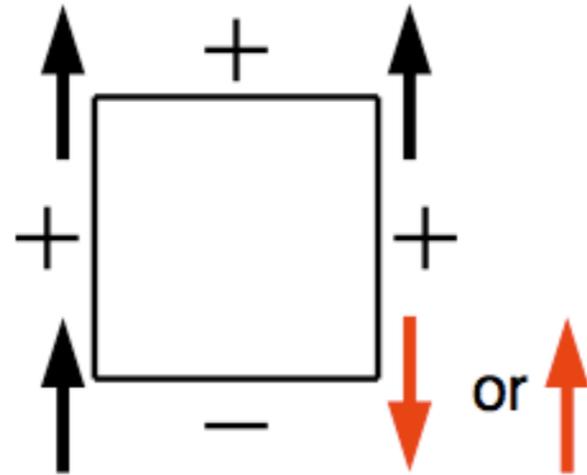


Overview

- Basic Introduction
 - What is a spin glass? Why are they important?
 - Why are Monte Carlo simulations for spin glasses hard?
- Try to answer two important questions concerning phase transitions in spin glasses:
 - Is there a phase transition in an isotropic Heisenberg spin glass?
 - Is there a transition in an Ising spin glass in a magnetic field (Almeida-Thouless line)?

What is a spin glass?

A system with **disorder** and **frustration**



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

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i .$$

Interactions are **quenched** and are random (have either sign).

Take a **Gaussian** distribution: $[J_{ij}]_{\text{av}} = 0$; $[J_{ij}^2]_{\text{av}}^{1/2} = J (= 1)$

Spins, \mathbf{S}_i , **fluctuate** and have m -components:

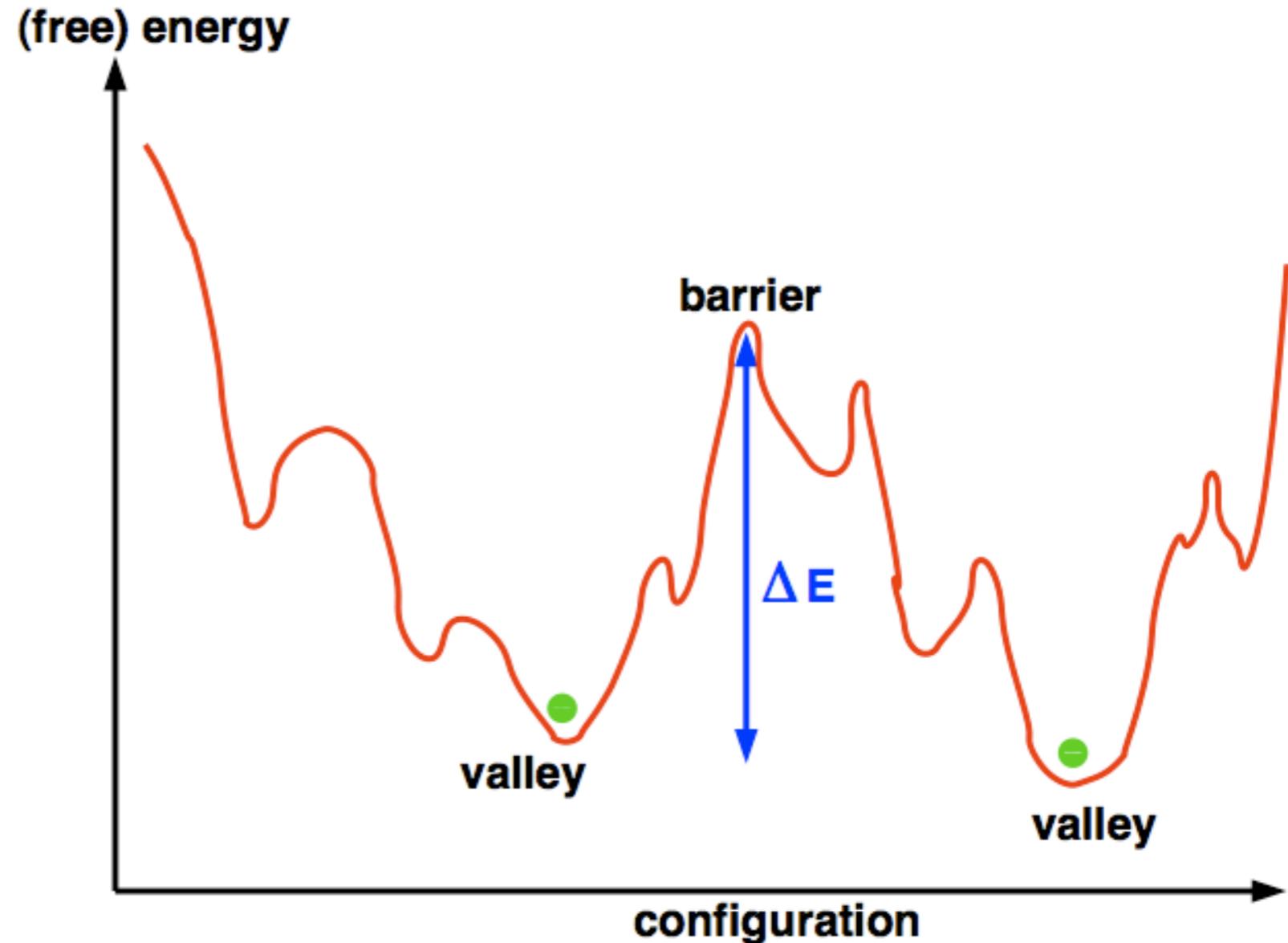
$$m = 1 \quad (\text{Ising})$$

$$m = 2 \quad (\text{XY})$$

$$m = 3 \quad (\text{Heisenberg}).$$

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 \Rightarrow frustration
- Important because relevant to other systems with complex energy landscape.
 - “Vortex glass” transition in high- T_c superconductors
 - Optimization problems
 - Protein folding
 - Error correcting codes
 -
- Advantage of spin glasses:
 - very precise experiments (coupling to field)
 - “simple” models which can be easily simulated

Spin Glass Phase Transition

Phase transition at $T = T_{SG}$.

