Simulations of Spin Glasses and Related Systems

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Hierarchical Systems Research Foundation.

Recent collaborators: H. G. Katzgraber, L. W. Lee, J. Pixley, D. Larson, V. Martin-Mayor, A. Tarancon, L. A. Fernandez, S. Gaviro, H. Bokil, C. Wengel, M. Körner

Talk for the RAHMAN PRIZE at APS March Meeting, Pittsburgh, March 19, 2009.

Overview

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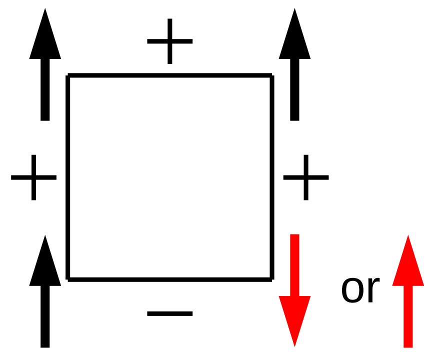
  - Is there a phase transition in an isotropic Heisenberg spin glass?
  - Is there a transition in an Ising spin glass in a magnetic field (Almeida-Thouless line)?

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: $[J_{ij}]_{\mathrm{av}} = 0; \quad [J_{ij}^2]_{\mathrm{av}}^{1/2} = J \; (= 1)$

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

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

Spin Glass Systems

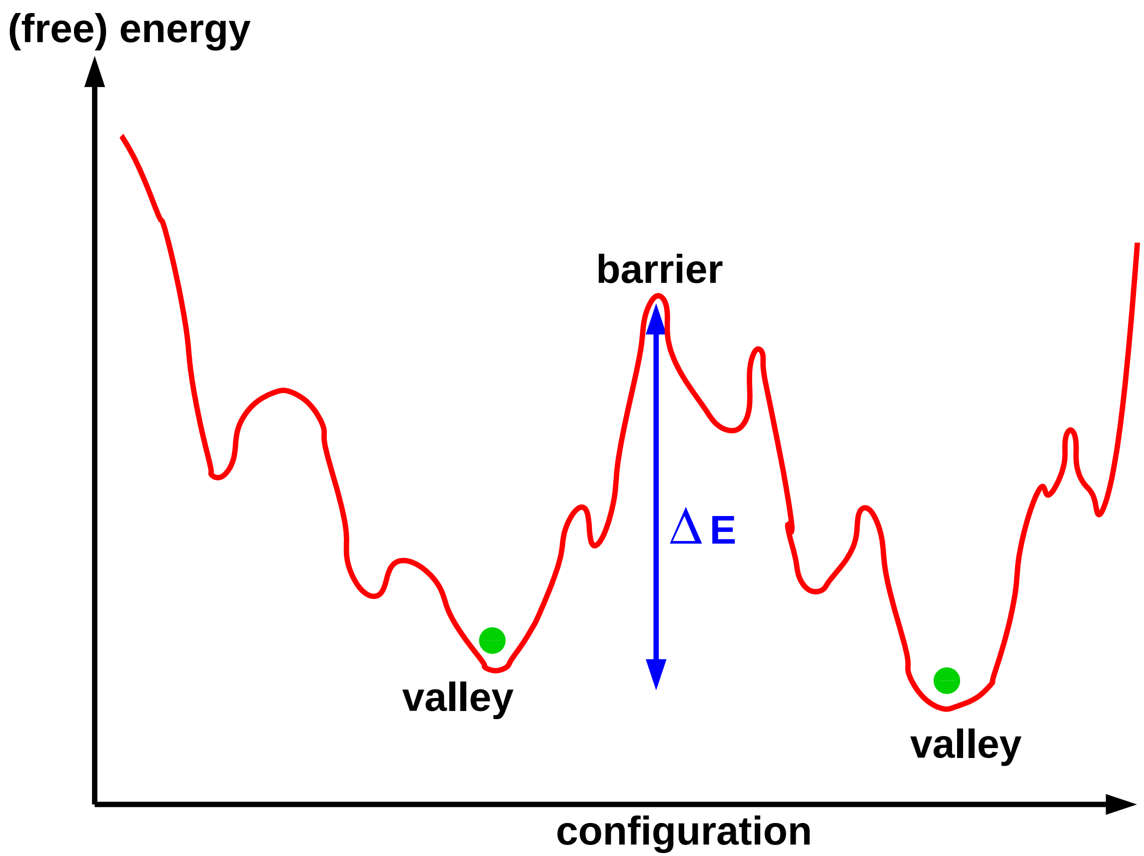
- Metals:
  Diluted magnetic atoms, e.g. Mn, in non-magnetic metal, e.g. Cu.
  RKKY interaction:

$$J_{ij} \sim \frac{\cos(2k_F R_{ij})}{R_{ij}^3}$$

  Random in magnitude and sign, which gives frustration.
  Note: Mn (S-state ion) has little anisotropy; $\rightarrow$ Heisenberg spin glass.
- Important because relevant to other systems:
  - "Vortex glass" transition in superconductors
  - Optimization problems in computer science
    (including solving optimization problems on a quantum computer)
  - Protein folding
  - Error correcting codes

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.



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 $T^3 \chi_{nl} = \chi_{SG} - \frac{2}{3}$.

Theory

- Mean Field Theory (Edwards-Anderson, Sherrington-Kirkpatrick, Parisi).
  Exact solution of an infinite range (SK) model. Finite T_{SG}.
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- Short-range (EA) models. Simulations on Ising systems also indicate a finite T_{SG} (see later) in $d = 3$. Vector spin glasses? (See later.)
- Equilibrium state below T_{SG}. Two main scenarios:

"Replica Symmetry Breaking" (RSB), (Parisi).

