Phase Transition in Spin Glasses

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UNIVERSITY OF CALIFORNIA SANTA CRUZ

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

Collaborators:
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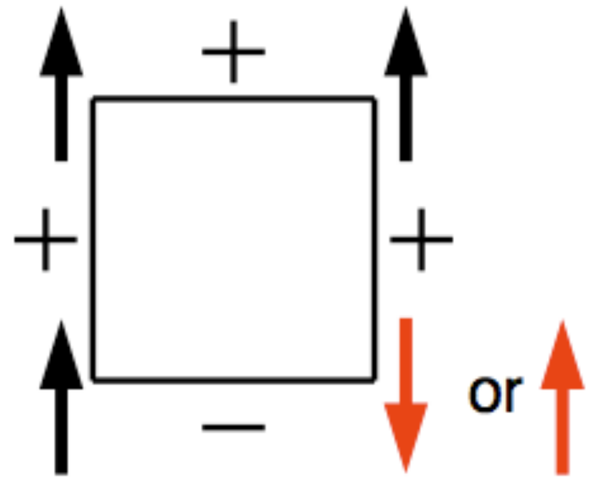
Overview

- 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).

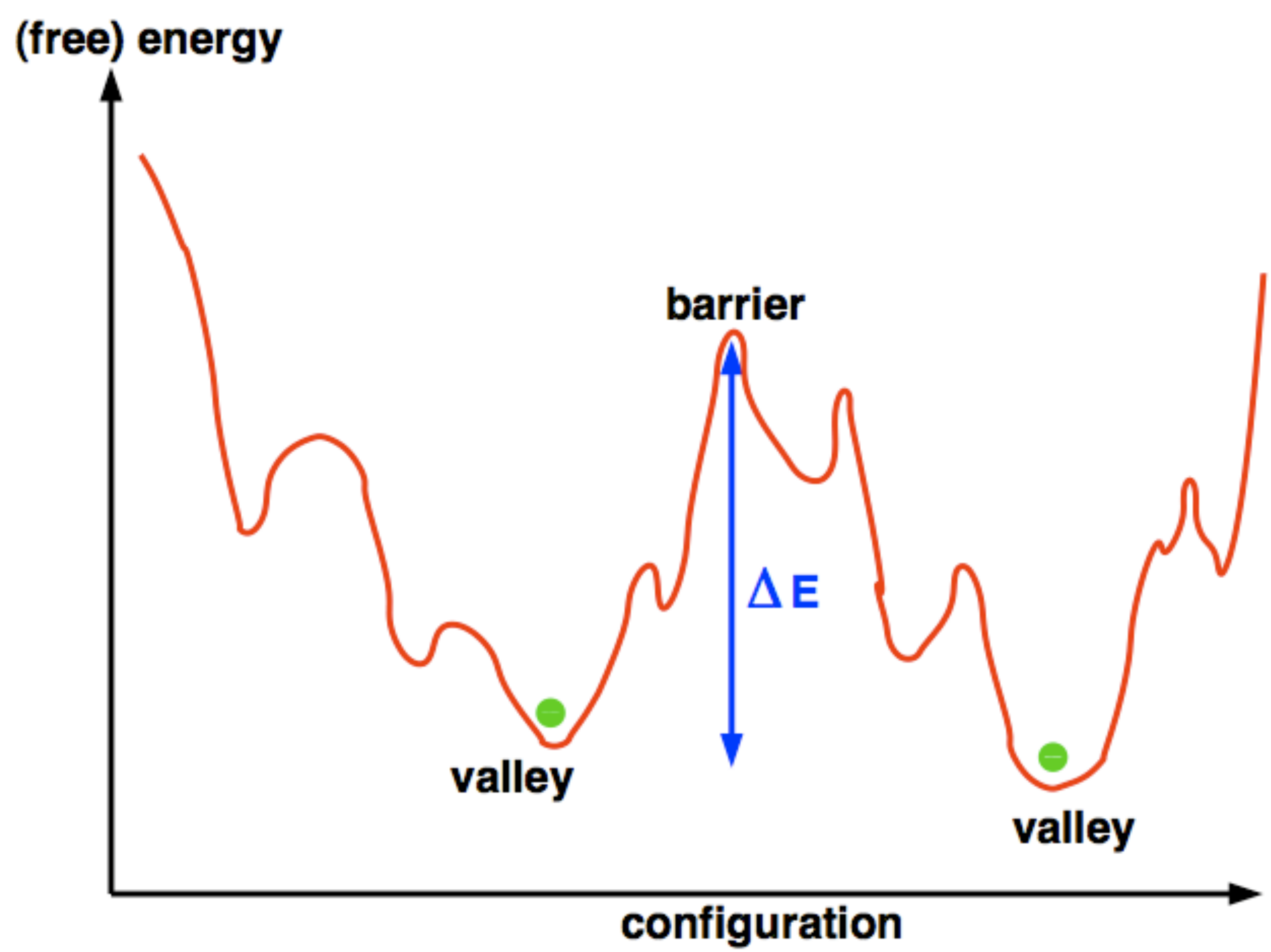
Take a Gaussian distribution: $[J_{ij}]_{\rm av} = 0; \quad [J_{ij}^2]_{\rm av}^{1/2} = J \; (= 1)$

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

$$\begin{aligned} \mathrm{m} &= 1 \quad \text{(Ising)} \\ \mathrm{m} &= 2 \quad \text{(XY)} \\ \mathrm{m} &= 3 \quad \text{(Heisenberg).} \end{aligned}$$

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
  - ....
- 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 $T \to T_{SG}^{+}$, 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

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

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

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

(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)?