For $T < T_{SG}$ the spin freeze in some random-looking orientation.

As $T \rightarrow T_{SG}^+$, the correlation length ξ_{SG} diverges.

The correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ becomes significant for $R_{ij} < \xi_{SG}$, though the sign is random. A quantity which diverges is the spin glass susceptibility

$$\chi_{SG} = \frac{1}{N} \sum_{i,j} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2]_{av},$$

(notice the square) which is accessible in simulations. It is also essentially the same as the non-linear susceptibility, χ_{nl} , defined by

$$m = \chi h - \chi_{nl} h^3 + \dots$$

(m is magnetization, h is field), which can be measured experimentally.

For the EA model $T^3 \chi_{nl} = \chi_{SG} - \frac{2}{3}$.

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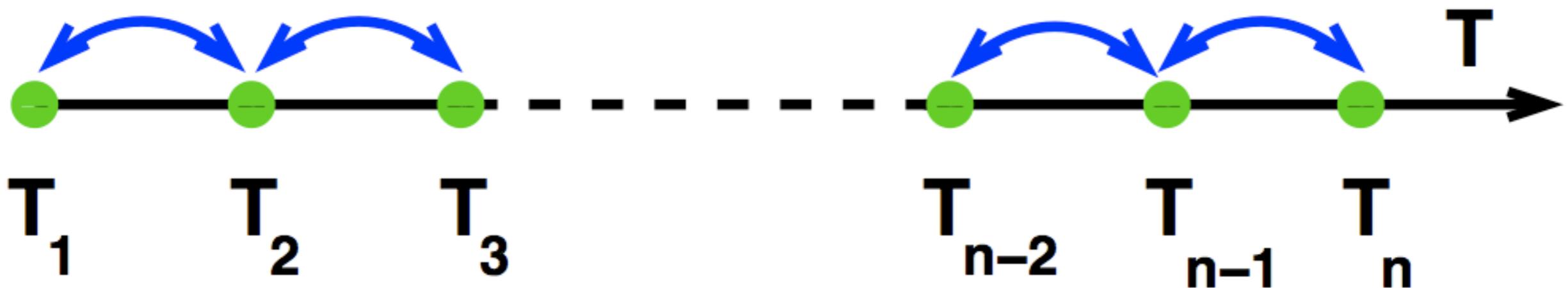
Why is Monte Carlo hard (for SG)?

- **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 T_1 and T_n .

Advantage: Speeds up equilibration at low- T .

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Finite Size Scaling

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

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

is the **bulk** correlation length.

In particular, the **finite-size** correlation length **varies as**

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

since ξ_L/L is **dimensionless** (and so has no power of L multiplying the scaling function X).

Hence data for ξ_L/L for different sizes should

intersect at T_{SG} and splay out below T_{SG} .

Let's first see how this works for the **Ising SG** ...

Results for Ising SG

FSS of the correlation length of the Ising SG

(from Katzgraber et al (2006))

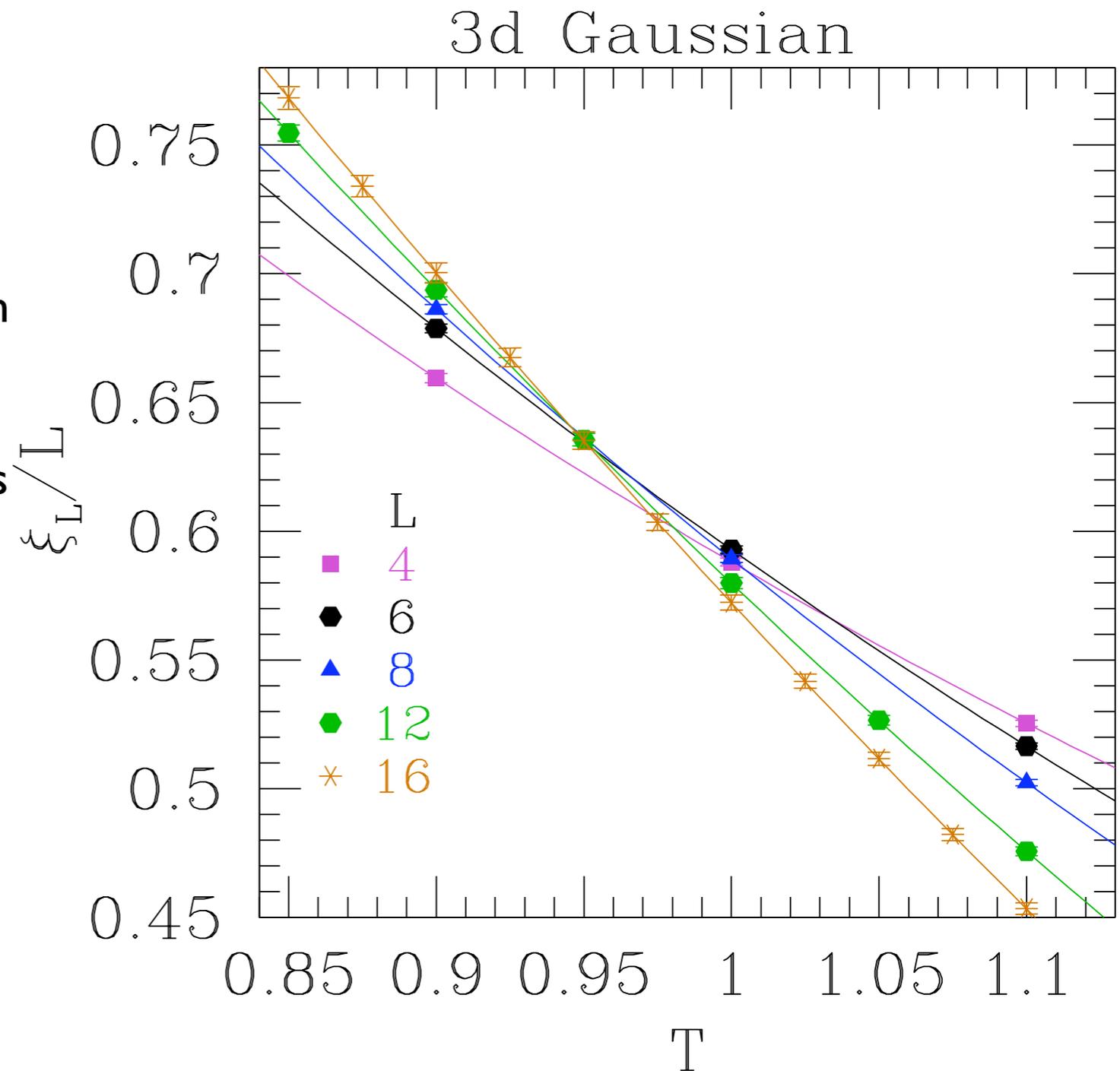
Correlation length determined from **k-dependence** of the FT of the spin-spin correlations $\langle S_i S_j \rangle^2$.