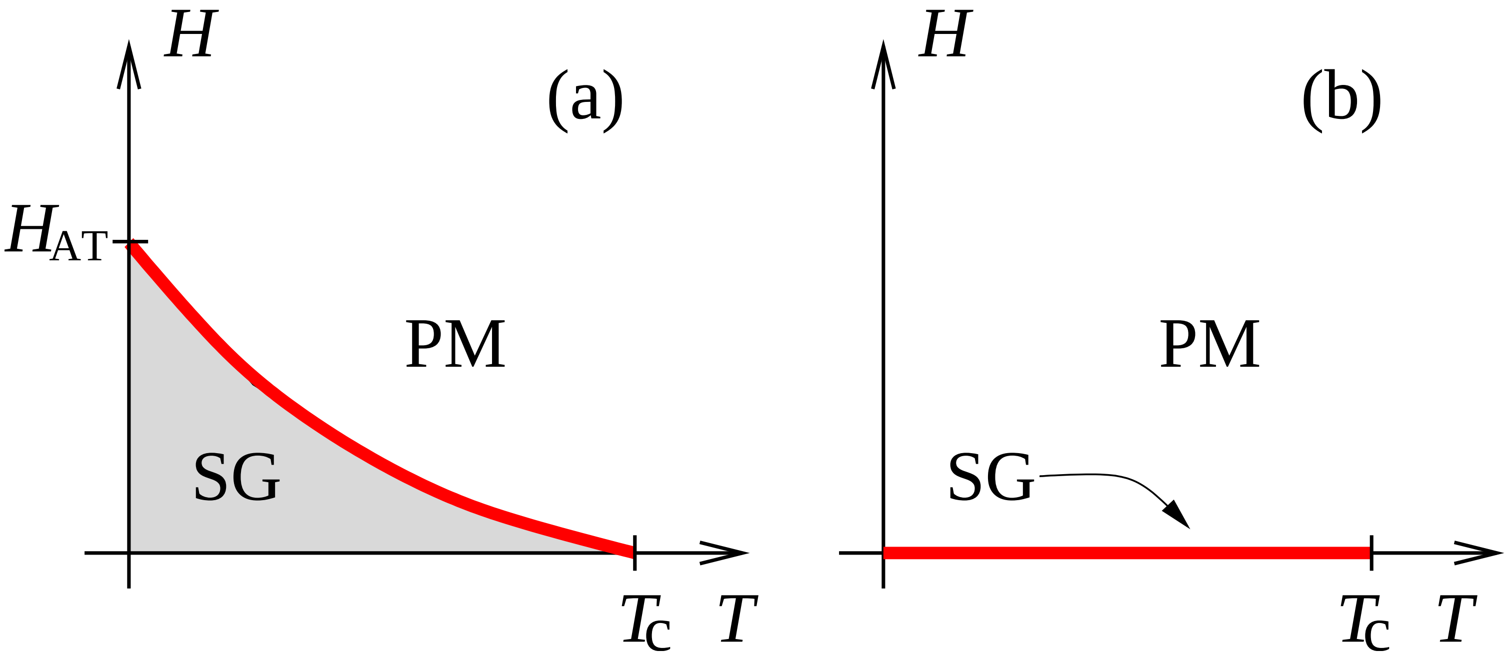
Assume short-range is similar to infinite-range. There is an AT line.

"Droplet picture" (DP) (Fisher and Huse, Bray and Moore, McMillan).

Focus on the geometrical aspects of the low-energy excitations. No AT line in any d.

Is there an AT line? (Ising)

In MFT there's a transition in a field for an Ising spin glass, the Almeida Thouless (AT) line, from a spin glass (divergent relaxation times, RSB) to a paramagnetic (finite relaxation times, "replica symmetric") phase.
The AT line is a ergodic-non ergodic transition with no symmetry change.



Does an AT line occur in short range systems?

- RSB: yes (see (a)) DP: no (see (b))
- Experiments (dynamics) (Uppsala group): no
- Theory: conflicting claims.

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Why is Monte Carlo Hard?

- Dynamics is very slow.

  System is trapped in valley separated by barriers.

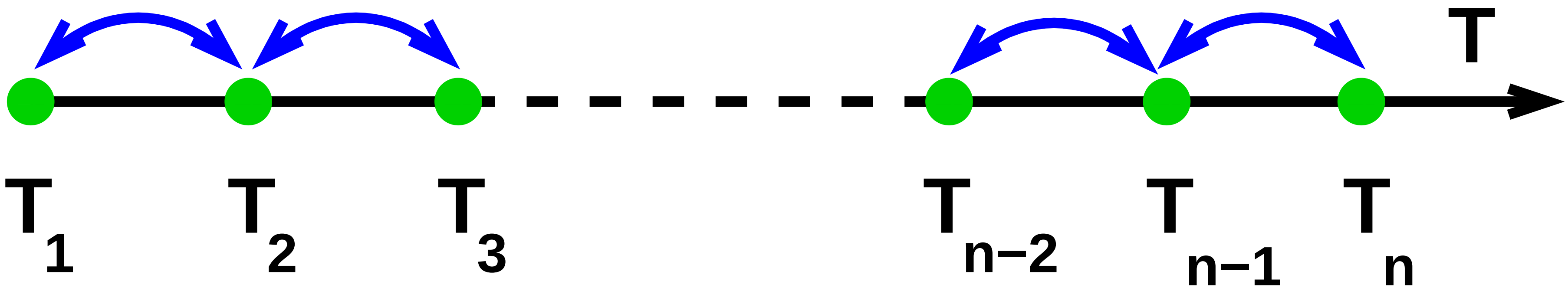
- Have to repeat the simulations for very many samples.

  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.

Equilibration

Equilibration test (for Gaussian distribution) e.g. for Ising

$$[q_l - 1]_{av} = \frac{2}{z} T\,[U]_{av},$$

where $U = -\frac{1}{N} \sum_{\langle i,j \rangle} J_{ij} \langle S_i S_j \rangle$ (energy)

$$q_l = \frac{1}{N_b} \sum_{\langle i,j \rangle} \langle S_i S_j \rangle^2$$ "link overlap", $N_b = Nz/2.$

z is the no. of neighbors, and $J = 1$.

