Numerical results on phase transitions in spin glasses

Peter Young

http://physics.ucsc.edu/~peter

e-mail:peter@physics.ucsc.edu

UNIVERSITY OF CALIFORNIA SANTA CRUZ

Work supported by the Hierarchical Systems Research Foundation.

With H. G. Katzgraber, D. Larson, V. Martin-Mayor, A. Tarancon, L. A. Fernandez, S. Gaviro

Talk at Disordered Systems, Spin Glasses, Montreal June 10, 2009.

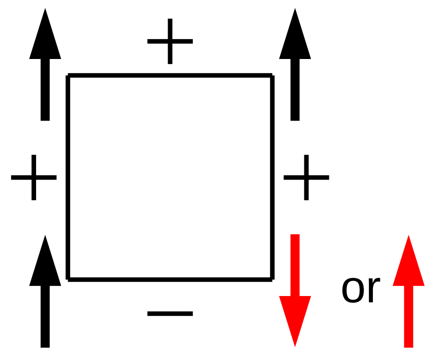
Can be downloaded from http://physics.ucsc.edu/~peter/talks/montreal.pdf

Overview

- Basic Introduction
  - Review of theory
  - Finite size scaling for the correlation length
- Try to answer two long-standing questions for 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)?

The Model

A system with disorder and frustration.



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

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

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

The $\mathbf{S}_i$ have m–components:

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

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

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

Will take a **Gaussian** distribution for the $\mathbf{J_{ij}}$.

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 1

Mean Field Theory (Edwards-Anderson, Sherrington-Kirkpatrick, Parisi). Exact solution of an infinite range (SK) model. Finite T_{SG}.

The Parisi solution is a “tour-de-force”. Has an infinite number of order parameters.

More than a quarter of a century after it was obtained using the replica trick, (needed “replica symmetry breaking” (RSB)) Tallegrand proved rigorously! that the Parisi free energy is exact for the SK model.

Theory 2

- Short-range (EA) models. Simulations on Ising systems also indicate a finite T_{SG} (see later) in $d = 3$. Heisenberg spin glasses? (See later.)

Theory 2

- Short-range (EA) models. Simulations on Ising systems also indicate a finite T_{SG} (see later) in $d = 3$. Heisenberg spin glasses? (See later.)
- Equilibrium state below T_{SG}. Two main scenarios:

Theory 2

- Short-range (EA) models. Simulations on Ising systems also indicate a finite T_{SG} (see later) in $d = 3$. Heisenberg spin glasses? (See later.)
- Equilibrium state below T_{SG}. Two main scenarios:

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

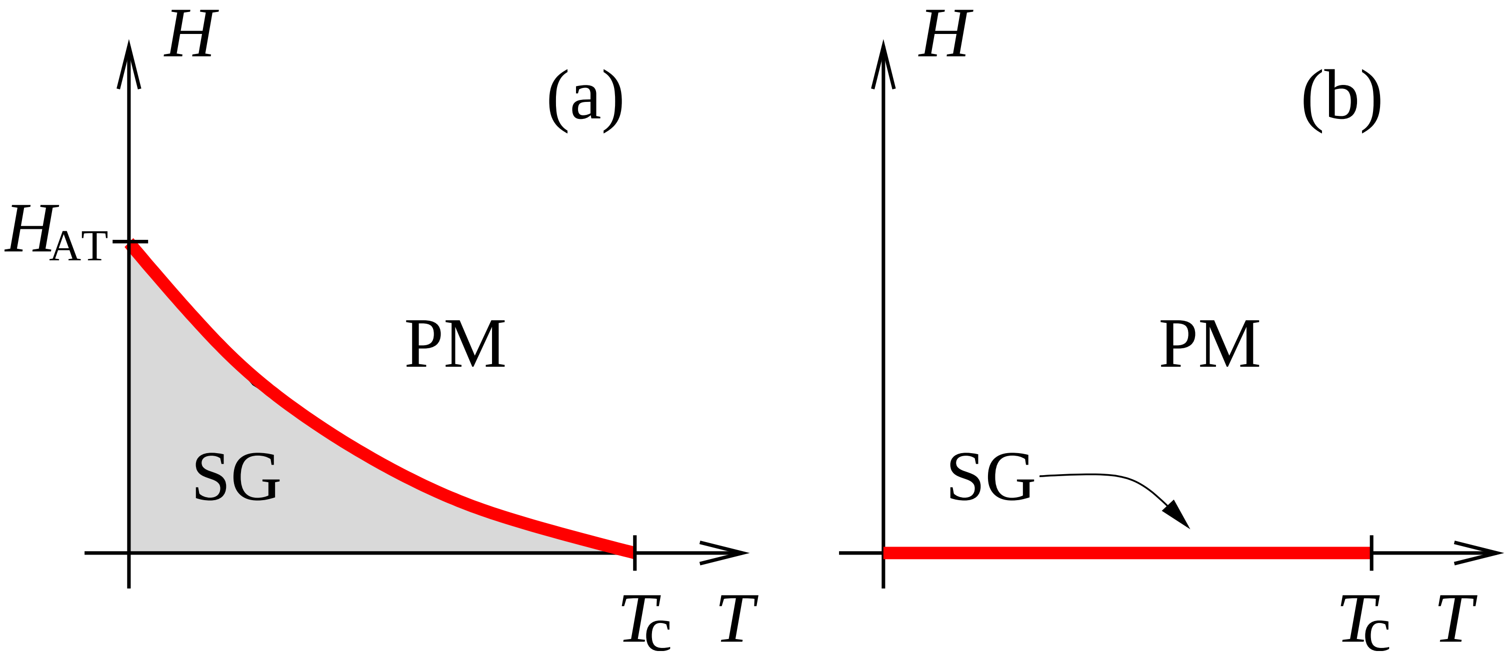
Assume short-range is similar to infinite-range. There is an AT line.