Method first used for SG by Ballesteros et al. but for the $\pm J$ 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.

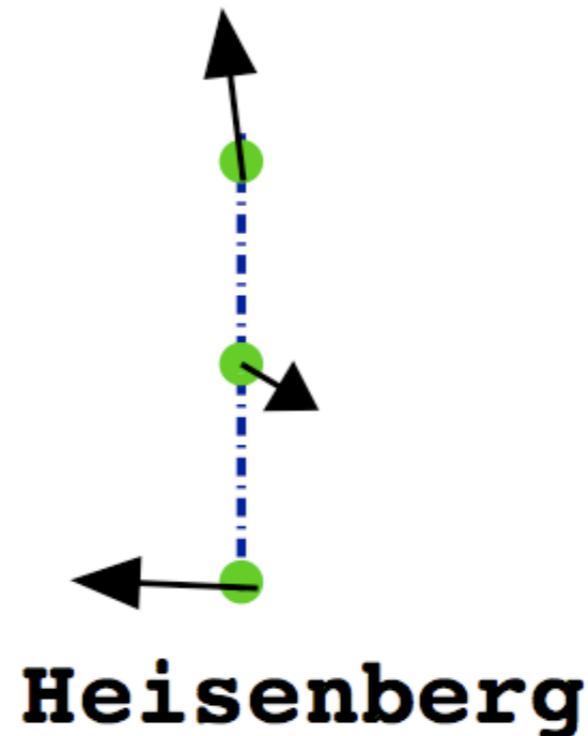
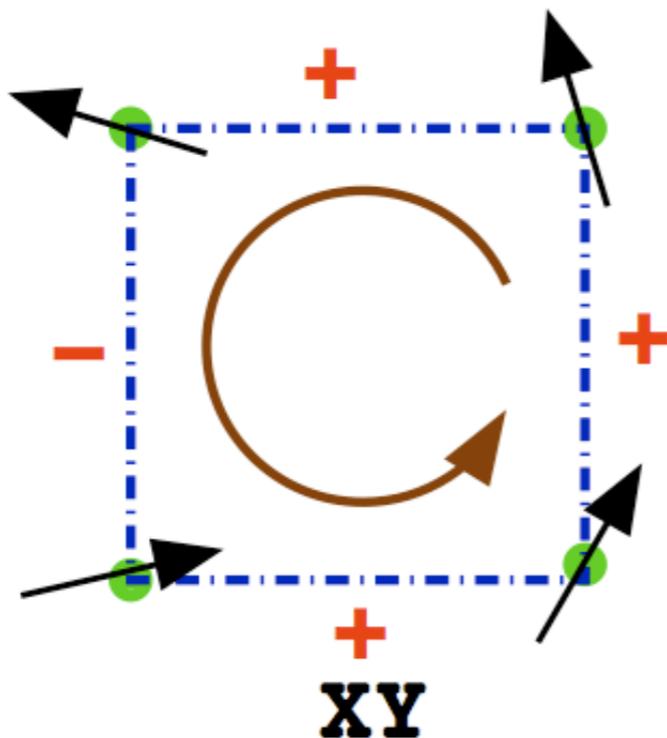


Chirality

- **Unfrustrated**: Thermally activated chiralities (vortices) drive the Kosterlitz-Thouless Berezinskii transition in 2d XY ferromagnet
- **Frustrated**: Chiralities are **quenched in** by the disorder at low-T because the ground state is **non-collinear**.

Define Chirality by (Kawamura)

$$\kappa_i^\mu = \begin{cases} \frac{1}{2\sqrt{2}} \sum'_{\langle l,m \rangle} \text{sgn}(J_{lm}) \sin(\theta_l - \theta_m), & \text{XY } (\mu \perp \text{square}) \\ \mathbf{S}_{i+\hat{\mu}} \cdot \mathbf{S}_i \times \mathbf{S}_{i-\hat{\mu}}, & \text{Heisenberg} \end{cases}$$



Motivation for Vector Model

- Old Monte Carlo for Heisenberg: T_{SG} , if any, seems very low, probably zero.
- Kawamura: $T_{SG} = 0$, but transition in the chiralities, $T_{CG} > 0$, this implies “spin-chirality decoupling”. Subsequently Kawamura suggests that $T_{SG} > 0$ but $T_{SG} < T_{CG}$.
- But: alternative of a single transition proposed by Nakamura and Endoh, Lee and APY, Campos et al, Pixley and APY.