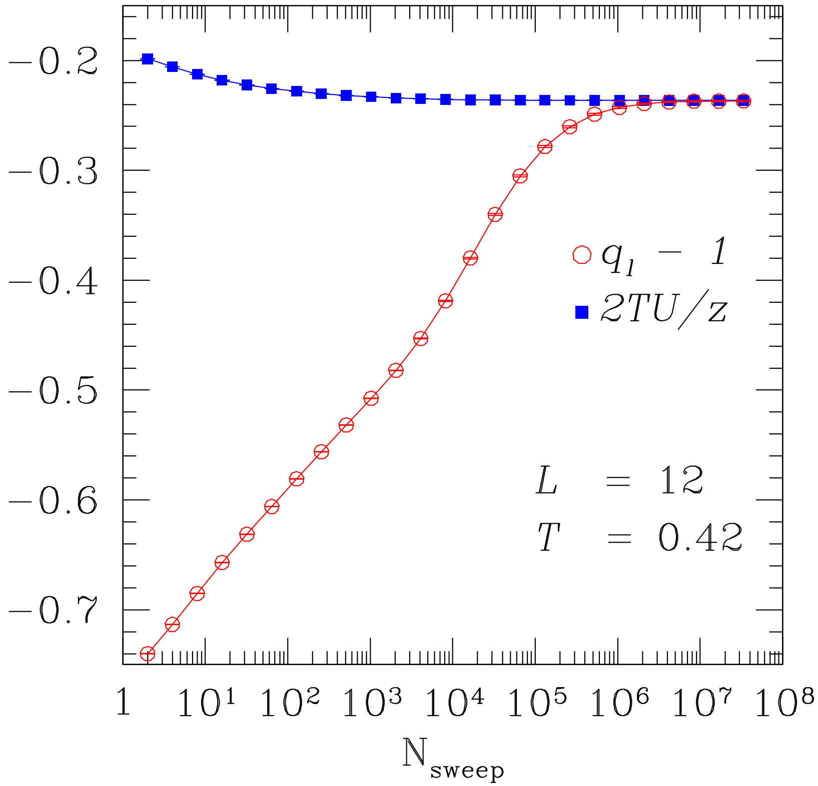
$[\cdots]_{av}$ is an average over samples.

Data for Ising spin glass (H. Katzgraber)

$[q_l - 1]_{av}$ and $(2/z)T[U]_{av}$

approach a common value from *opposite* directions,

and, once they agree with each other, the **results don't change if N_{sweep} is increased further**.



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$$\mathcal{H}_{\mathrm{GG}} = - \sum_{\langle i,j \rangle} \cos\left[\phi_i - \phi_j - A_{ij}\right] ,$$

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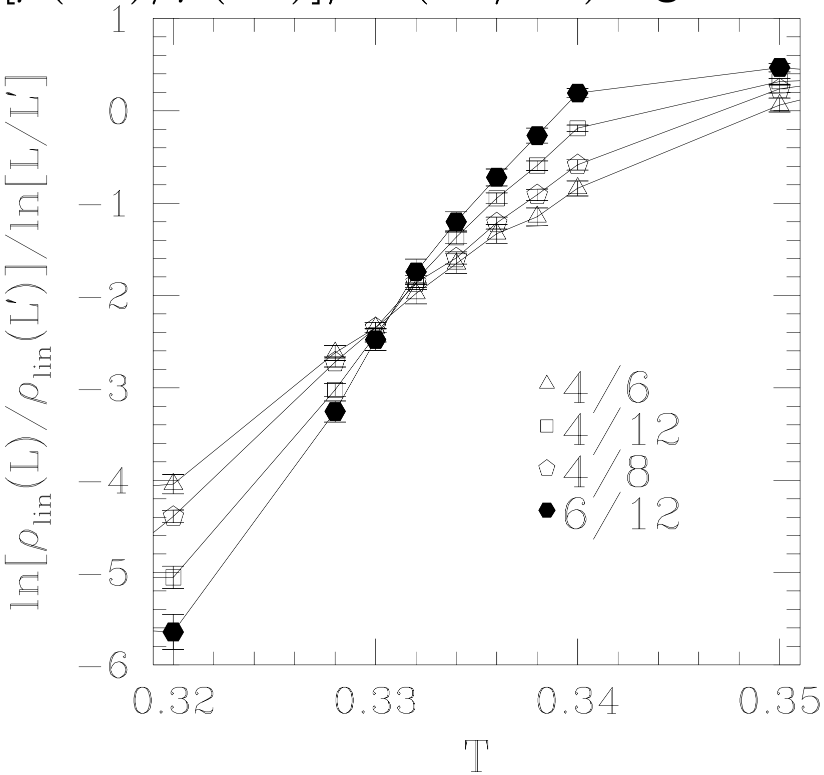
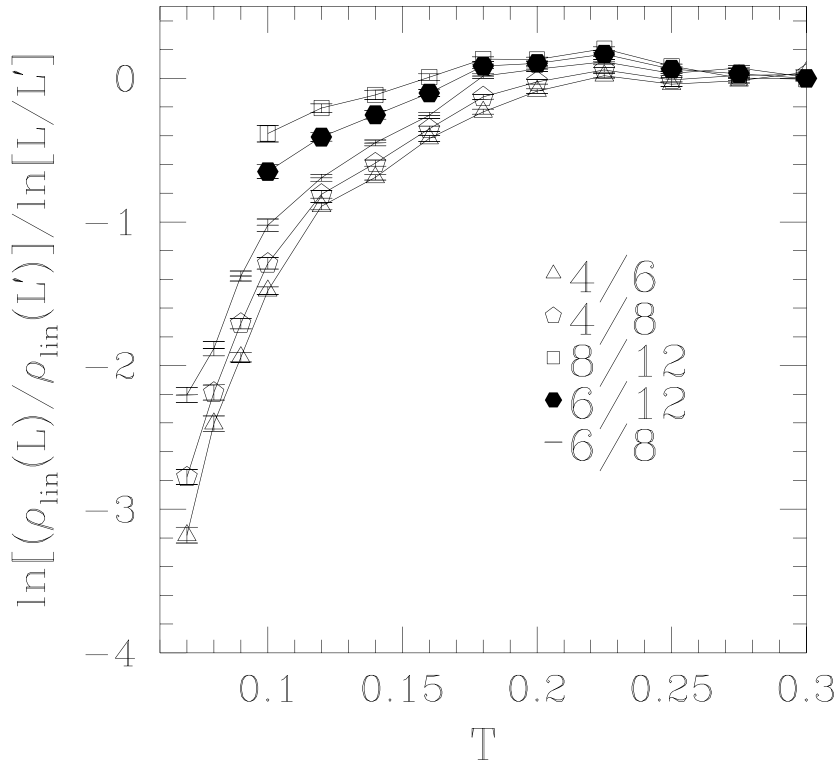
- Numerics: $\Longrightarrow$ the gauge glass has a vortex glass transition.
- Real superconductors have screening of the vortex-vortex interaction. "Relevant" only very close to T_c (FFH).
- Investigated role of screening with H. Bokil (1995) and C. Wengel (1996). Added fluctuating vector potential. (Vortex representation).

