Phase Transition in Spin Glasses

A.P. Young

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

Collaborators:

Work supported by the NSF
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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:

\[ \mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i \cdot S_j - \sum_i h_i \cdot S_i. \]

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

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

Spins, \( S_i \), fluctuate and have \( m \)-components:

\[ m = 1 \quad (\text{Ising}) \]
\[ m = 2 \quad (\text{XY}) \]
\[ m = 3 \quad (\text{Heisenberg}). \]
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 $\xi_{SG}$ diverges.

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

$$\chi_{SG} = \frac{1}{N} \sum_{i,j} \langle S_i \cdot S_j \rangle^2_{av},$$

(notice the square) which is accessible in simulations. It is also essentially the same as the non-linear susceptibility, $\chi_{nl}$, 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:

$$
\begin{align*}
    & T_1 & T_2 & T_3 & \quad & T_{n-2} & T_{n-1} & T_n \\
\end{align*}
$$

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-$T$.

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 $L/\xi_{\text{bulk}}$ 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 $\xi_L/L$ is dimensionless (and so has no power of $L$ multiplying the scaling function $X$).

Hence data for $\xi_L/L$ 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

$T_{SG} \approx 0.96$

Previously, Marinari et al found $T_{SG} \approx 0.95 \pm 0.04$ 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)

\[
\kappa_{ij}^{\mu} = \begin{cases} \\
\frac{1}{2\sqrt{2}} \sum'_\langle l,m \rangle \text{sgn}(J_{lm}) \sin(\theta_l - \theta_m), & \text{XY (}\mu \perp \text{ square)} \\
S_{i+\hat{\mu}} \cdot S_i \times S_{i-\hat{\mu}}, & \text{Heisenberg} \\
\end{cases}
\]
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)

Are there two (nearby) transitions or just one?
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Viet and Kawamura, $L \leq 24$, claim $T_{CG} = 0.145$, $T_{SG} = 0.120$
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Are there two (nearby) transitions or just one?

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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)
In MFT, \( \chi_{SG} \) diverges on AT line where now

\[
\chi_{SG}(k) = \frac{1}{N} \sum_{i,j} [(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle)^2]_{av} e^{ik \cdot (R_i - R_j)}.
\]

Convert this to correlation length \( \xi_L \)

\( \chi_{SG} \) in a field not accessible in experiment is in simulations.

Best to use FSS of \( \frac{\xi_L}{L} \) to look for transition.

i.e. look for intersections:

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

no sign of a transition. (Katzgraber, APY)
Results of Simulations

In MFT, $\chi_{BG}$ diverges on AT line where now

$$\chi_{BG}(k) = \frac{1}{N} \sum_{i,j} [(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle)^2]_{av} e^{ik \cdot (R_i - R_j)}.$$ 

Convert this to correlation length $\xi_L$.

$\chi_{BG}$ in a field not accessible in experiment is in simulations.

Best to use FSS of $\xi_L/L$ to look for transition.

i.e. look for intersections:

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

no sign of a transition. (Katzgraber, APY)

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

• Spin glasses are related to a range of problems in science, and have the advantage that there are “simple” models which can be simulated, and experiments can probe them in exquisite detail since they couple to a magnetic field.
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  • (The last two are not yet universally accepted.)