Here: describe recent work on **FSS of the correlation lengths** of both spins and chiralities for the **Heisenberg** spin glass.

Useful because

- this was the most successful approach for the Ising spin glass
- treat spins and chiralities on equal footing

Over-relaxation Moves

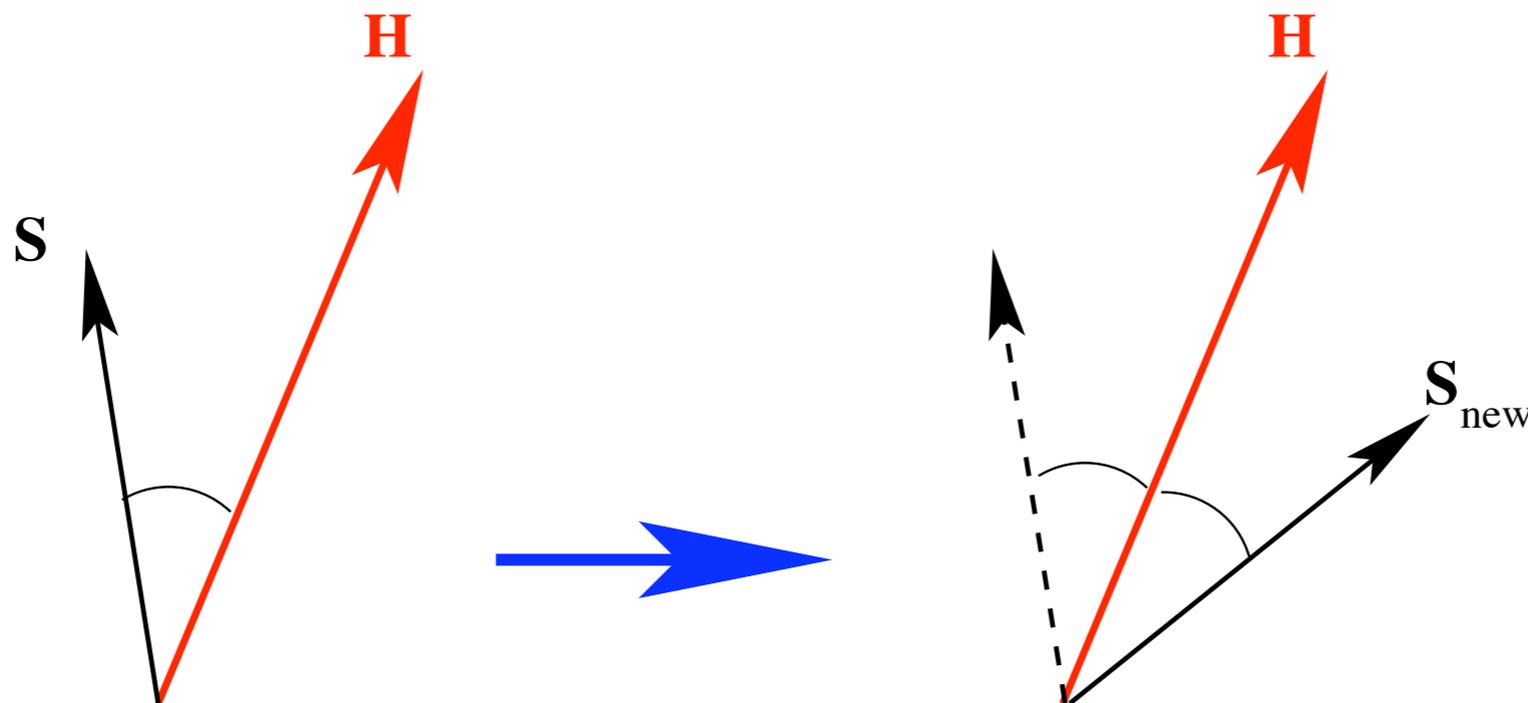
In addition to

- Heat bath (single spin) moves, and
- Parallel tempering moves,

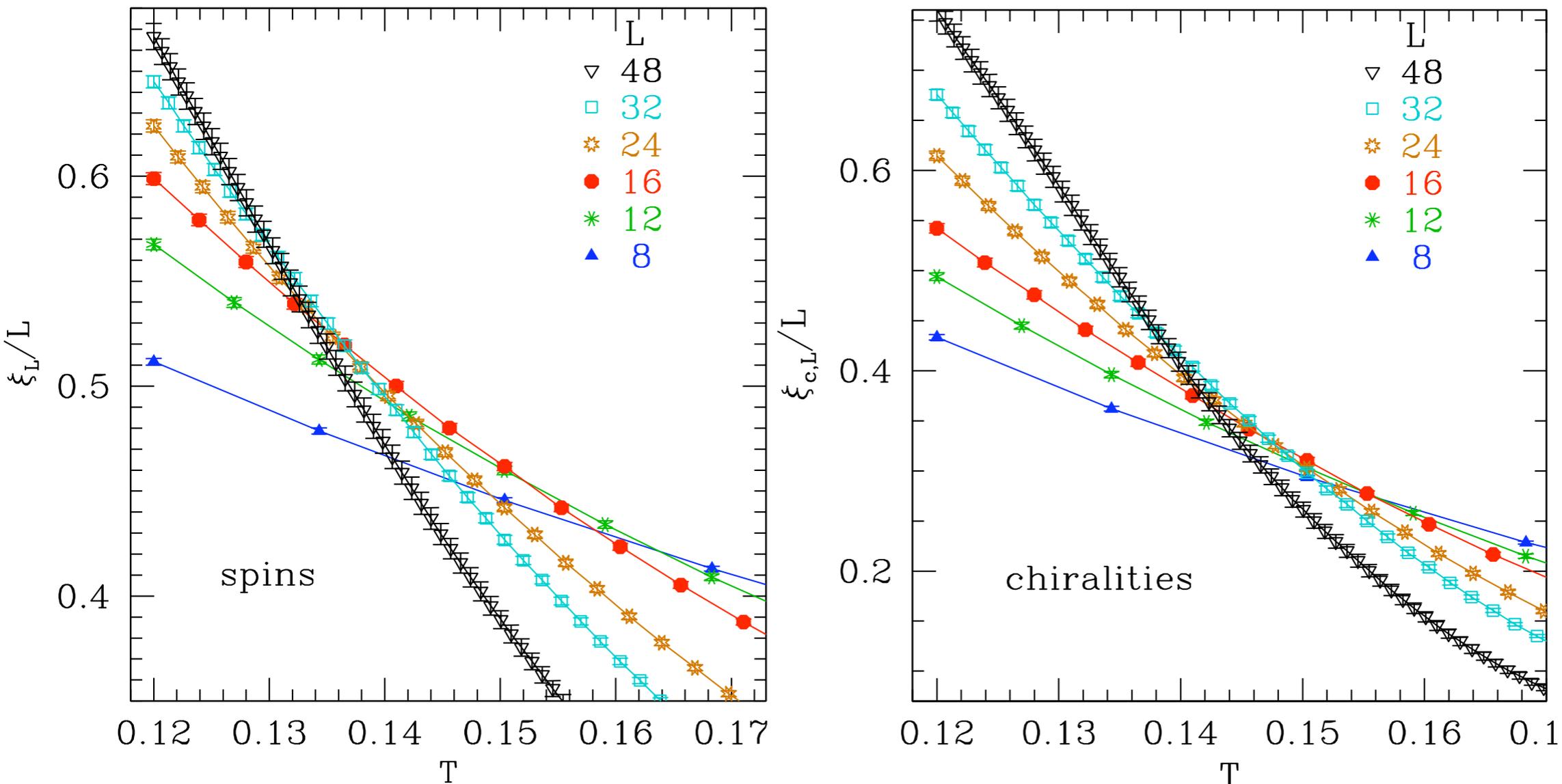
the simulation is **considerably speeded up** by mainly using “**over-relaxation**” moves.

Advantages:

- Over-relaxation sweep takes less CPU time than heatbath sweep
- **Many fewer sweeps are needed to equilibrate** (surprising)