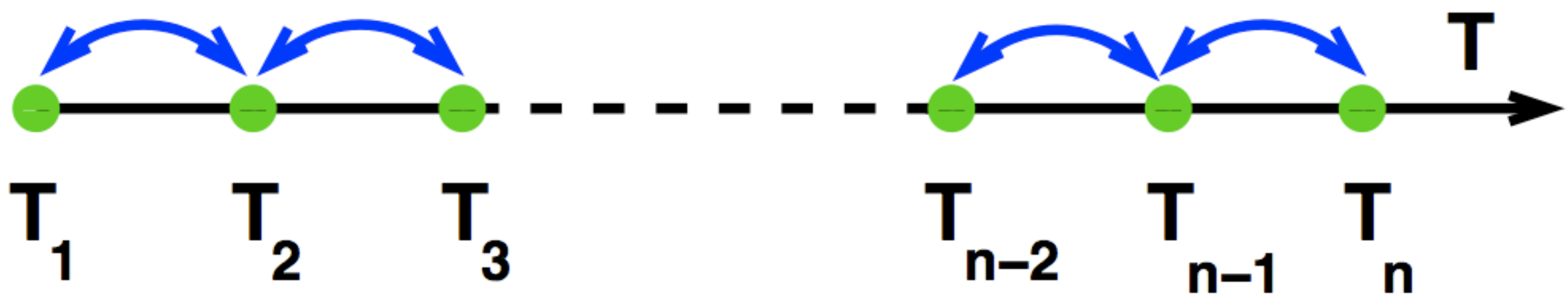
- Dynamics is very slow.
  System is trapped in valley separated by barriers.
  Use parallel tempering to speed things up.

- 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 $\mathbf{T_1}$ and $\mathbf{T_n}$.

Advantage: Speeds up equilibration at low-T.

c.f. previous talks at this meeting by Machta and Yllanes

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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))

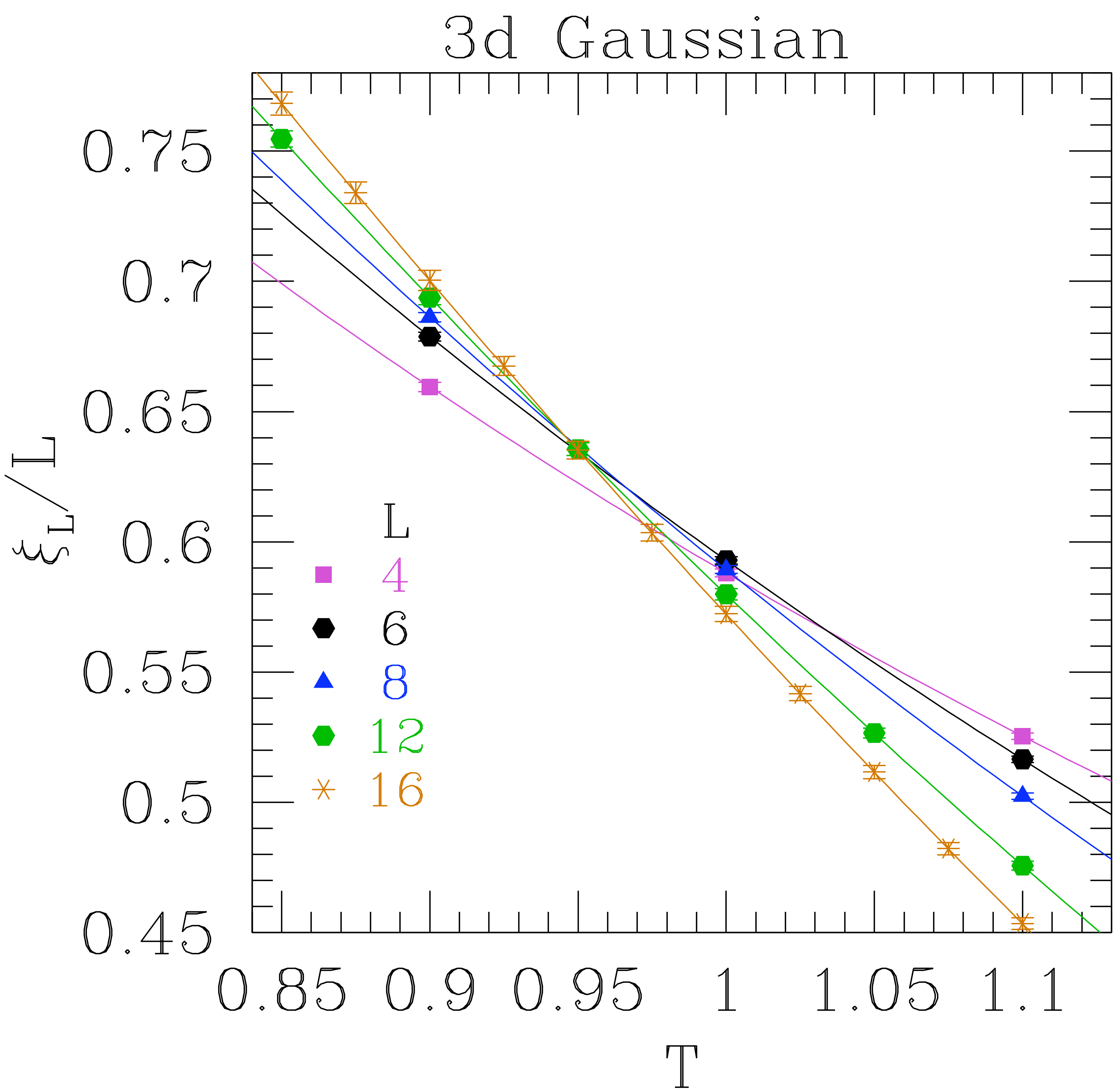
Correlation length determined from **k**-dependence of the FT of the spin-spin correlations $\langle S_i \, S_j \rangle^2$.