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

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

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.

Overview

- Basic Introduction
  - Review of theory
  - Finite size scaling for the correlation length
- Try to answer two long-standing questions for 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)?

Correlation Length

Spin glass correlation Function

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

Note: $\chi_{nl} \sim \chi_{SG}(\mathbf{k}=0)$, which is essentially the "correlation volume".

Determine the finite-size spin glass correlation length ξ_L from the Ornstein Zernicke equation:

$$\chi_{SG}(\mathbf{k}) = \frac{\chi_{SG}(0)}{1+\xi_L^2\mathbf{k}^2+\ldots},$$

by fitting to $k=0$ and $k=k_{\mathrm{min}}=\frac{2\pi}{L}(1,0,0)$.

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

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

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: Ising

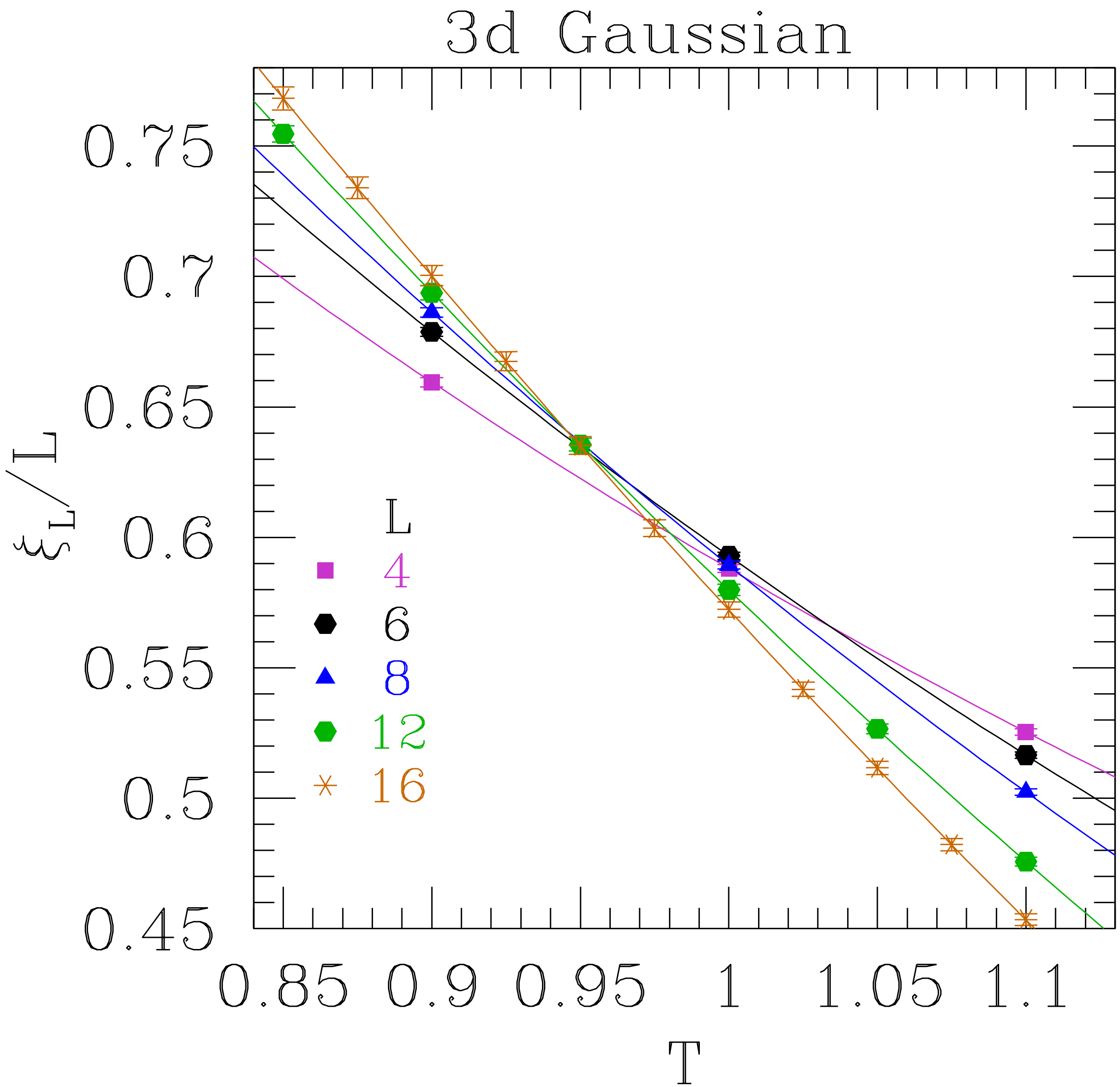
FSS of the correlation length for the Ising spin glass. (from Katzgraber, Körner and APY Phys. Rev. B **73**, 224432 (2006).)