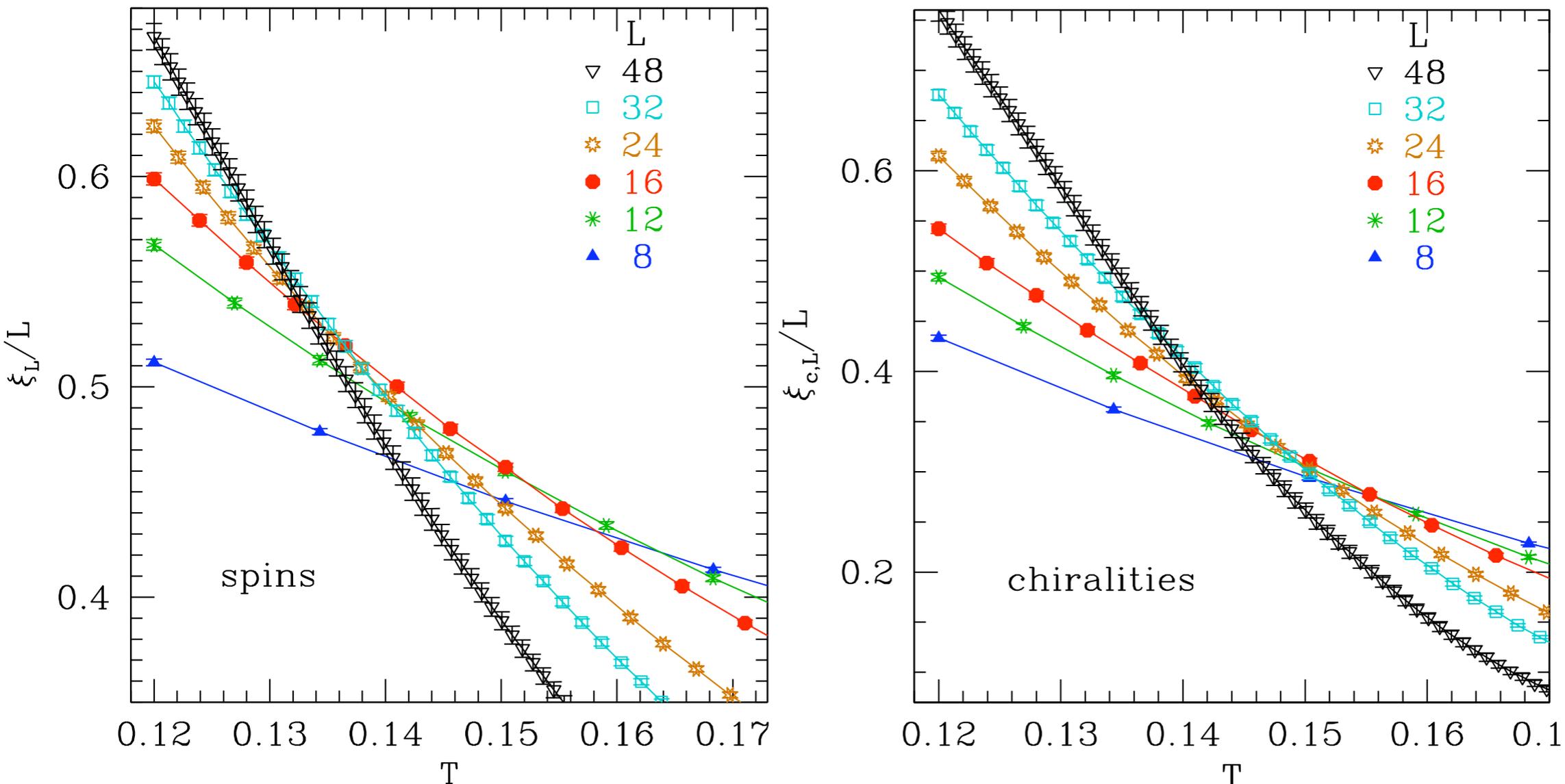
Results for Heisenberg Spin Glass



(Fernandez, Gavira, Martin-Mayor, Tarancon, APY (2009). Equilibration tested on a sample-by-sample basis, see the previous talk by David Yllanes)

