Recent Numerical Results on Spin Glasses

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Abstract

After giving an introduction to spin glasses, I will discuss recent numerical results on two topics which have been of interest in the field for many years: (i) whether there is a finite temperature phase transition in isotropic vector (e.g. Heisenberg) spin glasses, and (ii) whether there is a phase transition (called the AT line) in a spin glass in a magnetic field.

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1 Introduction

Since this is a presentation to a general audience I will start by giving an introduction to spin glasses, and then discuss recent numerical results on two topics of interest in this fi eld.

Spin glasses are disordered systems in which there is also competition, or "frustration" between the interactions. A toy example illustrating frustration is shown in Fig. 1

Most theoretical work has used the simplest model with these properties, which is due to Edwards and Anderson [1]:

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

in which the spins $\mathbf{S}_i$ lie on the sites of a regular lattice, and the interactions J_{ij},

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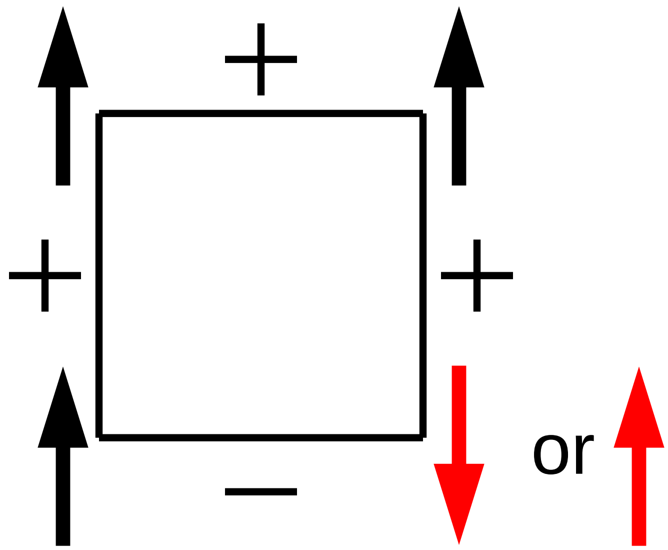

Fig. 1. A toy model which shows frustration. If the interaction on the bond is a "+", the spins want to be parallel and if it is a "−" they want to be antiparallel. Clearly all these conditions can not be met so there is competition or "frustration".

which we take to be between nearest neighbors only, are independent random variables with mean and standard deviation given by

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

A zero mean is chosen to avoid any bias towards ferromagnetism or antiferromagnetism, and it is convenient, in the simulations, to take a Gaussian distribution for the J_{ij}. The $\mathbf{S}_i$ are of unit length and have m–components:

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

Experimentally, there are different types of spin glass, for example:

- Metals:
  Diluted magnetic atoms, e.g. Mn, in a non-magnetic metal such as Cu, interact with the RKKY interaction whose sign depends on the distance between the atoms. Note that Mn is an S-state ion and so has little anisotropy. It should therefore correspond to a *Heisenberg* spin glass.
- Insulators:
  An example is $Fe_{0.5}Mn_{0.5}TiO_3$, which comprises hexagonal layers. The spins align perpendicular to layers (hence it is *Ising*-like). Since it is an insulator, the

interactions are short-range.

Spin glass ideas have also been useful in other areas of science such as protein folding and optimization problems in computer science.

After considerable work, it became clear that a spin glass has a sharp thermodynamic phase transition at temperature $T = T_{SG}$, such that for $T < T_{SG}$ the spins freeze in some random-looking orientation. As $T \to T_{SG}^{+}$, the spin glass correlation length, discussed below, diverges. A quantity which diverges, therefore, is the *spin glass susceptibility*

$$\chi_{SG} = \frac{1}{N} \sum_{\langle i,j \rangle} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2]_{\rm av} \,, \tag{4}$$

(notice the square) which is accessible in simulations. It is also essentially the same as the *non-linear susceptibility*, χ_{nl}, which can be measured experimentally and is defined by the coefficient of h^3 in the expansion of the magnetization m,

$$m = \chi h - \chi_{nl} h^3 + \cdots \,, \tag{5}$$

where h is the magnetic field. We expect that χ_{nl} diverges at T_{SG} like

$$\chi_{nl} \sim (T - T_{SG})^{-\gamma} \,, \tag{6}$$

where γ is a critical exponent. This divergent behavior has been seen in many experiments. A nice example is the data of Omari et al. [2] on 1% Mn in Cu which shows a clear divergence.