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

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

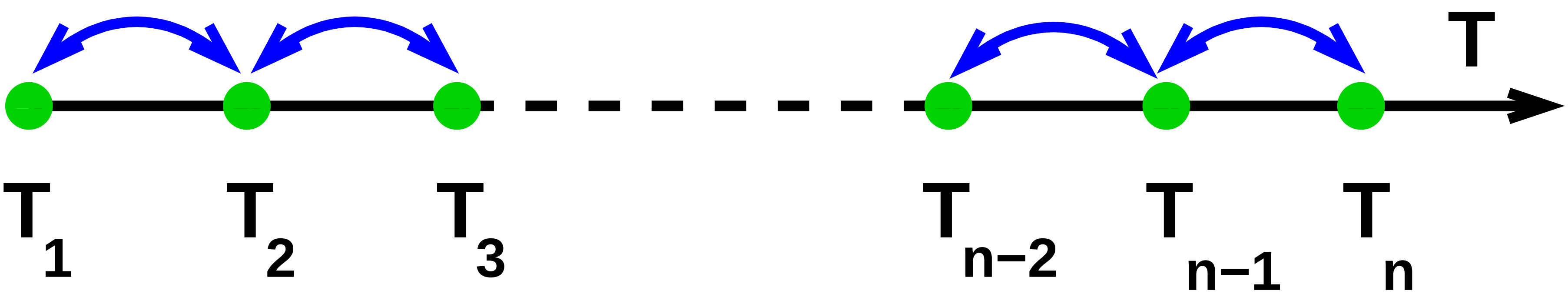
Prevously Marinari et al. found $T_{SG} = 0.95 \pm 0.04$ using a different analysis



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: T of each copy performs a random walk between T_1 and T_n.

- satisfies detailed balance
- simple
- system visits many valleys at low-T (with correct relative weight)

Overview

- Basic Introduction
  - Review of theory
  - Finite size scaling for the correlation length
- Try to answer two long-standing questions for spin glasses
  - Is there a phase transition in a Heisenberg spin glass?

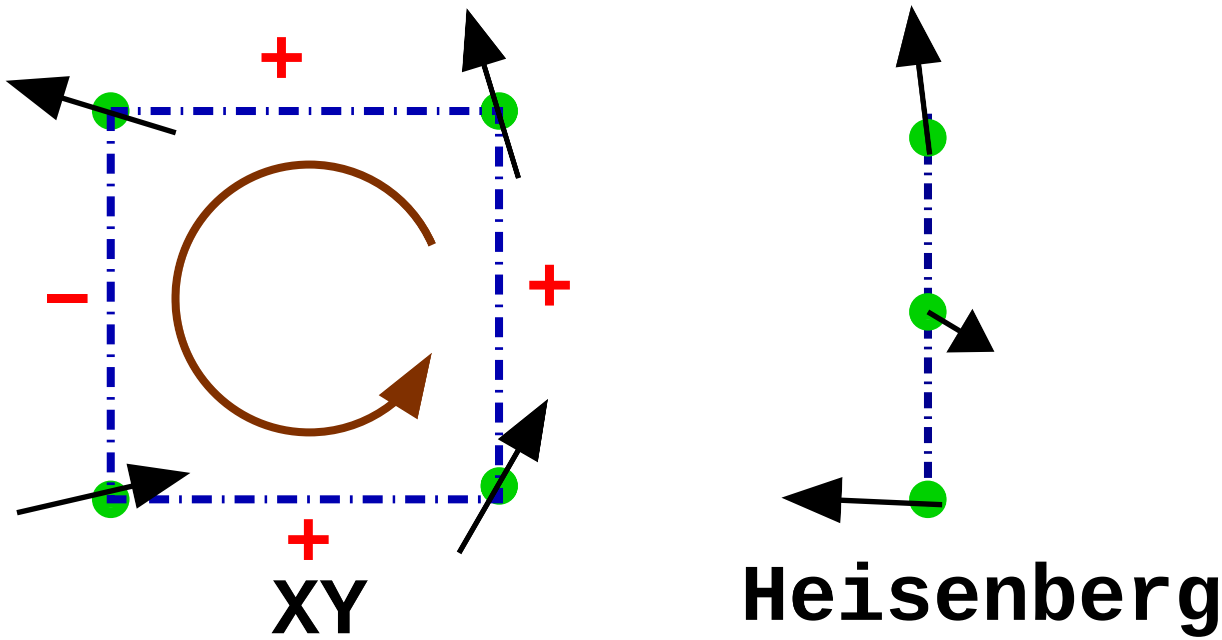
    Martin-Mayor, Tarancon, Fernandez, Gaviro, and APY (arXiv:0905.0322)
  - Is there a transition in an Ising spin glass in a magnetic field (Almeida-Thouless line)?

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

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, if any, seems very low, probably zero.

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, 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 $\mathbf{T_{SG} < T_{CG}}$.

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, 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.

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, 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

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, 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.

Motivation for vector model

- Most theory done for the Ising ($S_i = \pm 1$) spin glass. Clear evidence for finite $\mathbf{T_{SG}}$. Best evidence: finite size scaling (FSS) of correlation length (Ballesteros et al.)
- Many experiments closer to a vector spin glass $\mathbf{S}_i$. Theoretical situation less clear:
  - Old Monte Carlo: $\mathbf{T_{SG}}$, 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.

Equilibration: 1

The condition

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

is satisfied in equilibrium (for Gaussian distribution), where

$$U = -\frac{1}{N} \sum_{\langle i,j \rangle} J_{ij} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \quad \text{(energy)}$$

$$q_l = \frac{1}{N_b} \sum_{\langle i,j \rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2 \quad \text{“link overlap”}$$

$$q_s = \frac{1}{N_b} \sum_{\langle i,j \rangle} \langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle \quad \text{with } N_b = Nz/2,$$

Note: $z\,(= 6)$ is the lattice coordination number, and we have set $J = 1$.