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

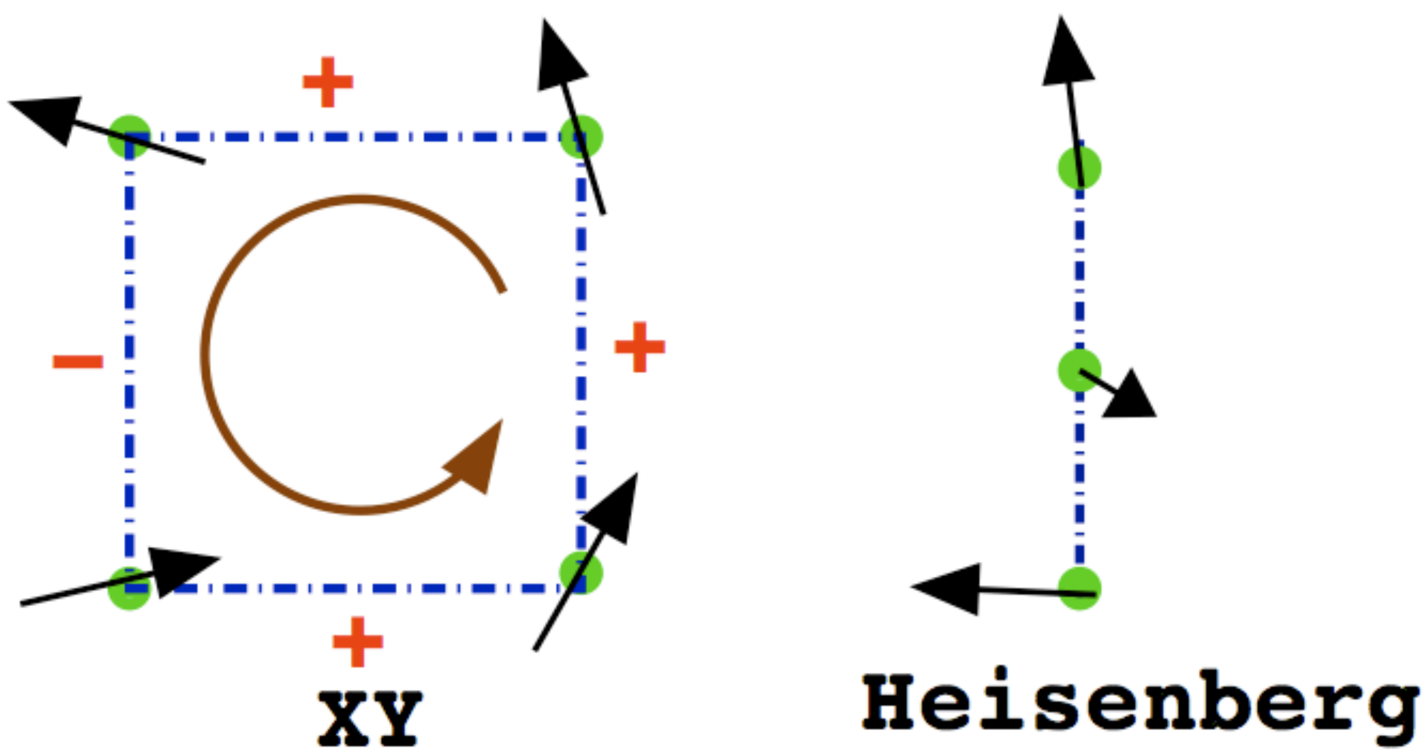


Chirality

- 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)