At low temperatures, the dynamics of spin glasses becomes very slow, such that below T_{SG} the system is never fully in equilibrium. This is because the “energy landscape” becomes very complicated with many “valleys” separated by “barriers”. The (free) energies of the valleys can be very similar and yet the spin configurations rather different. Hence there are large-scale, low-energy excitations in spin glasses.

This non-equilibrium behavior has been extensively studied in recent years. Of particular note has been the study of “aging” in spin glasses, pioneered by the Uppsala group [3]. One cools the system below T_{SG} and waits for a “waiting time” t_w. The system is then perturbed in some way, e.g. by applying a magnetic field, and the subsequent response is measured. It is found that the nature of the response depends on t_w, providing clear evidence that the system was not in equilibrium. However, in this talk, I will not be discussing non-equilibrium behavior.

2 Finite size scaling of the correlation length

We shall see that a particularly useful quantity to calculate numerically is the spin glass correlation length of the finite-size system, ξ_L, which can be determined from the Ornstein Zernicke equation:

$$\chi_{SG}(\mathbf{k}) = \frac{\chi_{SG}(\mathbf{0})}{1 + \xi_L^2 \mathbf{k}^2 + \ldots}, \tag{7}$$

by fitting to $\mathbf{k} = 0$ and $\mathbf{k} = \mathbf{k}_{\min} = \frac{2\pi}{L}(1, 0, 0)$. The precise formula is

$$\xi_L = \frac{1}{2\sin(k_{\min}/2)} \left(\frac{\chi_{SG}(0)}{\chi_{SG}(\mathbf{k}_{\min})} - 1 \right)^{1/2}. \tag{8}$$

In order to locate the transition we use the technique of finite-size scaling (FSS). The basic assumption of FSS is that the size dependence comes from the ratio L/ξ_{bulk} where

$$\xi_{\text{bulk}} \sim (T - T_{SG})^{-\nu} \tag{9}$$

is the *bulk* spin glass correlation length. In particular, the *finite-size* correlation length is expected to vary as

$$\frac{\xi_L}{L} = X\left(L^{1/\nu}(T - T_{SG}) \right), \tag{10}$$

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}. For quantities with dimension, like χ_{SG}, there will be an unknown power of L multiplying the scaling function in Eq. (10) which makes the analysis more complicated.

One of the problems that we will discuss is the phase transition in a Heisenberg spin glass, for which the question of a finite temperature transition has been much less well established than for the Ising case. Kawamura [4,5] argued that $T_{SG} = 0$ for a purely isotropic spin glass, but there can be a glass-like transition at $T = T_{CG}$ in the “chiralities” (i.e. vortices). In Kawamura’s picture, the observed spin glass transition is due to anisotropy in the system which couples spins and chiralities. To define chirality we follow Kawamura [4]:

$$\kappa_i^\mu = \begin{cases} \dfrac{1}{2\sqrt{2}} \sum_{\langle l,m \rangle}' \operatorname{sgn}(J_{lm}) \sin(\theta_l - \theta_m), & \text{XY } (\mu \perp \text{square}), \\ \mathbf{S}_{i+\hat{\mu}} \cdot \mathbf{S}_i \times \mathbf{S}_{i-\hat{\mu}}, & \text{Heisenberg}, \end{cases} \tag{11}$$

see Fig. 2, where for the XY case i refers to the plaquette indicated, and for the Heisenberg model, i refers to the middle of the three sites.

However, the possibility of finite T_{SG} has been raised by various authors [6–10], so the situation was confusing.