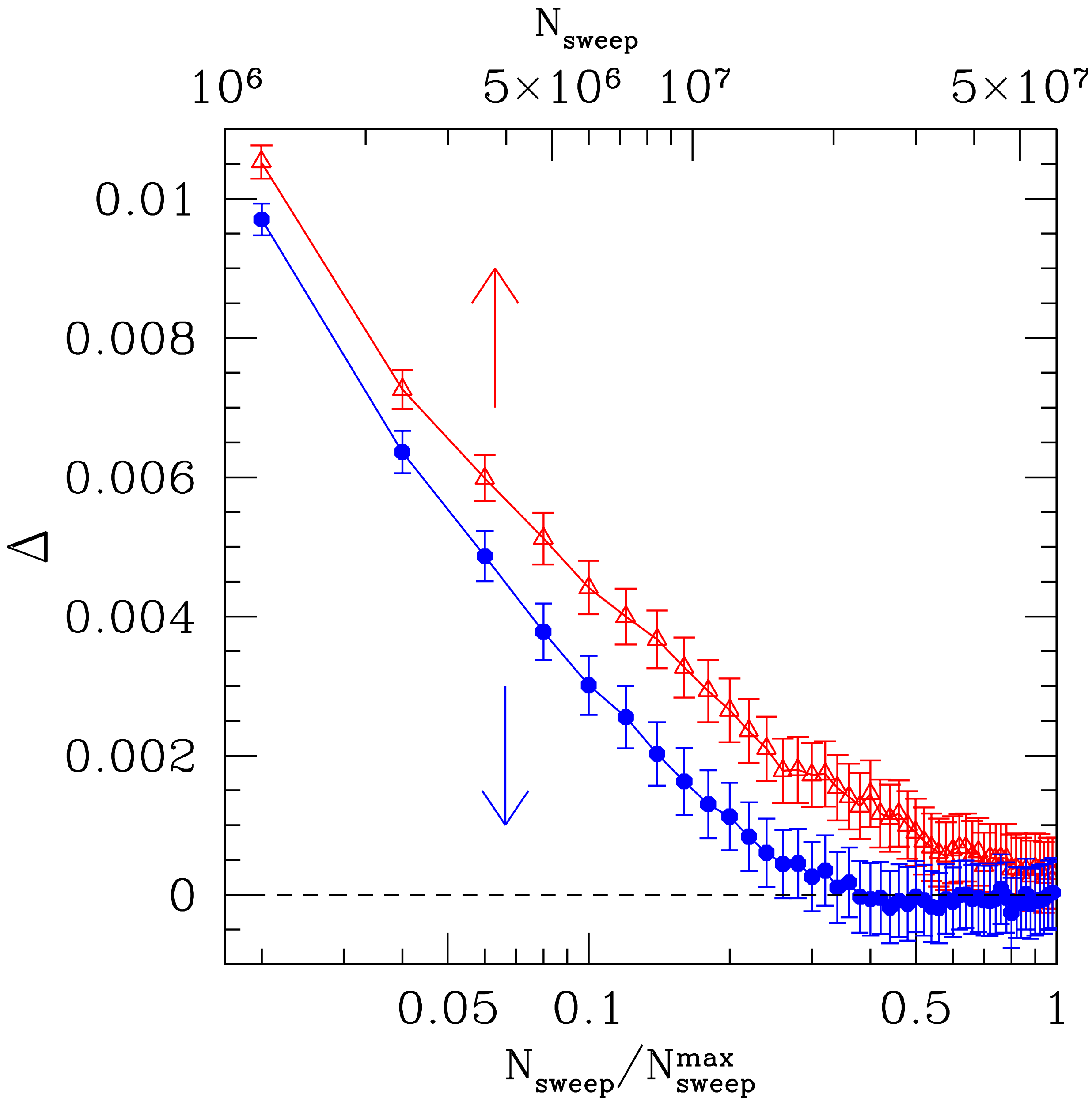
Not valid out of equilibrium (LHS $>$ RHS).

Equilibration: 2

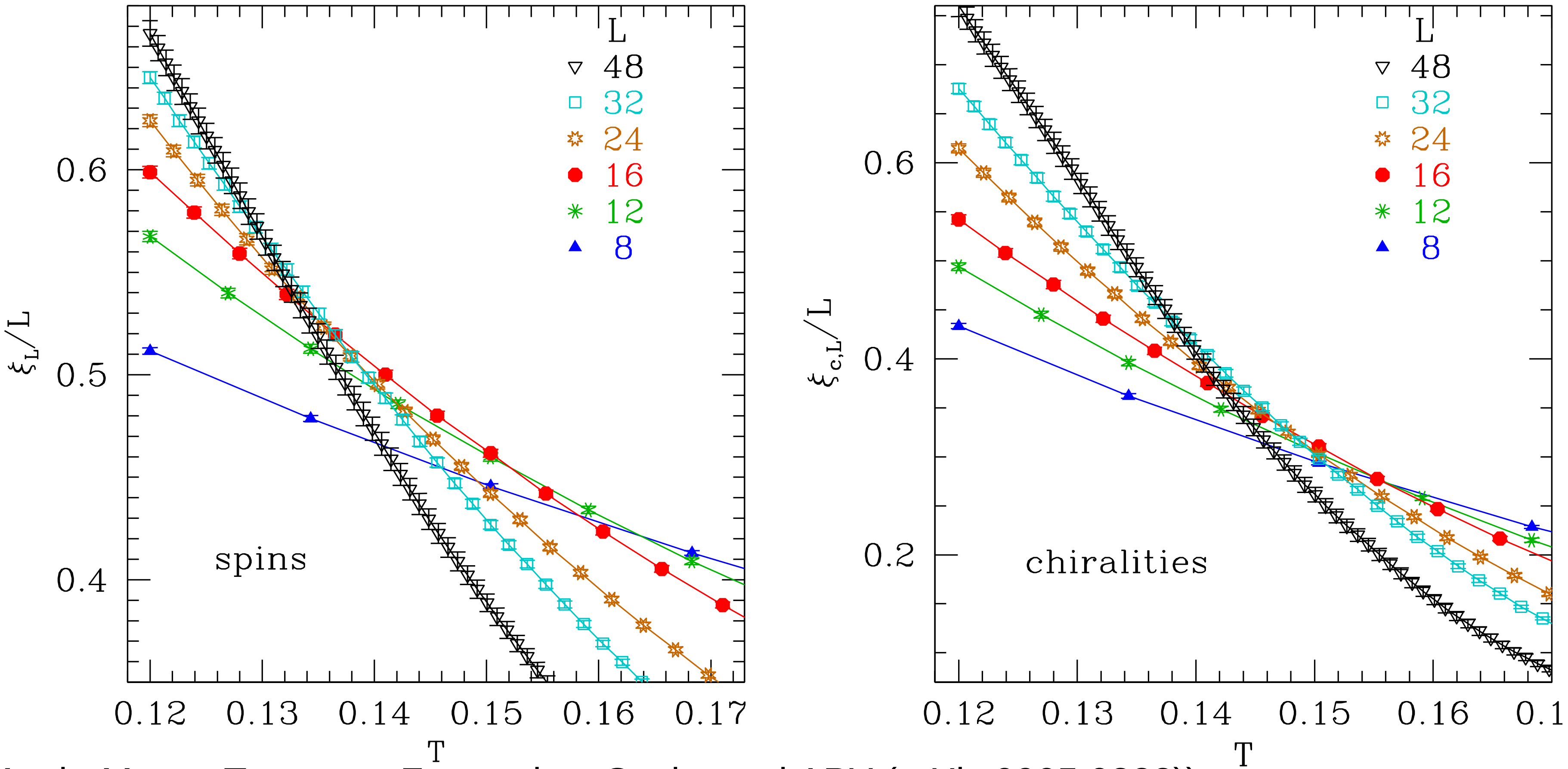
Equilibration test for
$T = 0.12, L = 48$
(largest size, lowest T).

