Some recent results concerning phase transitions in spin glasses

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Abstract. I give an introduction to spin glasses, including a short discussion of experiments and theoretical concepts. I then discuss recent results from Monte Carlo simulation about two topics (i) the transition in a Heisenberg spin glass, and (ii) the transition in a magnetic field (Almeida-Thouless line) for an Ising spin glass.

1. Introduction
Spin glasses are systems with two key ingredients: disorder, and frustration, i.e. competition between different terms in the Hamiltonian so they can not all be satisfied simultaneously. Figure 1 shows a toy example of frustration with a single square of Ising spins. (Ising spins can only point up or down.) The “+” or “−” on the bonds indicates a ferromagnetic or antiferromagnetic interaction respectively. In this example, with one negative bond, it is impossible to minimize the energy of all the bonds so there is competition or “frustration”.

Most theoretical work therefore uses the simplest model with the features of disorder and frustration, the Edwards Anderson [1] (EA) model, whose Hamiltonian is

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

(1)

**Figure 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 simultaneously so there is competition or “frustration”.
The spins $S_i$ are classical $m$-component vectors which lie on the sites $i$ of a three-dimensional, simple cubic lattice with $N = L^3$ sites. Periodic boundary conditions are applied. The interactions $J_{ij}$ are between nearest neighbors and are independent random variables with a symmetric distribution and standard deviation unity, i.e.

$$[J_{ij}]_{av} = 0; \quad [J_{ij}^2]^{1/2}_{av} = 1,$$

where $[\cdots]$ means an average over the disorder. We will also use the notation $\langle \cdots \rangle$ to indicate a thermal average for a particular set of interactions. The precise form of the distribution of the $J_{ij}$ is not very important but, for technical reasons, it will be convenient to take a Gaussian distribution in the simulations reported here. In some of what follows we shall also include a magnetic field $h_i$. We shall refer to the models with $m = 1, 2$ and 3 as follows:

$$m = 1 \text{ (Ising);} \quad m = 2 \text{ (XY);} \quad m = 3 \text{ (Heisenberg).} \quad (3)$$

Different types of experimental systems have the necessary ingredients of disorder and frustration:

- **Metals:**
  Diluted magnetic atoms, e.g. Mn, in a non-magnetic metal such as Cu, interact with the RKKY interaction,

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

where $k_F$ is the Fermi wavevector. We see that $J_{ij}$ is random in magnitude and sign, so there is frustration. 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). Within a layer the spins in pure FeTiO$_3$ are ferromagnetically coupled while spins in pure MnTiO$_3$ are antiferromagnetically coupled. Hence the mixture gives an Ising spin glass with short range interactions.

- **Spin glasses** are important because ideas developed for them have application in areas of science far beyond the rather narrow one of disordered magnets. Examples include:
  - Protein folding
  - Optimization problems in computer science
  - Polymer glasses, foams · · ·

A characteristic feature of spin glasses is their dynamics is very slow at low temperature, due to the development of a complicated “energy landscape” with many valleys separated by barriers, as shown in figure 2. This leads to interesting non-equilibrium effects at low temperatures. In this paper, however, we will focus on another important feature of spin glasses, namely that they can have a sharp thermodynamic phase transition, which will be reviewed in the next section.

2. Spin Glass Phase Transition

Despite frustration and strong disorder it turns out that one can have sharp equilibrium phase transitions in spin glasses. For temperature $T$ less than the spin glass transition temperature $T_{SG}$ the spins are frozen in an arrangement which looks random to the eye but which is such as to minimize the (free) energy of the system. As $T \to T_{SG}^+$ there is a correlation length $\xi_{SG}$ which diverges. The significance of $\xi_{SG}$ is that $\langle S_i \cdot S_j \rangle$ is significant for $|R_i - R_j| < \xi_{SG}$ but tends to zero at larger distances. However, the sign of the correlation is random and depends
on the particular values of the interactions in the system. Hence, a useful quantity to study, because it diverges, is the spin glass susceptibility $\chi_{SG}$ defined by

$$\chi_{SG} = \frac{1}{N} \sum_{i,j} [(S_i \cdot S_j)^2]_{\text{av}},$$

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

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

where $m$ is the magnetization and $h$ is the applied field, which can be measured experimentally. For the EA model with a symmetric distribution of $J_{ij}$, $\chi_{SG}$ and $\chi_{nl}$ are essentially the same: $T^3 \chi_{nl} = \chi_{SG} - \frac{2}{T}$.