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



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

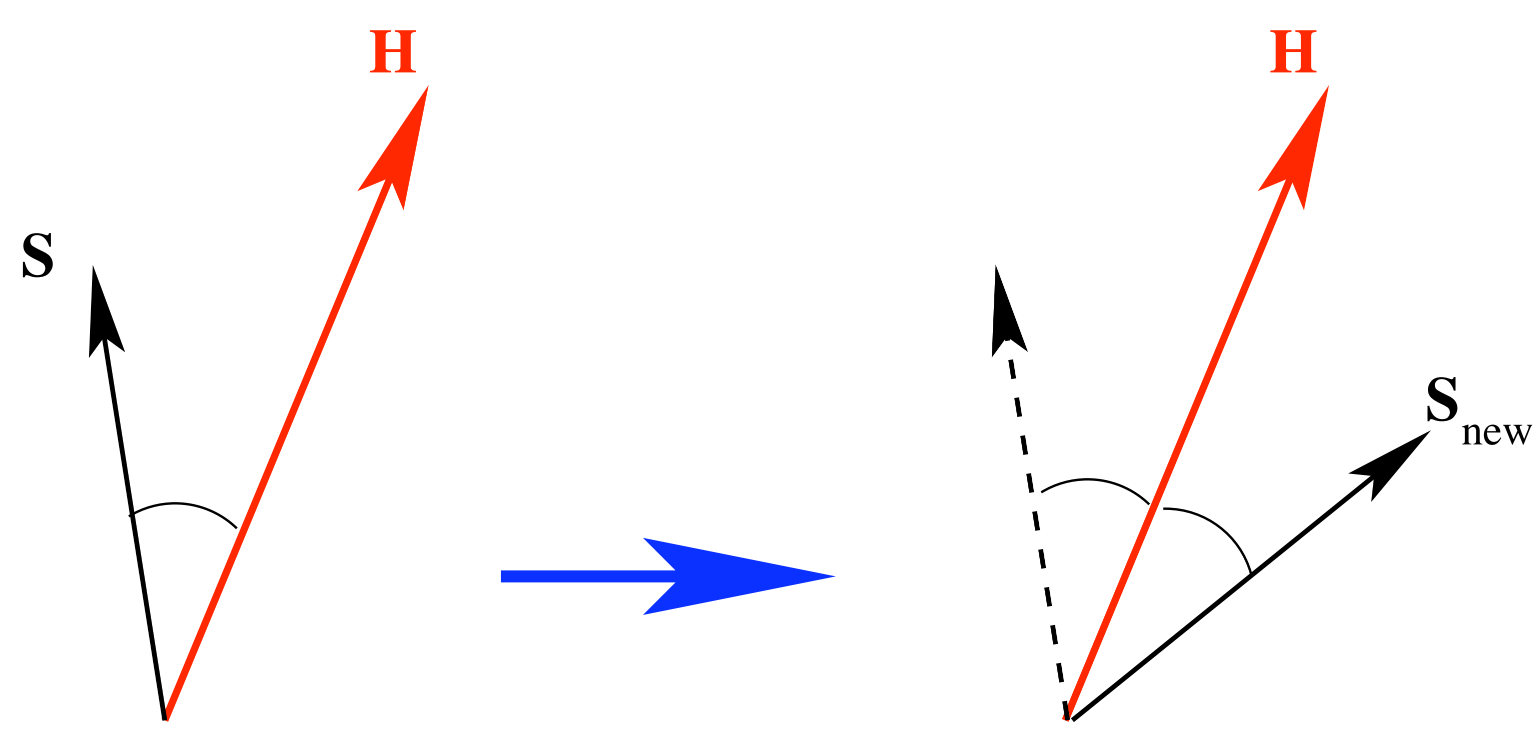
- Heat bath (single spin) moves, and
- Parallel tempering moves,

the simulation is considerably speeded up by mainly using

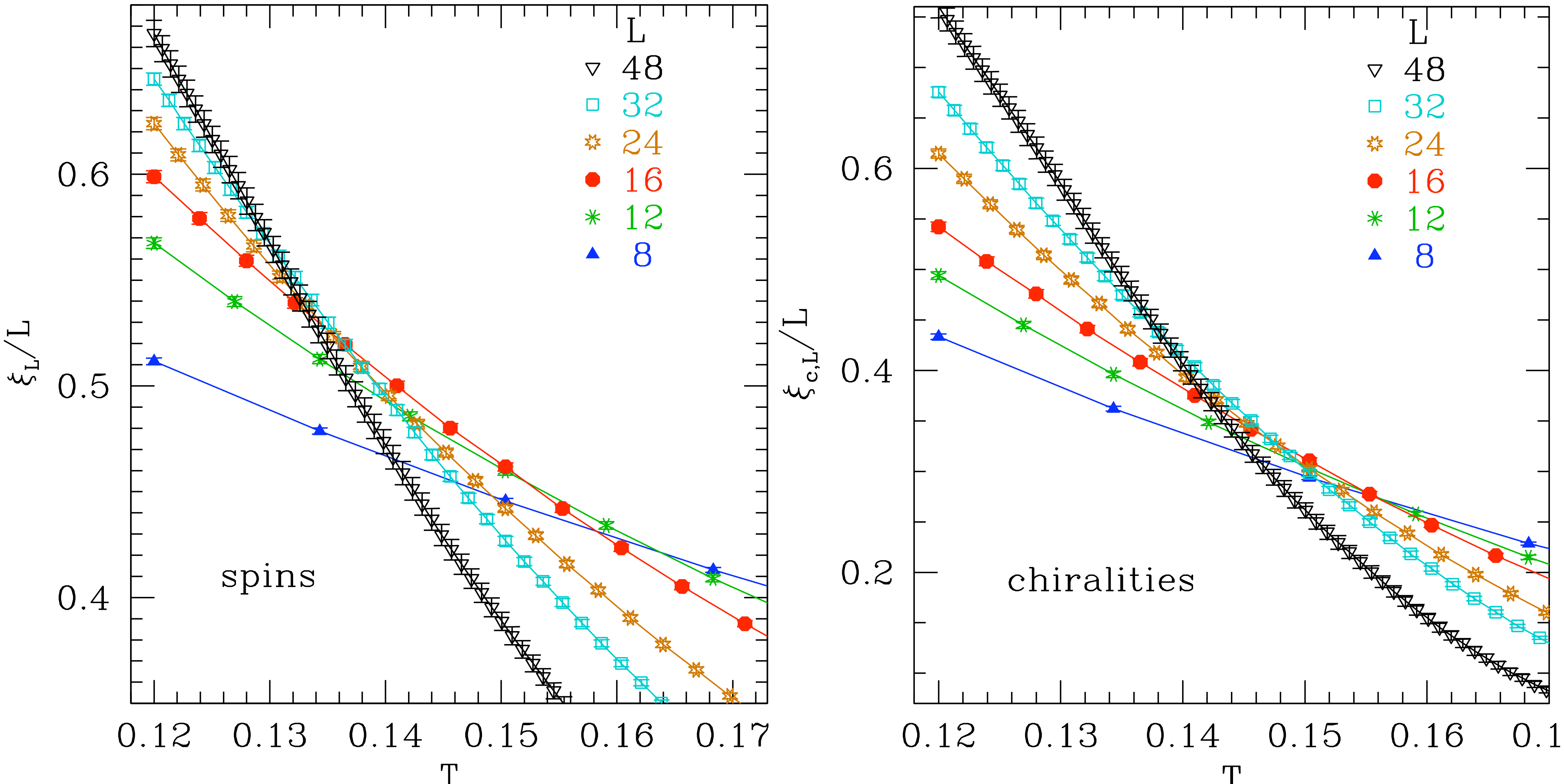
- "over-relaxation" moves.