Are there two (nearby) transitions or just one?

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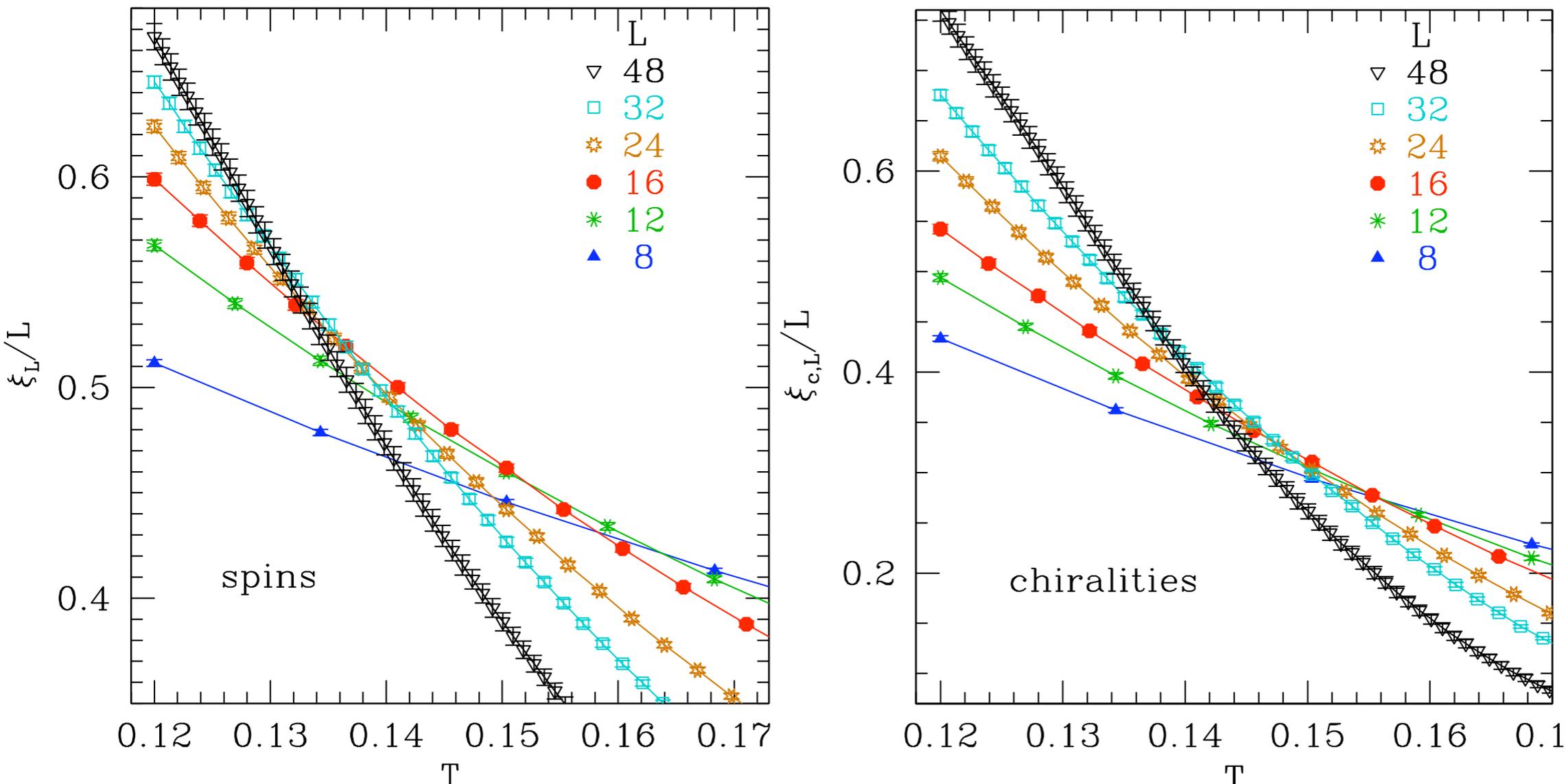


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Our data: difference in transition temps. is small, consistent with 0