$$\mathbf{\Delta} \equiv \left[\mathbf{q_s} - \mathbf{q_l} + \frac{\mathbf{2}}{\mathbf{z}}\mathbf{T}\,\mathbf{U}\right]_{\mathrm{av}}$$

is zero in equilibrium.



Heisenberg Spin Glass



(Martin-Mayor, Tarancon, Fernandez, Gaviro and APY (arXiv:0905.0322)).

Note: **much larger sizes** than for Ising (barriers smaller).

Are there two very close but distinct transitions?

Viet and Kawamura, $L \le 32$, claim $\boldsymbol{T_{CG} = 0.145 \pm 0.004, T_{SG} = 0.120 \pm 0.006}$.

We find, for $\boldsymbol{L \ge 16}$, $\boldsymbol{T_{\text{SG}} = 0.129^{+0.003}_{-0.016}}$. Chiral data needs subleading corrections for this range of sizes, but if we *assume* there is a single transition we get a good fit, for $\boldsymbol{L \ge 24}$, with $\boldsymbol{T_{\text{SG}} = T_{CG} = 0.120^{+0.010}_{-0.004}}$. Hence the data is compatible with a single transition.

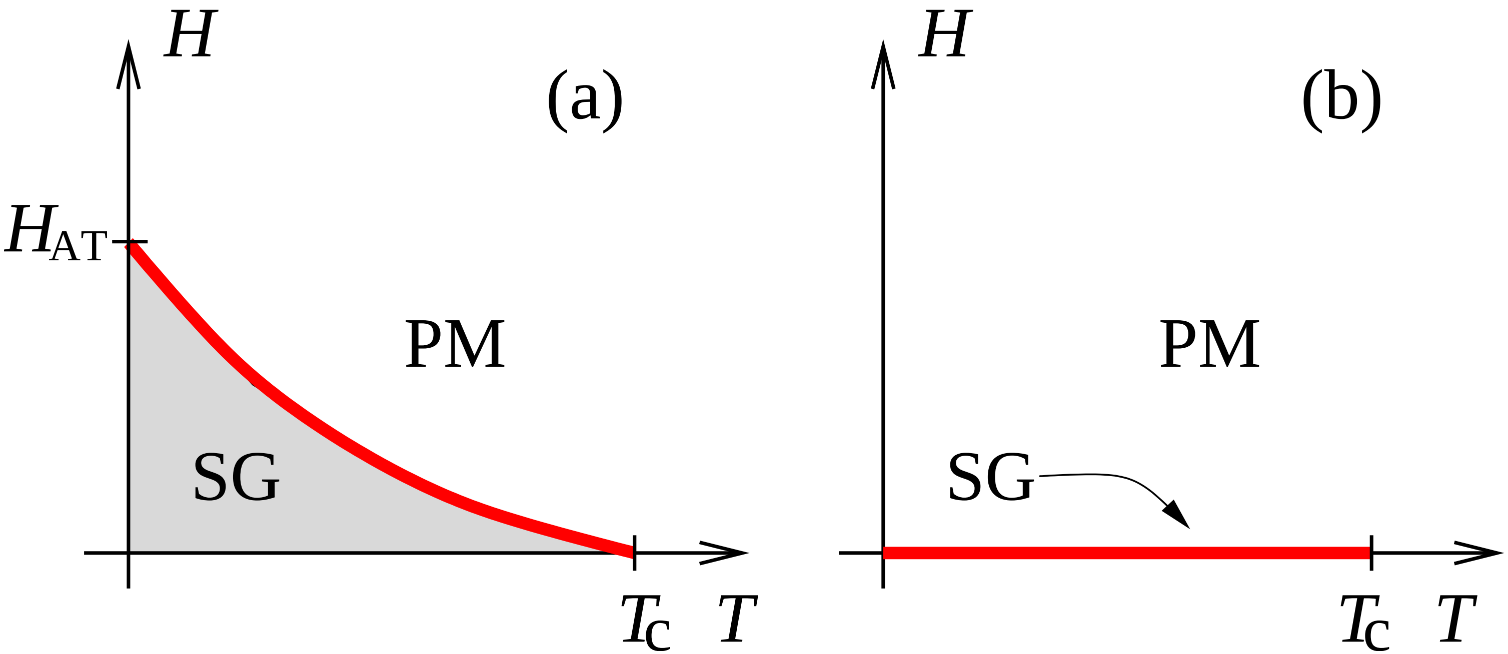
Overview

- Basic Introduction
  - Review of theory
  - Finite size scaling for the correlation length
- Try to answer two long-standing questions for spin glasses
  - Is there a phase transition in an isotropic Heisenberg spin glass?
  - Is there an phase transition in an Ising spin glass in a field?