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

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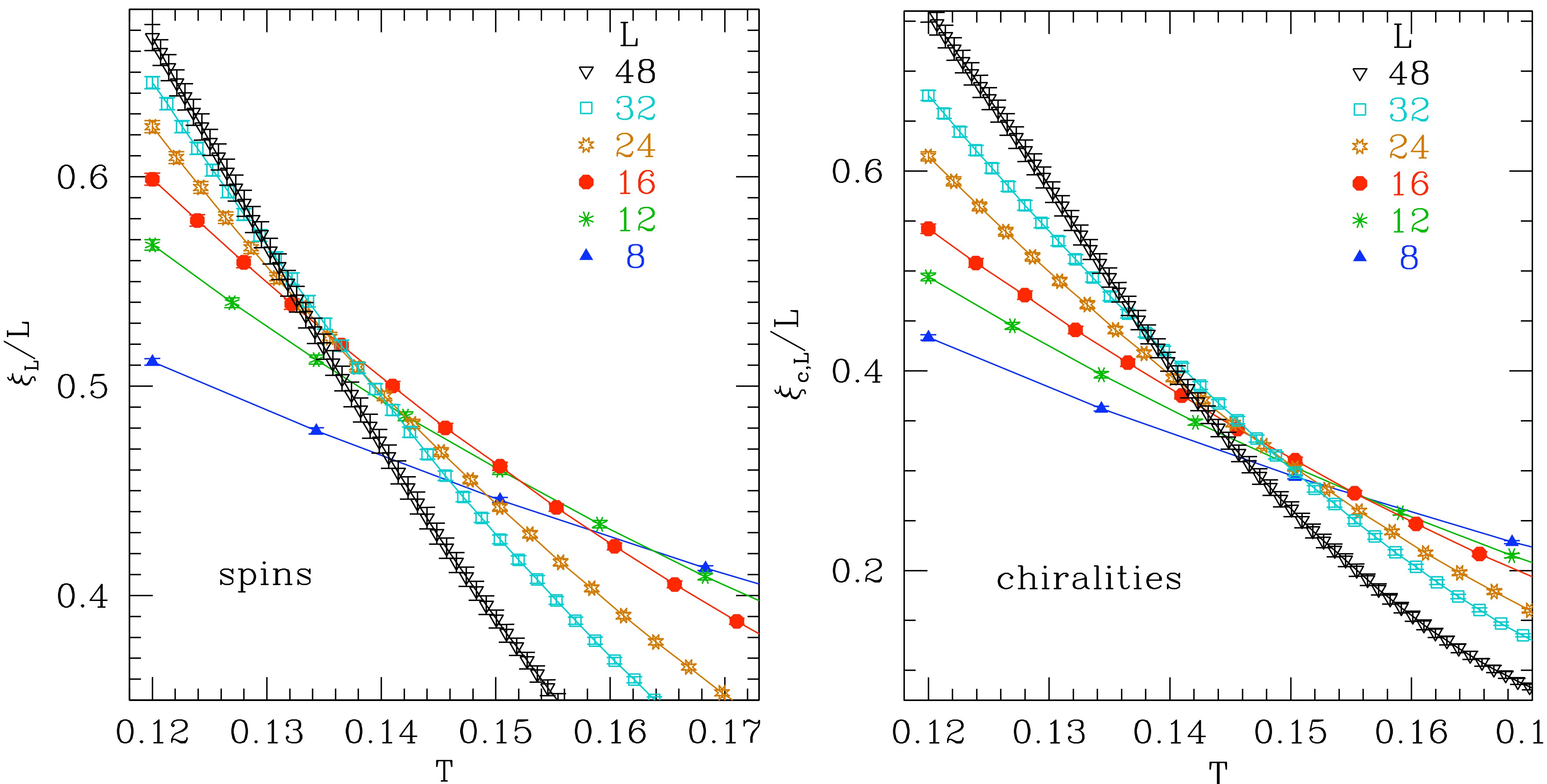