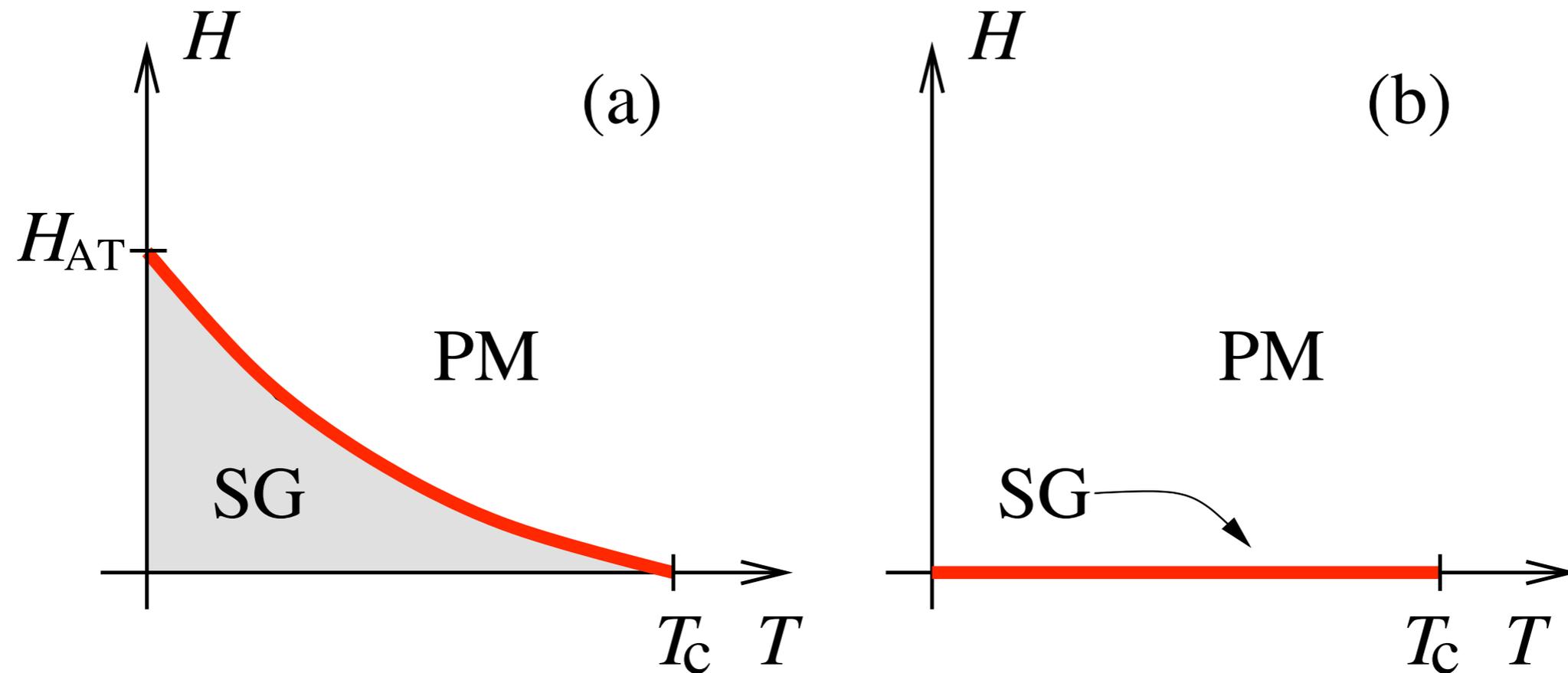
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Is there an AT line?

In MFT 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”).

The AT line is a **ergodic-non ergodic transition with no change in symmetry**



Does an AT line occur in real systems?

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

Results of Simulations

In MFT, χ_{SG} diverges on AT line where now

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

Convert this to correlation length ξ_L

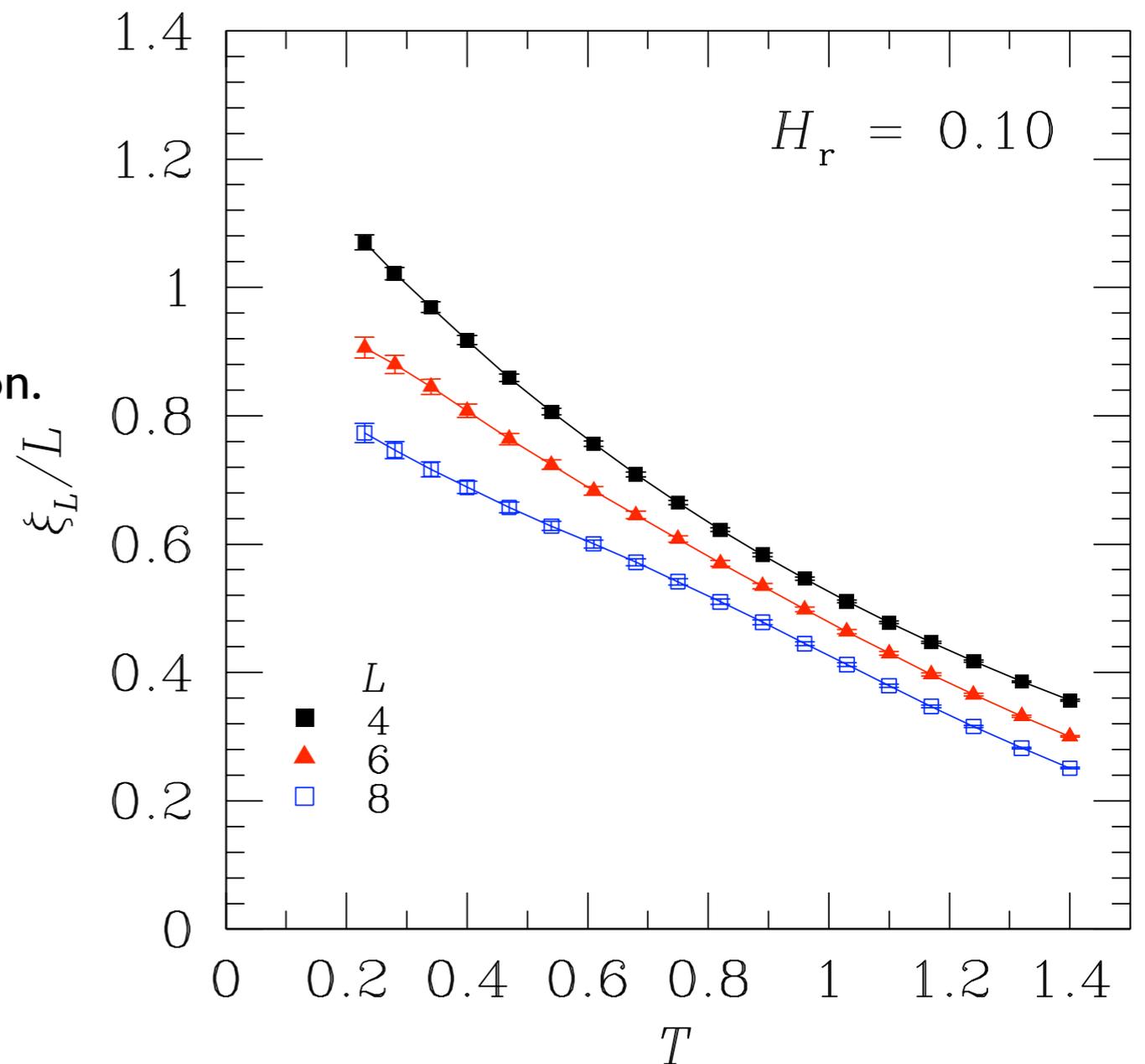
χ_{SG} in a field not accessible in experiment is in simulations.