Experimentally, it is found that $\chi_{nl}$ diverges,

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

with $\gamma$ generally in the range 2.5–3.5. This divergence is seen both for systems which are very anisotropic (i.e. Ising-like) and for systems which have little anisotropy and so are Heisenberg-like. An example of the former is Fe$_{0.5}$Mn$_{0.5}$TiO$_4$, and of the latter is Cu$_{1-x}$Mn$_x$ with $x$ typically a few atomic percent.

We now turn to the theoretical situation. The mean field theory (MFT) of spin glasses was initiated by Edwards and Anderson [1] and then pursued by Sherrington and Kirkpatrick [2] who argued that it should be take to be the exact solution of an Ising spin glass model with infinite-range interactions (now known as the SK-model). However, SK did not solve their model exactly; this was left to Parisi [3] who, in a tour-de-force, used a technique called “replica symmetry breaking” (RSB) to find the (very complicated) exact solution. The SK model has a spin glass phase transition in zero field, and, in addition, has a line of transitions, known as the Almeida-Thouless (AT) line, in a magnetic field. This line separates a non-ergodic (spin glass) phase at lower fields and temperatures from an ergodic (paramagnetic) phase at higher
temperatures and fields, see figure 3(a). Since the field breaks the up-down symmetry of the Hamiltonian, the AT line represents an ergodic to non-ergodic transition without symmetry change. It is perhaps the most striking prediction of the MFT of spin glasses. One topic discussed in this paper will be whether or not an AT line occurs in real three-dimensional Ising spin glass systems.

Much of what we know about more realistic (EA) models in three dimensions has come from numerical simulations. There has been general consensus that for Ising systems a spin glass transition occurs in zero field, especially since the work of Ballesteros et al. [4] who pioneered the use of the scaled correlation length in finite-size scaling analysis of spin glasses. However, the situation concerning vector spin glasses (XY or Heisenberg) has been less clear and is one of the topics discussed in this paper.

Although a real spin glass never truly equilibrates below $T_{SG}$ it is of interest to know what is the equilibrium state to which the system is trying to reach, even if it never quite gets there. There have been two principal proposals for this. Firstly, the “RSB” scenario, due to Parisi and collaborators, proposes that real spin glasses are quite similar to the infinite-range SK model. In particular there is an AT line for an Ising spin glass in a magnetic field. The other approach, known as the “droplet picture” [5], focuses on geometrical aspects of the large-scale, low energy excitations, which are, of course, not present in an infinite-range model which has no geometry. By making some plausible assumptions, predictions for many properties of the spin glass phase are obtained. For our purposes we note just one of them: the absence of an AT line for an Ising spin glass, in contrast to the RSB scenario. The phase diagram in the $H$–$T$ plane according to the two scenarios is shown in figure 3.

3. Finite-Size Scaling

In the later sections we will use numerical simulations to investigate phase transitions in spin glasses. Of course, a sharp transition can only occur in the thermodynamic limit, whereas simulations are carried out on finite-size lattices. We therefore use the technique of finite-size scaling (FSS) to extrapolate from results on a range of finite sizes to the thermodynamic limit. Following Ballesteros et al. [4], we shall find the correlation length of the finite system to be a particularly useful quantity to analyze by FSS.

To extract a correlation length we generalize the definition of the spin glass susceptibility in
equation (5) to finite wavevector $k$:

$$\chi_{SG}(k) = \frac{1}{N} \sum_{i,j} [(S_i \cdot S_j)^2]_{av} e^{i k \cdot (R_i - R_j)}. \quad (8)$$

We then determine the finite-size spin glass correlation length $\xi_L$ from the Ornstein-Zernicke equation:

$$\chi_{SG}(k) = \frac{\chi_{SG}(0)}{1 + \xi_k^2 k^2 + \ldots}, \quad (9)$$

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

The basic assumption in FSS is that the size dependence of the results comes from the ratio $L/\xi_{\text{bulk}}$ where

$$\xi_{\text{bulk}} \sim (T - T_{SG})^{-\nu} \quad (10)$$

is the bulk (i.e. infinite-system size) correlation length. In particular, the correlation length $\xi_L$ of the simulated system, which has linear size $L$, varies as

$$\frac{\xi_L}{L} = X \left( \frac{L^{1/\nu} (T - T_{SG})}{L} \right). \quad (11)$$

Since $\xi_L/L$ is dimensionless it turns out that there is no power of $L$ multiplying the scaling function $X$. This is very useful because, according to equation (11), data for different sizes intersect at $T_{SG}$. Hence the transition temperatures can be determined by eye. Furthermore, if there is long-range spin glass order then the data should splay out below $T_{SG}$. As noted above, this works very well for the Ising spin glass [4, 6] if we had used $\chi_{SG}$, rather than $\xi_L$ as the quantity to analyze, there would have been an additional factor of $L$ to an unknown power multiplying the scaling function in equation (11) which would have complicated the analysis.