  Region where relevant much larger than in experiments.

Screening: Results

At $\mathbf{T_c}$, $\rho_{\mathbf{lin}}$ varies as a power of system size $\mathbf{L}$, $\rho_{\mathbf{lin}} \propto L^{-\lambda}$. Hence $\ln[\rho(L_1)/\rho(L_2)] = -\lambda \ln(L_1/L_2)$, so look for intersections of $\ln[\rho(L_1)/\rho(L_2)]/\ln(L_1/L_2)$ against T (Wengel, APY (1996)):





Left: Pure system (quenched $\mathbf{A_{ij} = 0}$). Has the Meissner transition.
Right: Random system. Has no transition.

The vortex glass transition is rounded out very close to the putative T_c.

May have been seen: Strachan, Sullivan and Lobb, cond-mat/0206120.

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Finite size scaling

Assumption: size dependence comes from the ratio $\boldsymbol{L/\xi_{\mathrm{bulk}}}$ where

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

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

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

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

Hence data for $\boldsymbol{\xi_L/L}$ for different sizes should

intersect at $\boldsymbol{T_{SG}}$ and splay out below $\boldsymbol{T_{SG}}$.

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

Results: Ising

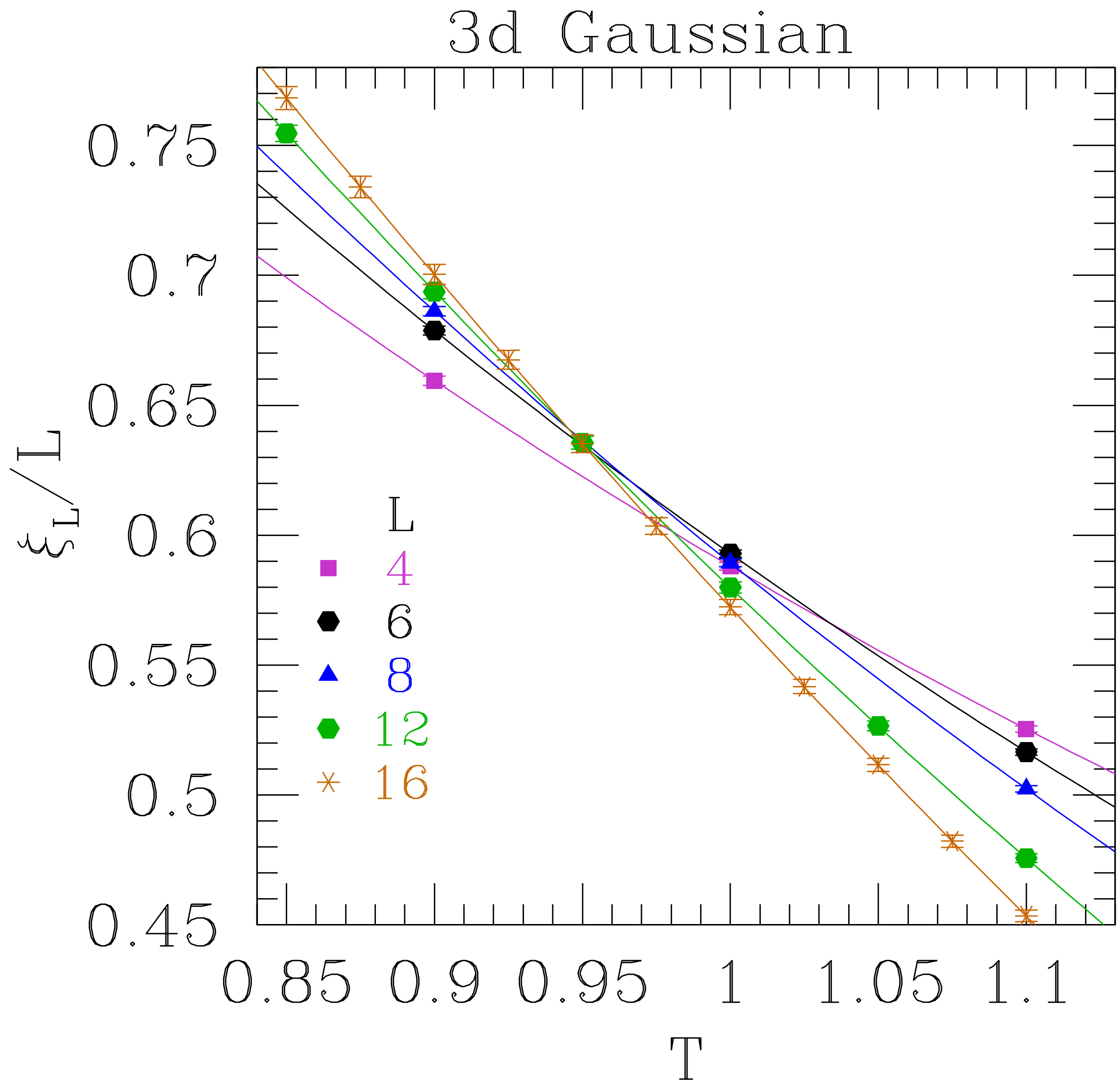
FSS of the correlation length for the Ising spin glass. (from Katzgraber, Körner and APY Phys. Rev. B **73**, 224432 (2006).)