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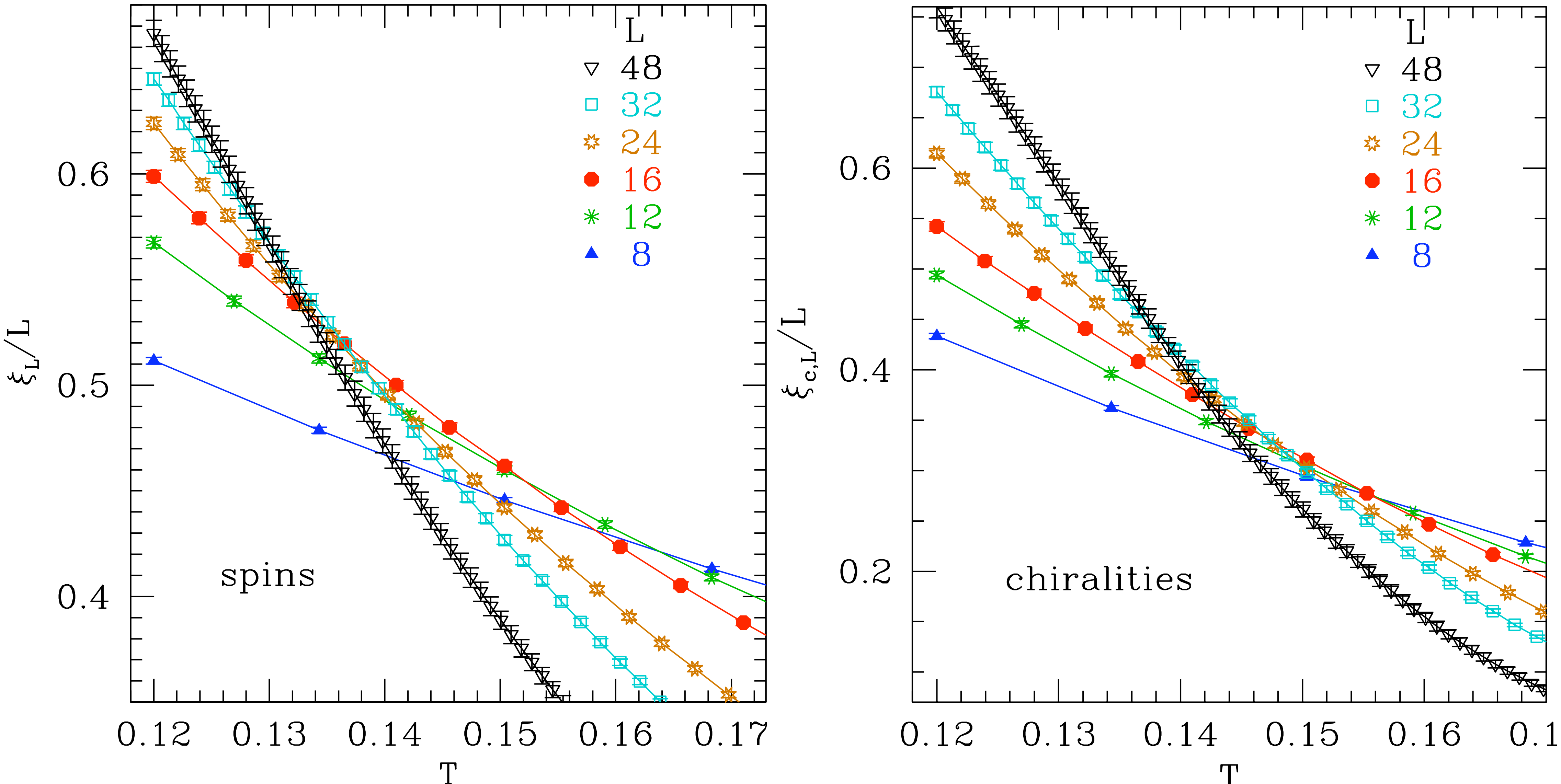

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Our data: difference in transition temps. is small, consistent with 0