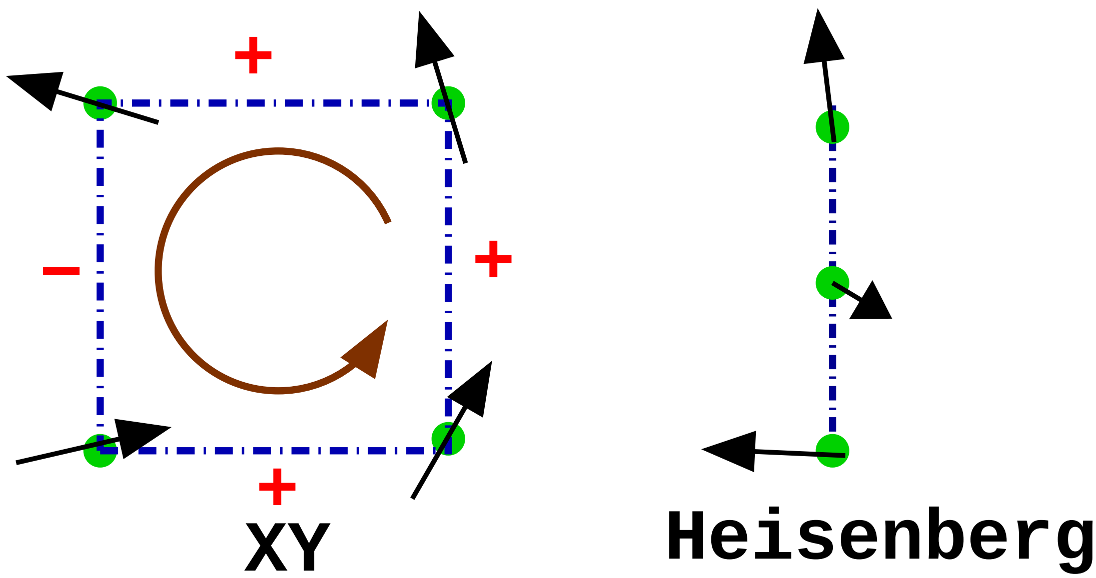

Fig. 2. An illustration of chirality for XY and Heisenberg spin glasses.

The chiral glass correlation length can be calculated in the same way as for the spin glass correlation length discussed above, so we can locate the transition(s) of both the spins and chiralities.

3 Phase transition in an isotropic Heisenberg spin glass

Our aim is to see if there is a single transition at which both spins and chiralities order or whether, as proposed by Kawamura, there is a finite-temperature transition in the chiralities but not the spins. The technique of finite size scaling of the correlation length discussed in the previous section seems ideally suited for this purpose. Data for ξ_L/L obtained from Monte Carlo simulations by Lee and myself [11] are shown in Fig. 3. There is a clear intersection showing that T_{SG} is finite.

Similar results for the chiral correlation length [11] show that the chiral glass transition occurs at the same temperature. We therefore conclude that there is a singel finite temperature transition in a Heisenberg spin glass in three dimensions.

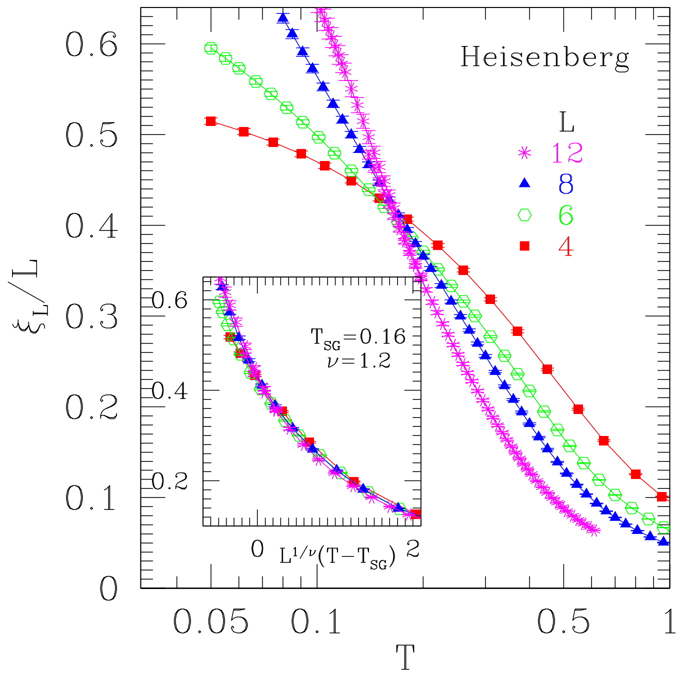

Fig. 3. Data for the spin glass correlation length of the Heisenberg spin glass divided by L (based on Ref. [11] with some additional data).