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

$$\boldsymbol{T_{SG} \simeq 0.96.}$$

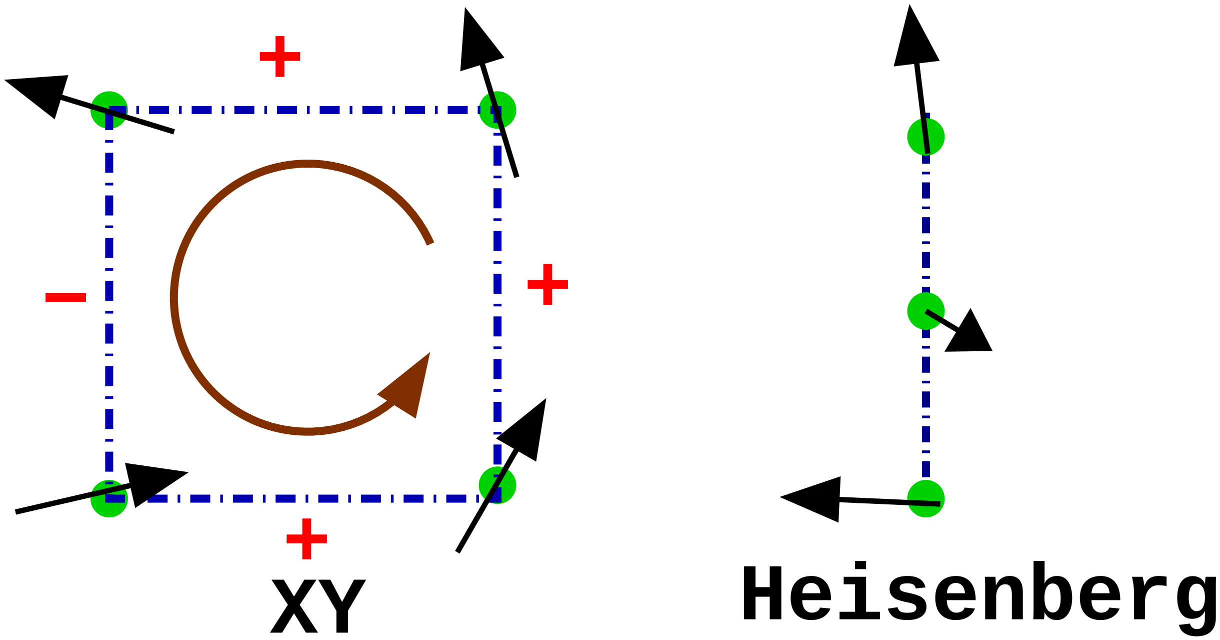
Prevously Marinari et al. found $T_{SG} = 0.95 \pm 0.04$ using a different analysis



Chirality

- Unfrustrated: Thermally activated chiralities (vortices) drive the Kosterlitz-Thouless-Berezinskii transition in the 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)