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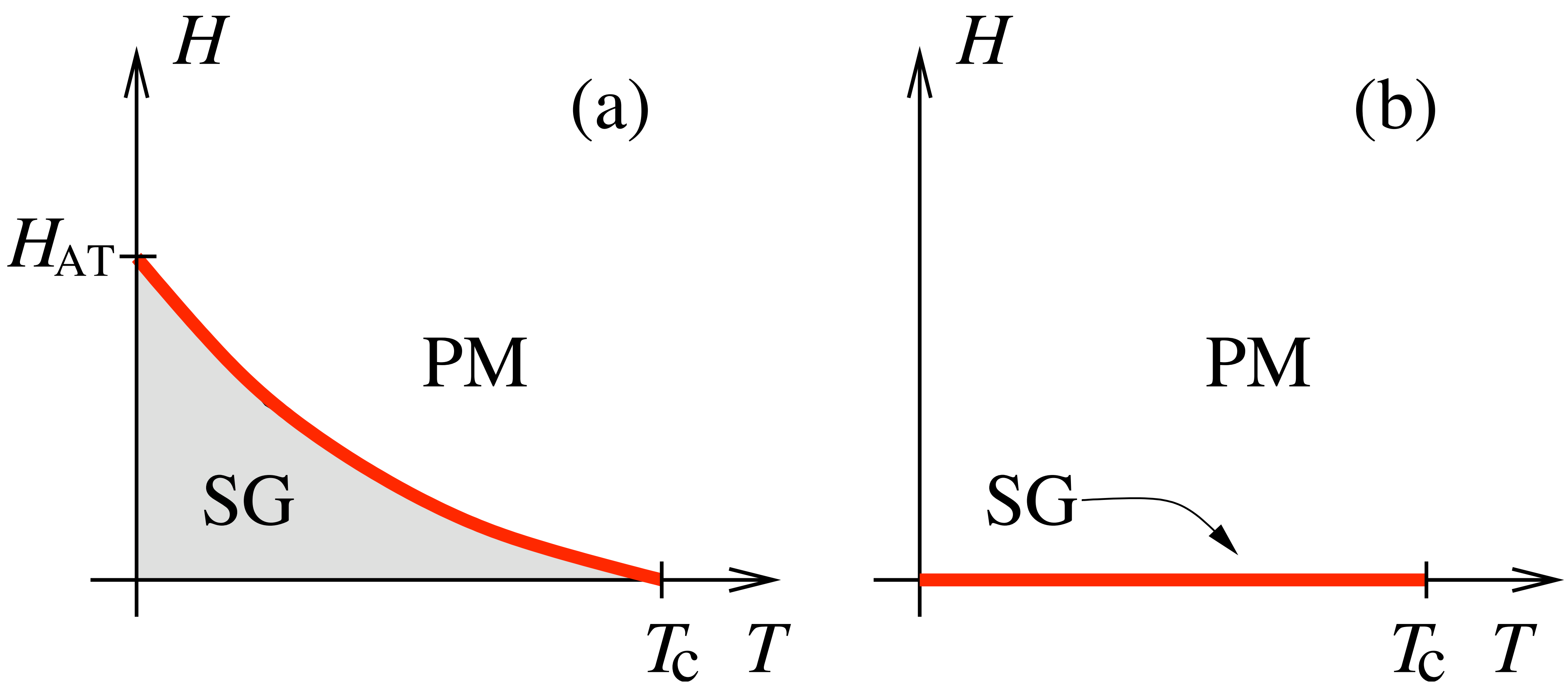
Is there an AT line?

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

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

Convert this to correlation length ξ_L

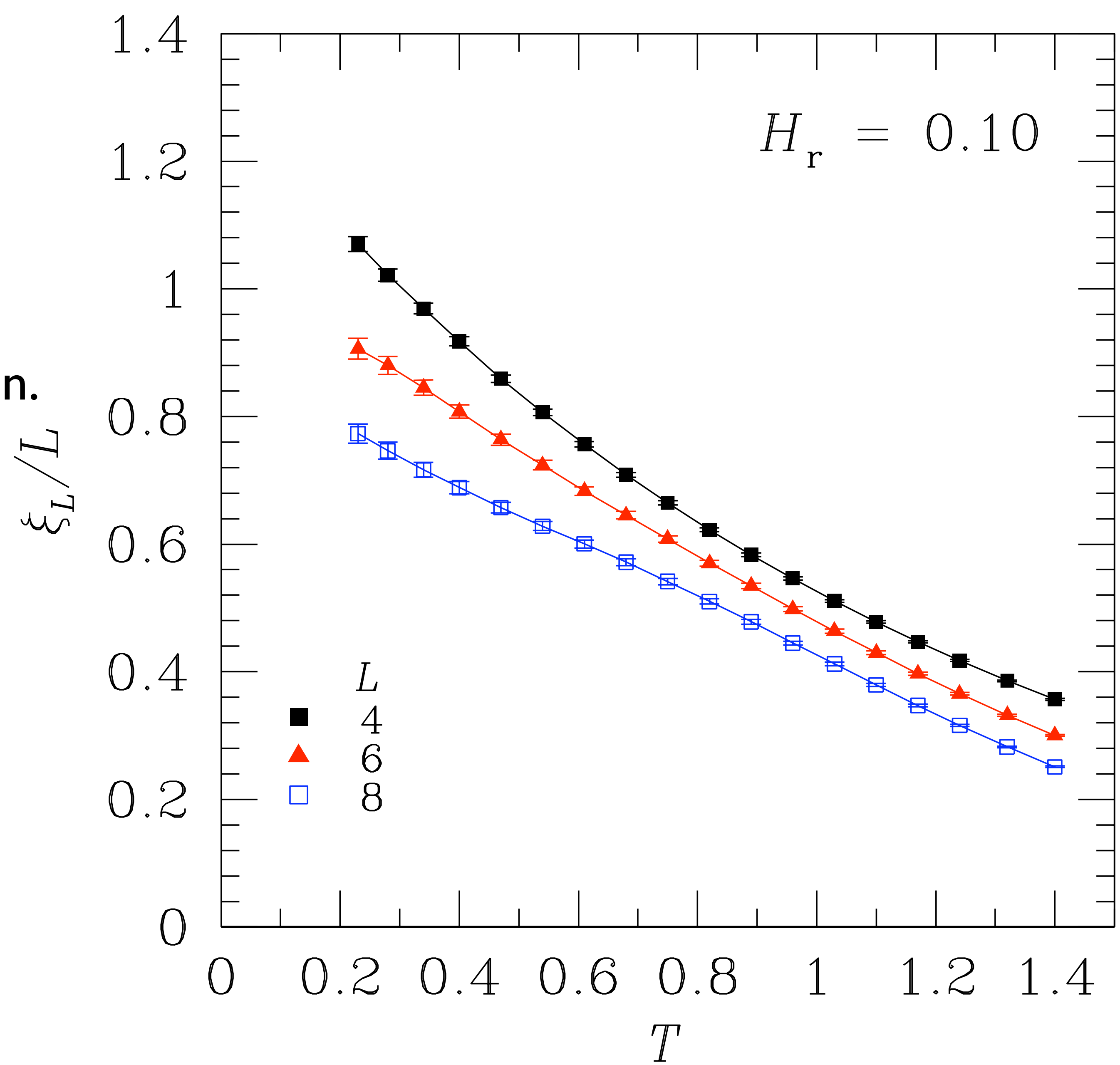
χ_{SG} **in a field not accessible in experiment is in simulations.**

