Phase Transition in Spin Glasses

A.P. Young

Invited talk at the DPG meeting, Regensburg, March 22, 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**:

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

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

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

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

- \(m = 1\) (Ising)
- \(m = 2\) (XY)
- \(m = 3\) (Heisenberg).
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.

Many interesting experiments on non-equilibrium effects (aging). Here concentrate on **equilibrium** phase transitions.
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:

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-$T$.
Equilibration

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

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

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

\[ q_l = \frac{1}{N_b} \sum_{i,j} \langle S_i S_j \rangle^2 \] “link overlap”, \[ N_b = N z / 2. \]

\( z \) is the no. of neighbors, and \( J = 1 \).
\[ [\cdots]_{av} \] is an average over samples.

Data for Ising spin glass (H. Katzgraber)

\[ [q_l - 1]_{av} \text{ and } (2/z)T\langle U \rangle_{av} \]

approach a common value from opposite directions,

and, once they agree with each other, the results don’t change if \( N_{\text{sweep}} \) is increased further.
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Finite Size Scaling

Assumption: size dependence comes from the ratio $\frac{L}{\xi_{\text{bulk}}}$ 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 spin correlations.

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)

\[
\kappa_{i_0}^{\mu} = \begin{cases} 
\frac{1}{2\sqrt{2}} \sum'_{l,m} \text{sgn}(J_{lm}) \sin(\theta_l - \theta_m), \\
S_{i_0+\hat{\mu}} \cdot S_i \times S_{i-\hat{\mu}},
\end{cases}
\]

**XY (\mu \perp square)**

**Heisenberg**
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
Results for Heisenberg Spin Glass

Are there two (nearby) transitions or just one?

(Fernandez, Gaviro, Martin-Mayor, Tarancon, APY (2009))
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Results for Heisenberg Spin Glass

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Are there two (nearby) transitions or just one?

Viet and Kawamura, $L \leq 24$, claim $T_{CG} = 0.145$, $T_{SG} = 0.120$

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

Convert this to correlation length $\xi_L/L$ not accessible in experiment but can use FSS of $\xi_L/L$ in simulations to look for transition.

Look for intersections:

With a small field of 0.1 (c.w. $TSG \approx 0.96$)

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

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Convert this to correlation length $\chi_{SG}$ not accessible in experiment but can use FSS of $\xi_L / L$ in simulations to look for transition.

Look for intersections:

With a small field of 0.1 (c.w. TSG $\cong 0.96$) 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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Danke Schön