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



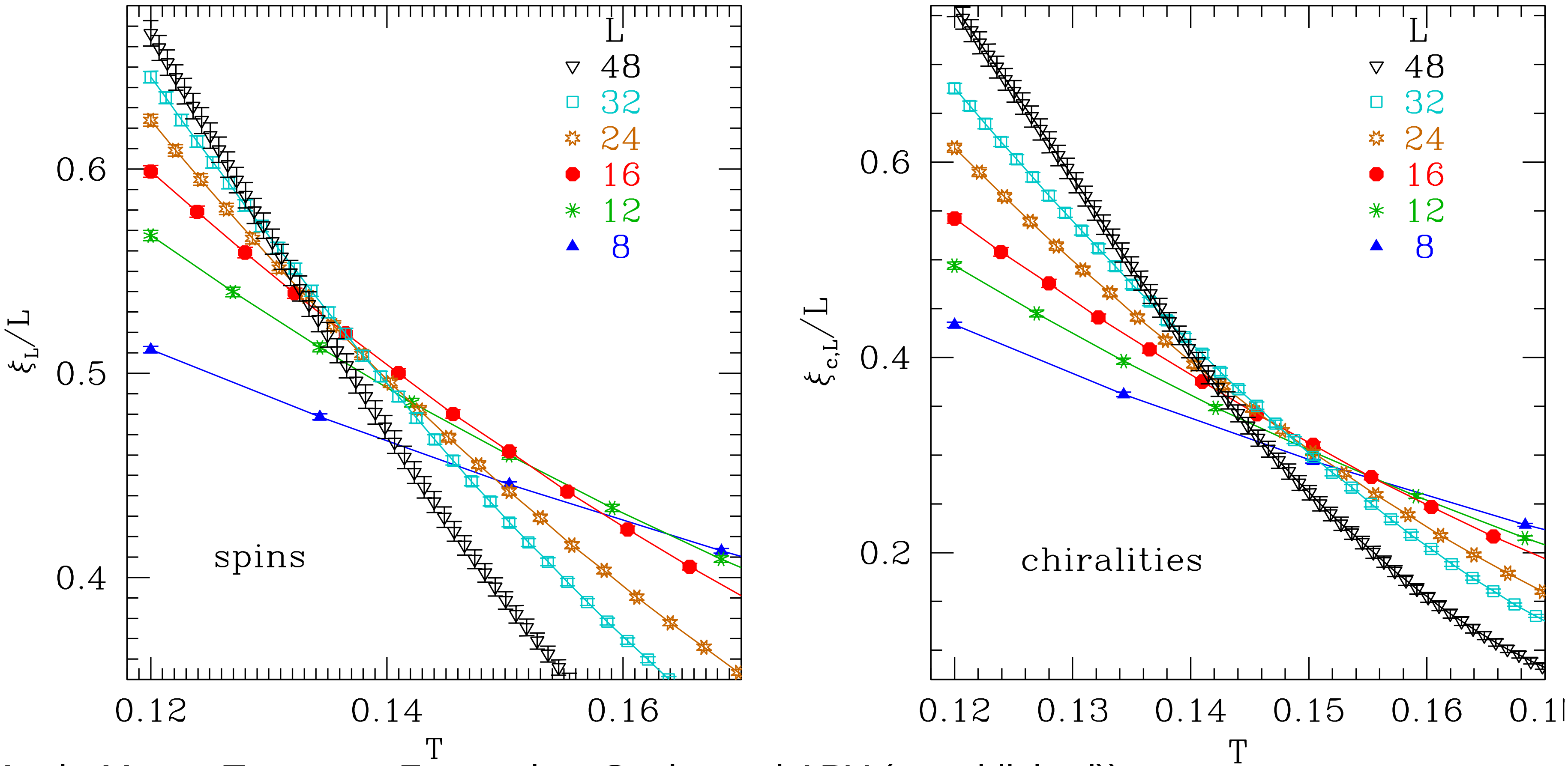
Motivation for vector model

- Old Monte Carlo for Heisenberg: $\mathbf{T_{SG}}$, if any, seems very low, probably zero.
- Kawamura: $\mathbf{T_{SG} = 0}$ but transition in the "chiralities", $\mathbf{T_{CG} > 0}$. This implies spin–chirality decoupling. Subsequently Kawamura suggests that $\mathbf{T_{SG} > 0}$ but $\mathbf{T_{SG} < T_{CG}}$.
- But: Alternative possibility 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 since

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

Heisenberg Spin Glass



(Martin-Mayor, Tarancon, Fernandez, Gaviro and APY (unpublished)).

Note: **much larger sizes** than for Ising (barriers smaller). Took 7.5 megahours of CPU time!

Spins and chiralities behave **very similarly** (but not identically) for this range of sizes.

Are there two very close but distinct transitions? Viet and Kawamura, $L \leq 32$, claim $T_{CG} = 0.145, T_{SG} = 0.120$. From our data, the difference seems less than this or zero. The apparent small difference in transition temperatures may be due to corrections to scaling.

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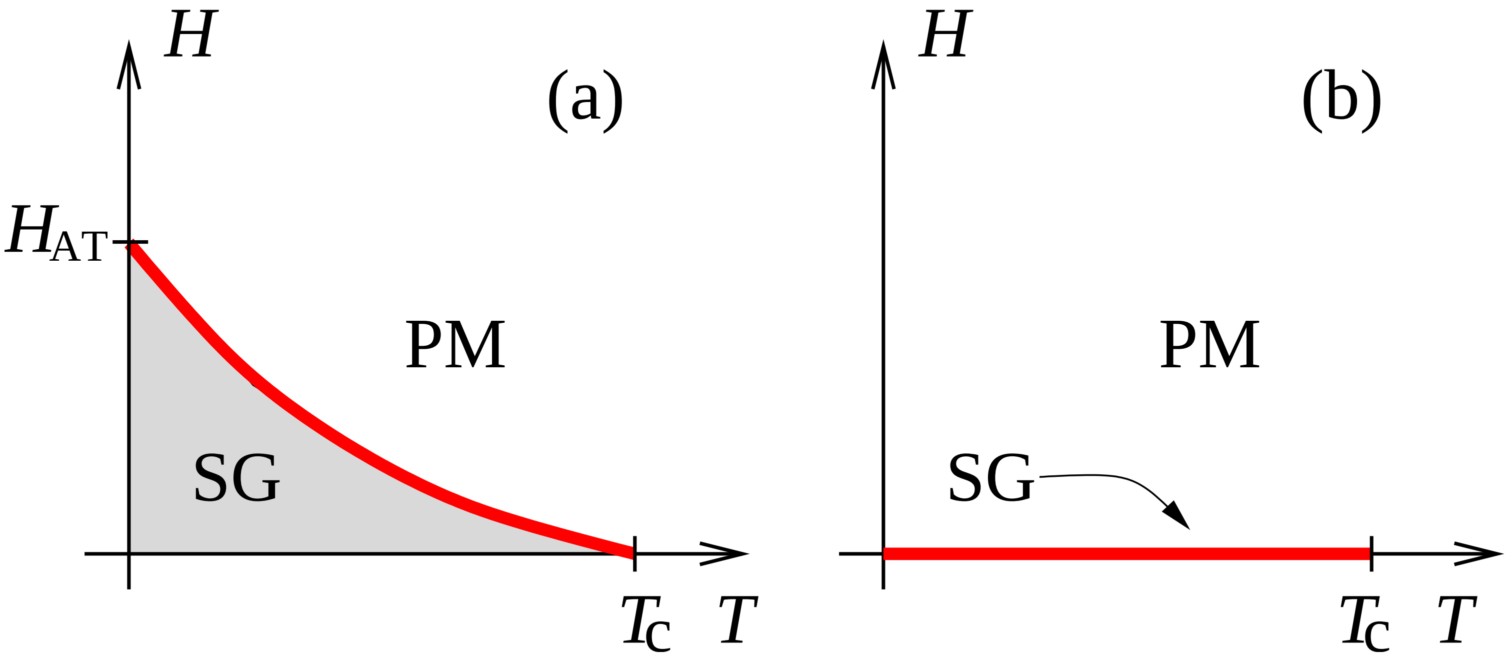

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- RSB: yes (see (a)) DP: no (see (b))
- Experiments (dynamics) (Uppsala group): no
- Theory: conflicting claims.