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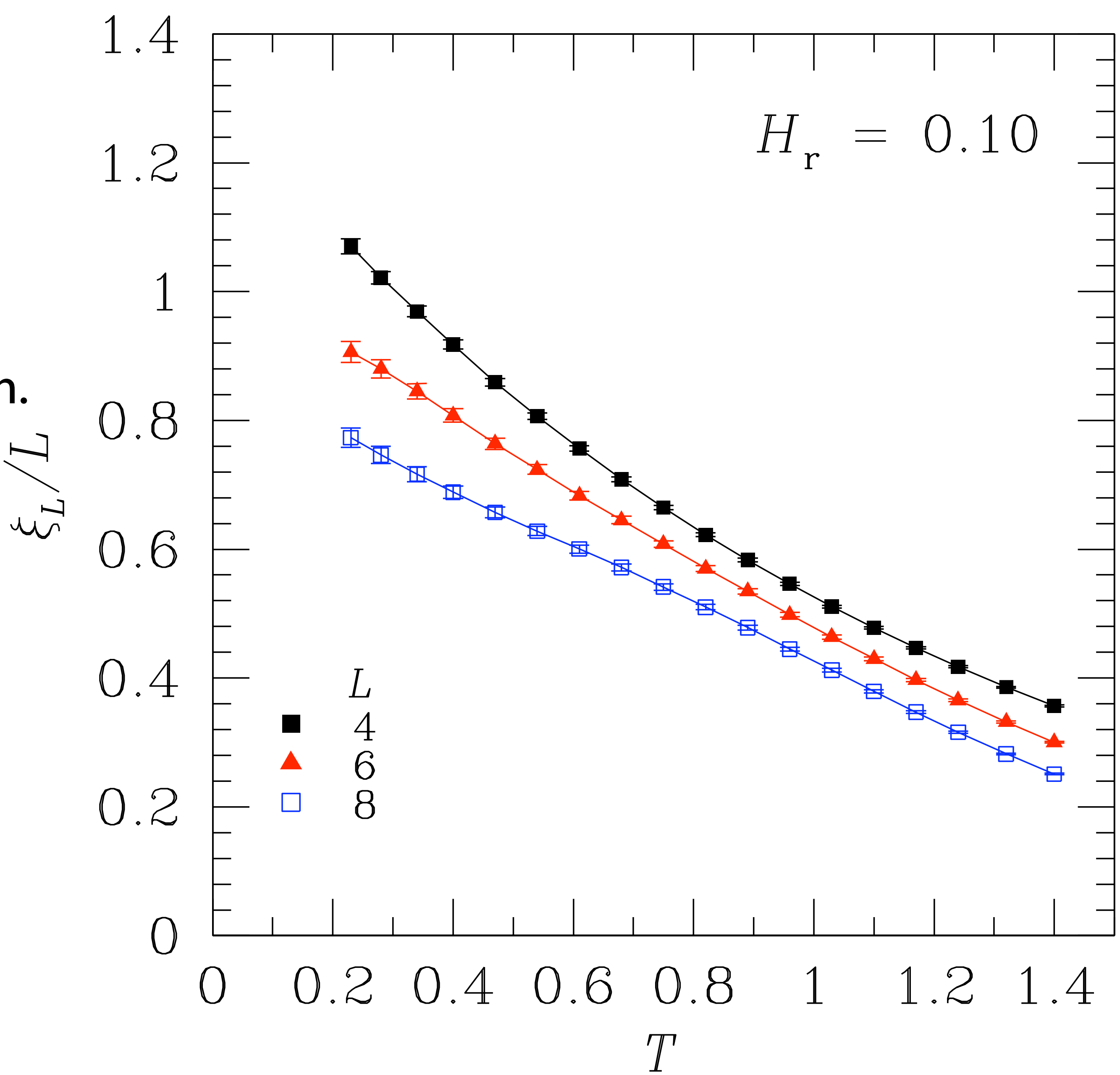
Seems to be no AT line in 3 dimensions (except perhaps at extremely small fields).



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  - (The last two are not yet universally accepted.)