Best to use FSS of ξ_L / L to look for transition.

i.e. look for intersections:

With a small field of 0.1 (c.w. $T_{SG} \cong 0.96$)

no sign of a transition. (Katzgraber, APY)



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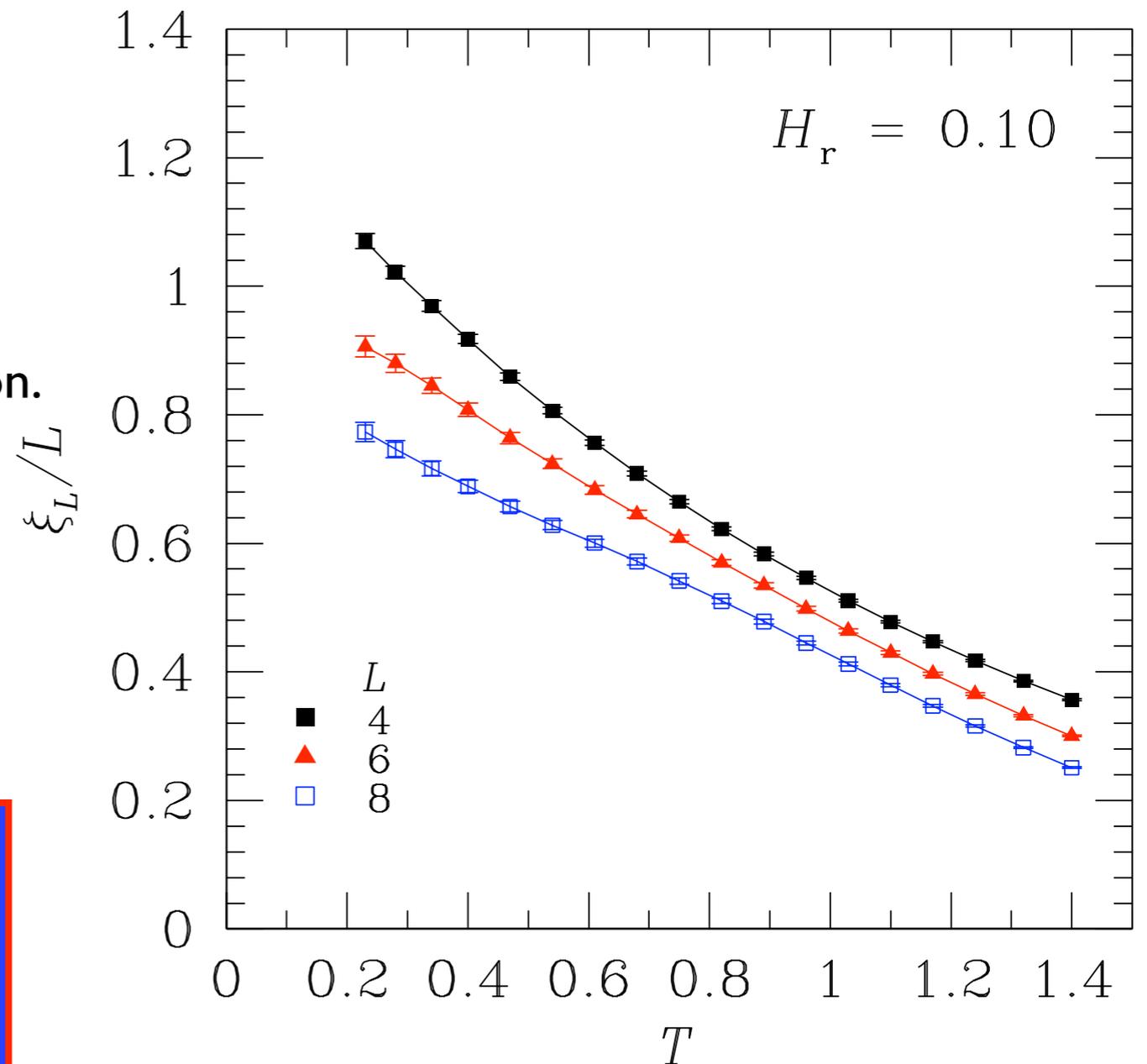
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Seems to be no AT line in 3 dimensions (except perhaps at extremely small fields).



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 - There does not appear to be an Almeida-Thouless line in three dimensions, though it may occur for d greater than a critical value (perhaps 6).
 - (The last two are not yet universally accepted.)