    Katzgraber, Larson and APY (Phys. Rev. Lett. **102**, 177205 (2009))

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.

Is there an AT Line?: 2

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; i.e. so we look for intersections.

Long-Range model in $d = 1$

(Kotliar, Stein and Anderson, 1983): $\boxed{[J_{ij}^2]_{av} \propto \frac{1}{r_{ij}^{2\sigma}},}$.

For the short-range model:

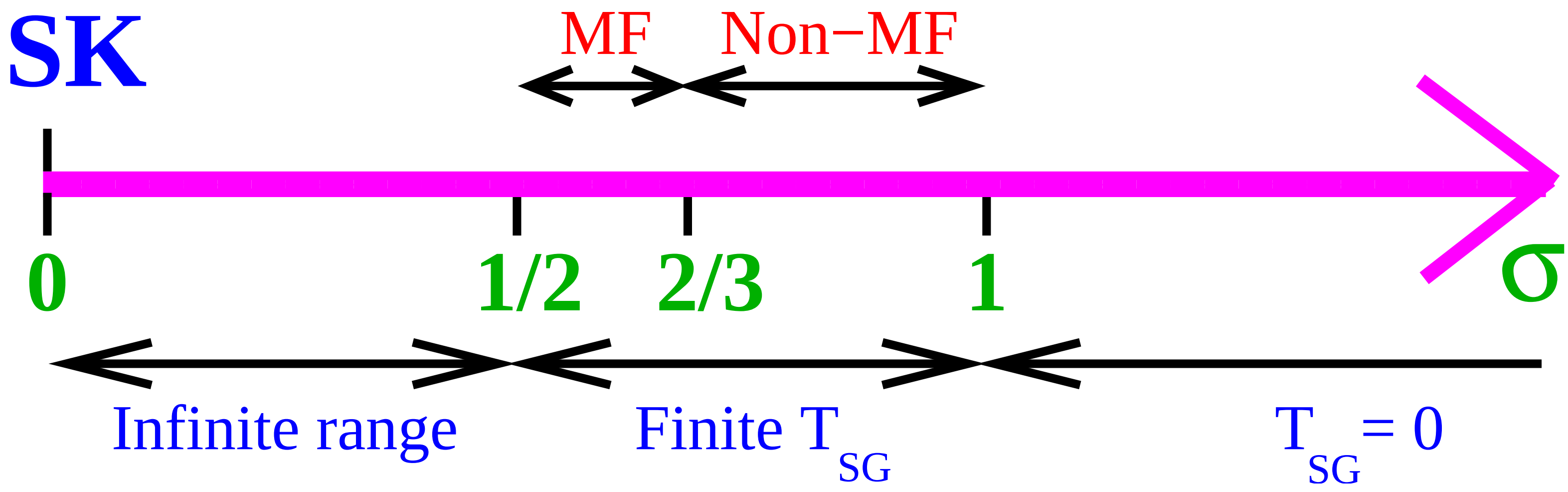
- there is a lower critical dimension d_l (equal to about 2.5),
- and an upper critical dimension d_u (equal to 6).

Make an analogy between varying d for short-range, and varying σ for long-range $d = 1$. (Works for ferromagnets, e.g. Fisher, Ma and Nickel.) In otherwords there is a σ_l *above* which $T_{SG} = 0$, and a σ_u *below* which the zero-field critical behavior is mean-field like, where

- $\sigma_l = 1,$ (Fisher and Huse)
- $\sigma_u = 2/3,$ (Kotliar, Stein and Anderson)
- The range $0 \le \sigma \le 1/2$ is infinite-range since $\sum_j [J_{ij}^2]_{\mathrm{av}}$ diverges.
- $\sigma = 0$ is the SK model.
- $\sigma \to \infty$ is the nearest-neighbor model.

Dependence on σ

The following figure summarizes the behavior of the $d = 1$ long-range model as a function of σ.



The interesting range is $\boxed{1/2 < \sigma < 1\,.}$

We use a (diluted) version of the model by Leuzzi et al (2008). The probability of a non-zero bond falls off like $1/r_{ij}^{2\sigma}$, but the strength of the bond does not fall off. We fix the mean coordination number to be 6.

Connection between d and σ

In finite-size scaling, the field h and reduced temperature t appear in arguments of scaling functions as $L^{y_T}\, t$ and $L^{y_H}\, h$, or equivalently

$$N^{y_T/d}\, t, \qquad N^{y_H/d}\, h,$$

where $N = L^d, y_H = (d+2-\eta)/2$ is the magnetic exponent, $y_T = 1/\nu$ is the thermal exponent. We make a plausible connection between the SR model in d-dimensions and the LR model in 1-dimension by

$$y_T^{SR}/d = y_T^{LR}, \qquad y_H^{SR}/d = y_H^{LR}.$$

The equation for y_H gives:

(since $\eta_{LR} = 3 - 2\sigma$ so $y_H^{LR} = \sigma$)