4 Absence of an Almeida-Thouless line

One of the surprising results of the mean field theory of spin glasses [1,12] is the existence of a paramagnetic to spin glass phase transition in a magnetic field [13] known as the Almeida-Thouless (or AT) line. Interestingly there is no change of symmetry at this transition.

It is important to know whether the AT line also occurs in more realistic short-range models, since the two main scenarios that have been proposed for the spin-glass state differ over this issue. In the "droplet picture" [14–16] there is *no* AT line in *any* finite-dimensional spin glass. By contrast, the "replica symmetry breaking" (RSB) picture [17,18] postulates that the behavior of short-range systems is quite similar to that found in mean field theory, which *does* have an AT line as just mentioned. Recently Katzgraber and I [19] have used finite size scaling of the correlation length, determined from Monte Carlo simulations, to investigate whether an AT line occurs in three dimensions. For technical reasons we used a Gaussian random field, of standard deviation H_r, rather than a uniform field. In mean field theory an AT line is expected in both. We also considered an Ising model, since this is the simplest case.

To determine the correlation length in a field we need the wavevector-dependent spin-glass susceptibility which is now given by

$$\chi_{SG}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} \left[\left(\langle S_i S_j \rangle_T - \langle S_i \rangle_T \langle S_j \rangle_T \right)^2 \right]_{\rm av} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} . \tag{12}$$

Figure 4 shows data for a particular value of H_r. Clearly there are no intersections, which implies the *absence* of an AT line, at least at this field. Similar results are found for different field strengths, and so we conclude that there is no AT line in short range spin glasses in three dimensions.

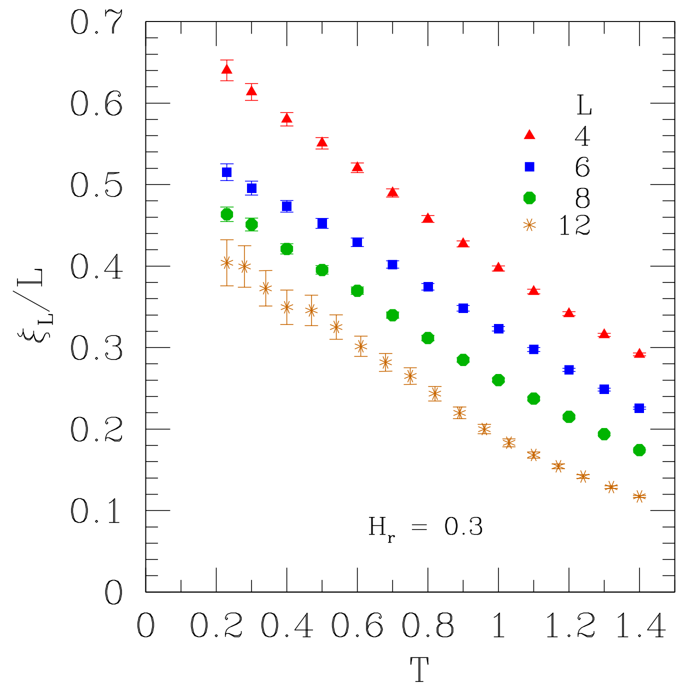

Fig. 4. Data for ξ_L/L for $H_{\rm r} = 0.3$ for different sizes. There is no sign of intersections down to the lowest temperature $T = 0.23$. (From Ref. [19].)

5 Conclusions

By using the finite size scaling of the correlation I have provided evidence that there *is* a phase transition in an isotropic Heisenberg spin glass in three dimensions, and that there *is not* a phase transition in a magnetic field (AT line). Much more remains to be done, particularly to understand the non-equilibrium behavior below T_{SG}.

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