Is there an AT Line? (ii)

Experiments:, no static divergent quantity; (χ_{nl} doesn't diverge in a field).

Simulations: According to RSB, χ_{SG} diverges in a field, where now

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

Hence can use FSS of ξ_L/L in the simulations to see if there is an AT line

ξ_L behaves as for the zero field case; so we look for intersections.

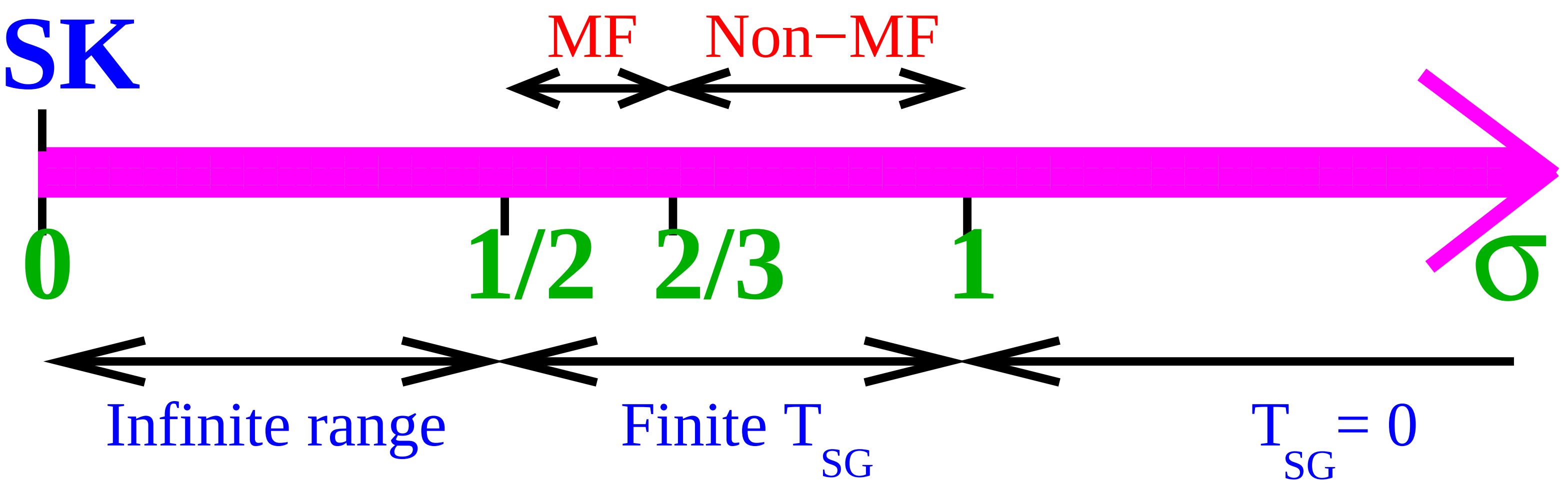
Long-Range model in $d = 1$

$$[J_{ij}^2]_{av} \propto \frac{1}{r_{ij}^{2\sigma}},.$$

Use diluted (diluted) version: Leuzzi et al (2008). The probability of a non-zero bond falls off like $1/r_{ij}^{2\sigma}$, but the strength bond does not fall off.

Analogy between short-range model in d-dimensions and the 1-d long-range model

d (SR)	σ [1–d (LR)]
∞	$1/2$
$6\ (= d_u)$	$2/3$
$2.5\ (= d_l)$	1



Results: AT-line (i)

FSS of the correlation length for the Ising spin glass in a (Gaussian random) field of $H_r = 0.1$ with $\sigma = 0.75$

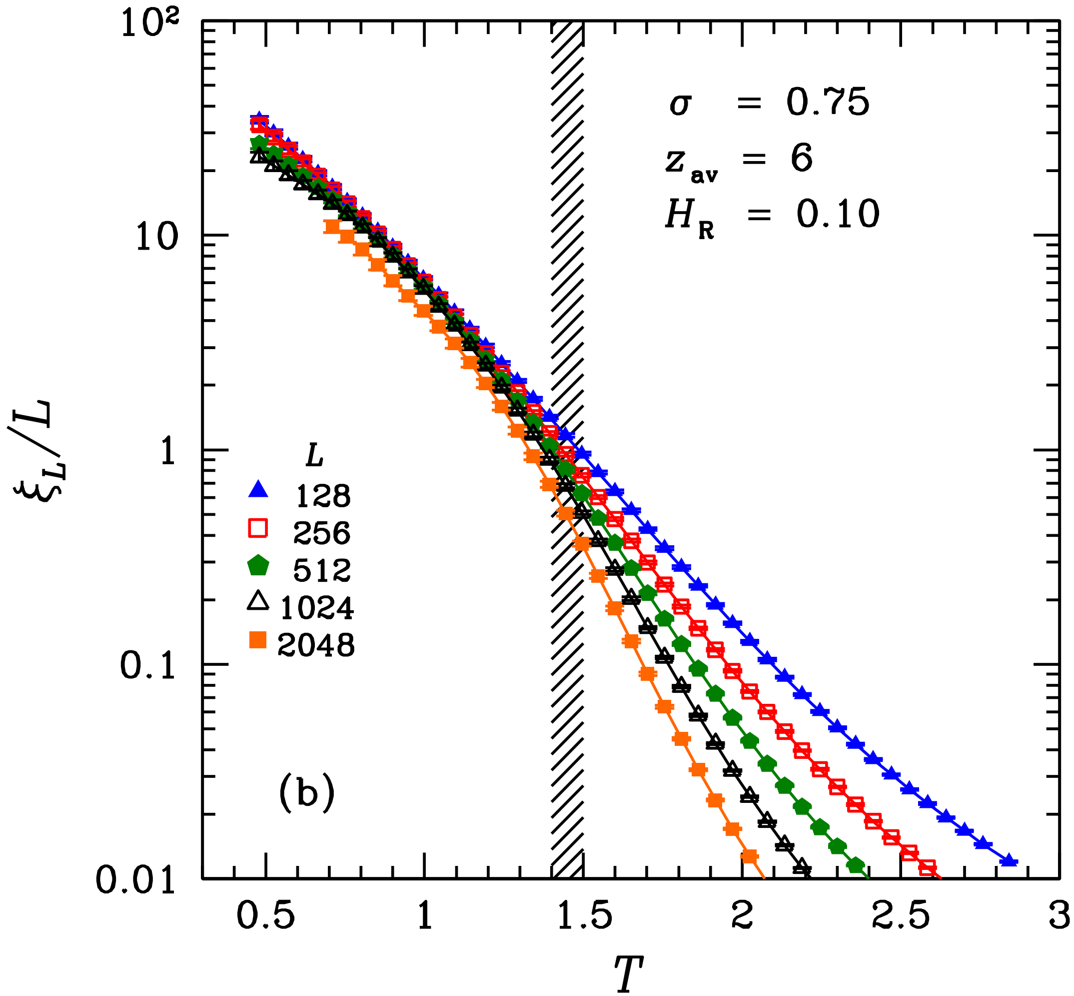
(non mean field region).