Also valid for y_T in the MF region

where $\nu_{SR} = 1/2, \eta_{SR} = 0, \nu_{LR} = 1/(2\sigma - 1)$

(and to 1st order in ϵ (M.A. Moore))

$$d = \frac{2 - \eta_{SR}(d)}{2\sigma - 1}.$$

σ	d
1/2	∞
3/5	10
2/3	6 (UCD)
0.75	4.6
0.85	3.3
0.9	3
1	2.5 (LCD)

Using information about η_{SR} we get

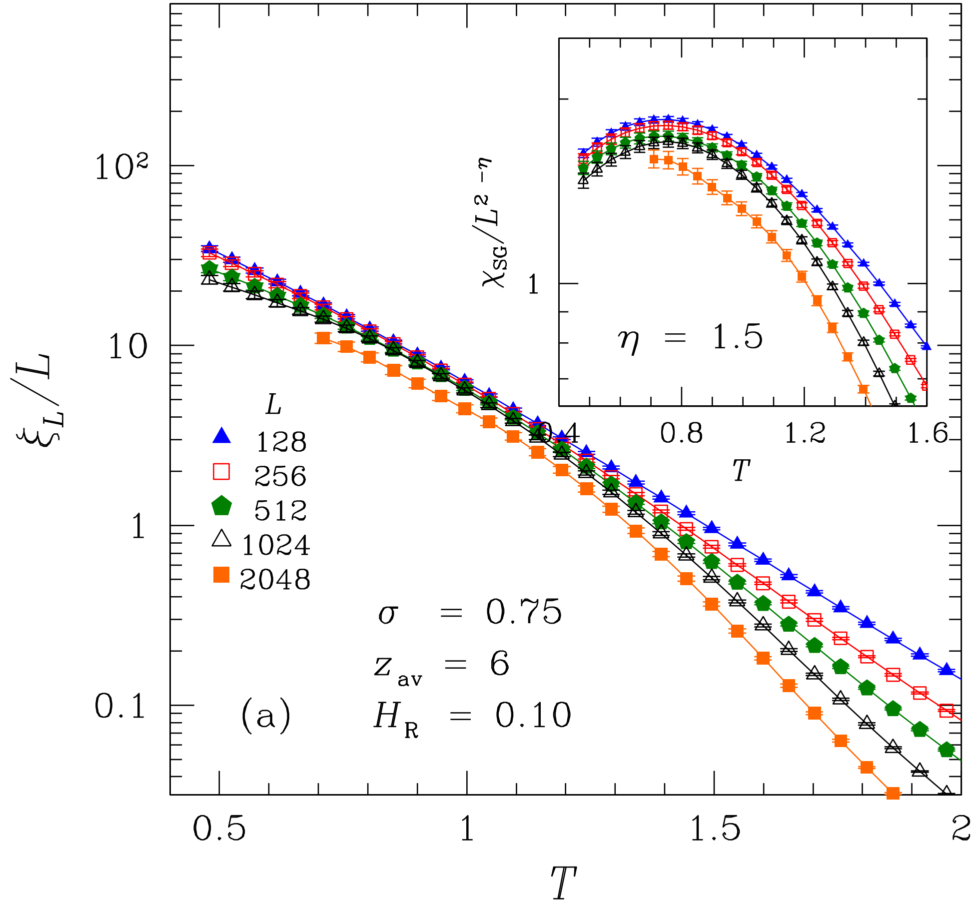
Results: AT-line

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.
Hence, if there is an AT line, it only occurs for extremely small fields

Katzgraber, Larson and APY

Phys. Rev. Lett. **102**, 177205 (2009)



Hence expect **no AT line** in the non mean field region, i.e. $d < 6$.
However, for the same model, with same σ and H_r, (but with ± 1 bonds), Parisi et al., **arXiv:0811.3435**, **claim an AT line.**