Lack of intersections implies no AT line down to this value of H_r.

(If there is an AT line, it only occurs for extremely small fields.)

Katzgraber, Larson and APY

Talk A29.00002, arXiv:0812.0421



Hence expect **no AT line** in the non mean field region, i.e. $\boldsymbol{d < 6}$.

However, for the same model, with same σ and H_r, (but with ± 1 bonds), Parisi et al., **arXiv:0811.3435**, find intersections and hence **claim an AT line.**

Results: AT-line (ii)

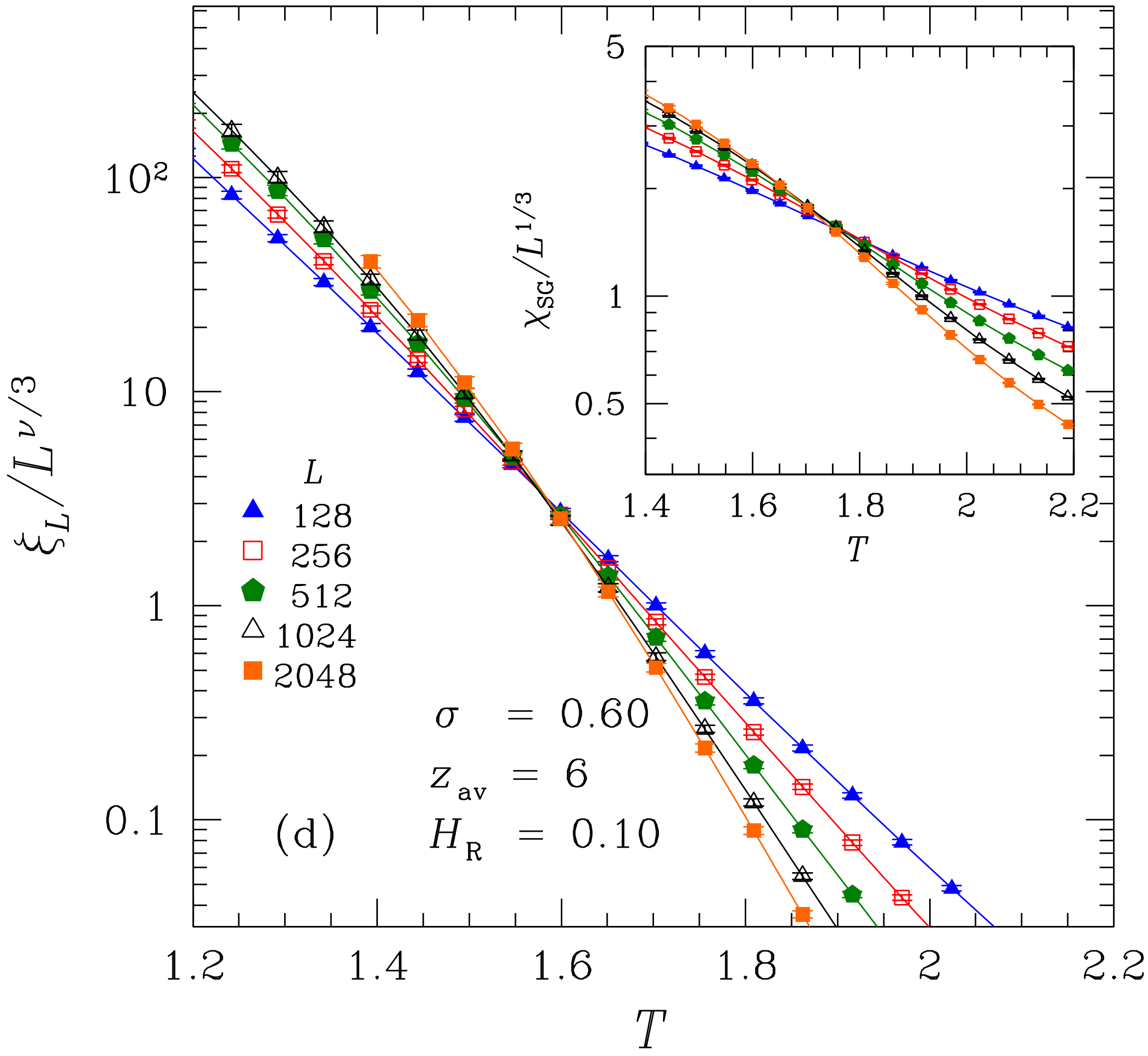
FSS of the correlation length for the Ising spin glass in a (Gaussian random) field of $H_r = 0.1$ with $\sigma = 0.60$

(mean field region).

(Katzgraber, Larson and APY).

The intersection implies

there is an AT line in the mean field region



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