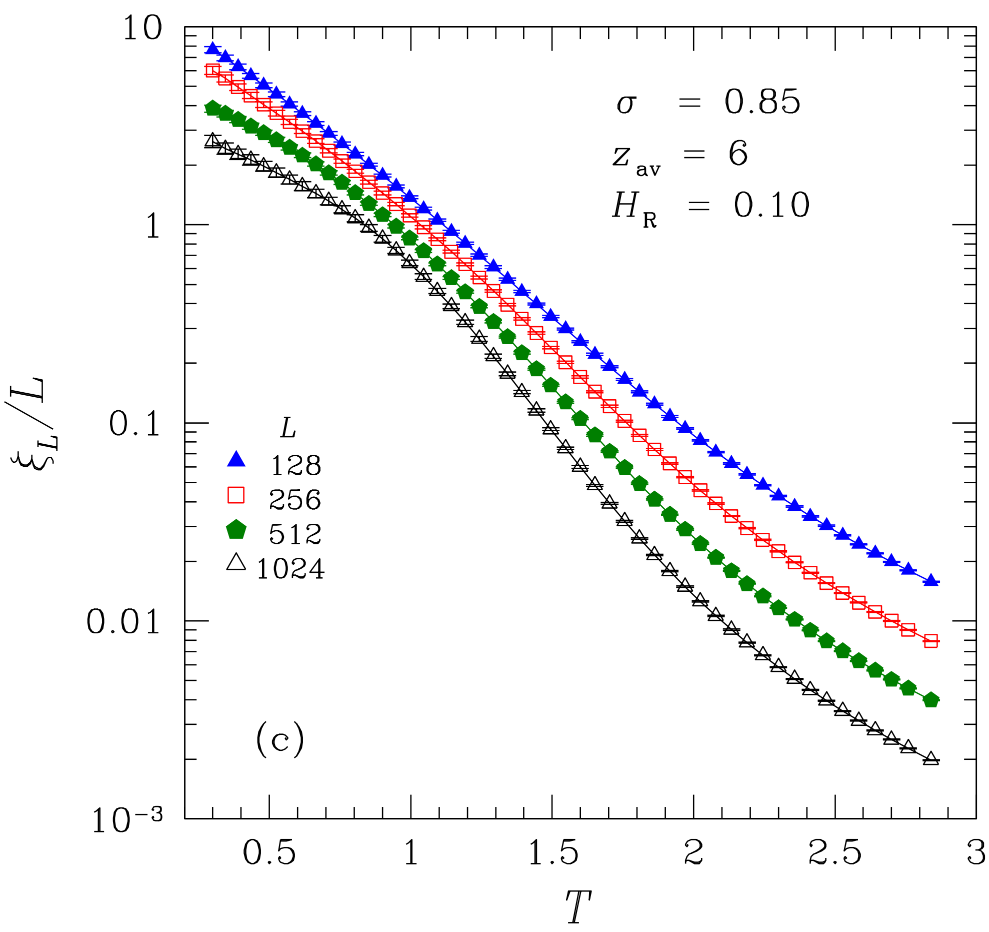
Results: AT-line

FSS of the correlation length for the Ising spin glass in a (Gaussian random) field of $H_r = 0.1$ with $\sigma = 0.85$ (further in the non mean field region).

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

Katzgraber, Larson and APY

Phys. Rev. Lett. **102**, 177205 (2009)

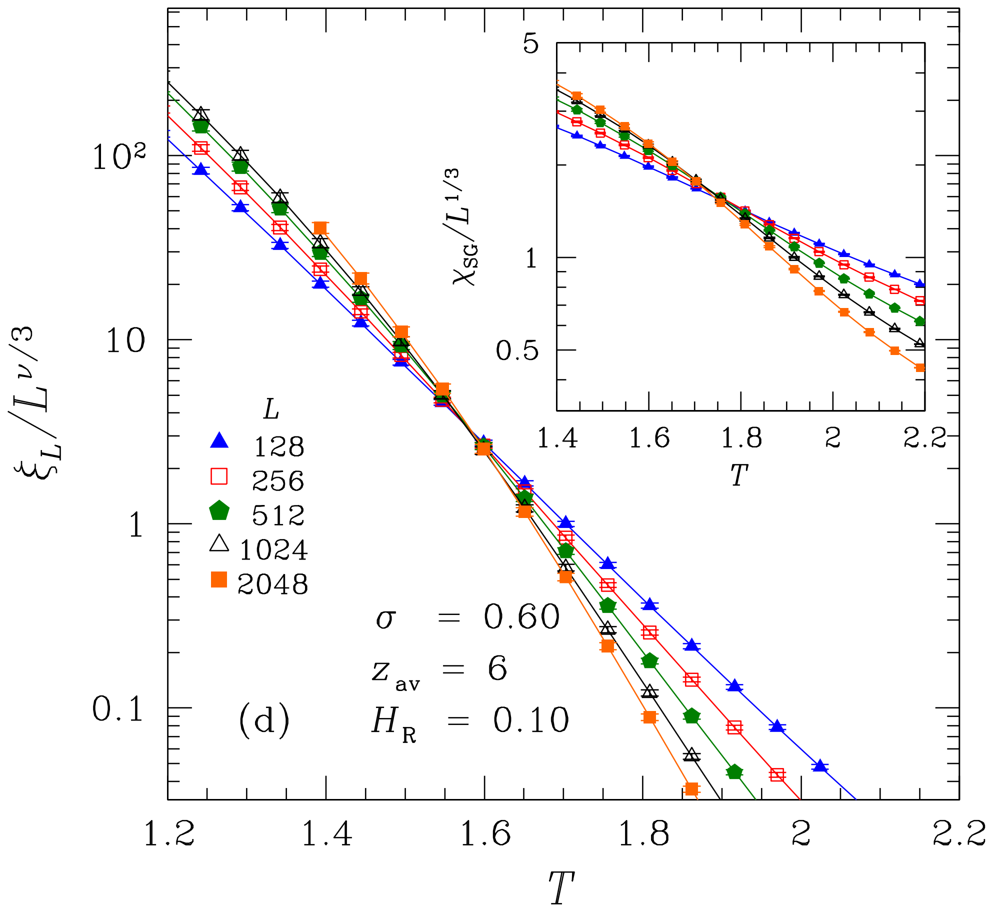


Results: AT-line

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 that there is an AT line in the mean field region



Conclusions

Do spin glasses have phase transitions?

Conclusions

Do spin glasses have phase transitions?

- In zero field YES, even for vector spin glasses, though whether the chiralities order at a slightly higher temperature is still controversial.
- In a magnetic field, NO, i.e. no AT line for Ising spin glasses, at least in three dimensions. Evidence for an AT line in high dimensions, perhaps $d > 6$.

Conclusions

Do spin glasses have phase transitions?

- In zero field YES, even for vector spin glasses, though whether the chiralities order at a slightly higher temperature is still controversial.
- In a magnetic field, NO, i.e. no AT line for Ising spin glasses, at least in three dimensions. Evidence for an AT line in high dimensions, perhaps $d > 6$.

Need to understand better:
Nature of the equilibrium state below T_{SG}. Absence of an AT line favors droplet theory, but other data (non-trivial order parameter distribution $P(q)$) favors RSB.

Conclusions

Do spin glasses have phase transitions?

- In zero field YES, even for vector spin glasses, though whether the chiralities order at a slightly higher temperature is still controversial.
- In a magnetic field, NO, i.e. no AT line for Ising spin glasses, at least in three dimensions. Evidence for an AT line in high dimensions, perhaps $d > 6$.

Need to understand better:

Nature of the equilibrium state below T_{SG}. Absence of an AT line favors droplet theory, but other data (non-trivial order parameter distribution $P(q)$) favors RSB.

THANK YOU