Before the work of Ballesteros et al. [4], another dimensionless quantity was use, the “Binder ratio”. However, in three dimensions, this does not splay out much [7, 8] below $T_{SG}$ and so gives less convincing evidence for a transition.

4. Parallel Tempering

Experimentally, spin glass dynamics becomes very slow at low temperatures, as discussed in section 1, because the system has a very complicated “energy landscape” with many “valleys”, separated by barriers, in which the system gets trapped. In Monte Carlo simulations too, the system gets trapped in a valley at low temperature, and conventional Monte Carlo simulations take a huge amount of time to equilibrate in this region. Most Monte Carlo simulations of spin glasses, including those described here, therefore use a modified approach known as parallel tempering (replica exchange) [9], which helps the system get over barriers and equilibrate at low temperature. This approach, which I now describe, is of quite general applicability to problems with a complicated energy landscape.

In this approach one simulates copies of the system, with the same interactions, at a set of $n$ temperatures between $T_{\text{min}} = T_1$ and $T_{\text{max}} = T_n$, see figure 4. The highest temperature is chosen so that the system equilibrates fast; it has enough energy to easily get over the barriers. The lowest temperature is chosen in the region one wants to study. In addition to the usual single-spin updates at each temperature, one also performs temperature swaps in which the entire spin configurations at neighboring temperatures, $T_i$ and $T_{i+1}$, are swapped with probability

$$P_{\text{swap}} = \exp \left[ \frac{(\beta_i - \beta_{i+1})(E_i - E_{i+1})}{k_B T} \right]. \quad (12)$$
Figure 4. Sketch illustrating the temperatures swaps in the parallel tempering method.

where \( \beta_l = 1/T_l \) and \( E_l \) is the total energy of the copy at temperature \( T_l \). It is not difficult to check that equation (12) satisfies the detailed balance condition, and so eventually the whole set of copies will come to thermal equilibrium.

The price one pays is that one has to simulate several (sometimes many) copies of the system. Not all this is wasted, though, since one usually does want results at several temperatures. However, there is an overhead because one ends up doing more sweeps than necessary at high temperatures, and quite often one is forced to use more temperatures than are really needed. This is particularly the case for large sizes because the spacing between temperatures has to vary with \( N \) as \( N^{-1/2} \), so the number of temperatures varies as \( N^{1/2} \), in order that the probability in equation (12) is significant. Physically this is because the same spin configuration must occur with significant probability at both \( T_l \) and \( T_{l+1} \). However, at low temperature, one finds that the speed up of the relaxation time more than compensates for the overhead in simulating a large number of temperatures.

5. Heisenberg Spin Glass

Although the numerical evidence for a finite temperature spin glass transition in three dimensions is very strong for Ising spin glasses, the situation for isotropic vector spin glasses has been more controversial.

We have already mentioned that experimentally systems with rather little anisotropy, which should be close to a Heisenberg system, are found to have a divergent non-linear susceptibility, as well as more anisotropic (Ising-like) systems. However, old Monte Carlo simulations [10, 11] did not find evidence for a transition and concluded that \( T_{SG} \), is probably zero. Based in this, Kawamura [12, 13, 14, 15] proposed that \( T_{SG} = 0 \) but there can be a transition involving “chiralities” at \( T = T_{CG} \ (> 0) \).

Chirality (i.e. vorticity) arises for non-collinear (XY) or non-coplanar (Heisenberg) systems. For unfrustrated systems, the ground state is collinear so chiralities have to be thermally activated. However, they can be important and are responsible for the Kosterlitz-Thouless-Berezinskii (KTB) transition in the 2d XY ferromagnet. For frustrated systems like spin glasses, chiralities are quenched in by the disorder, since the spins splay out in all possible directions to try to relieve the frustration, and so there are chiralities even in the the ground state.

Following Kawamura, we define chirality by

\[
\kappa_i^\mu = \begin{cases} 
\frac{1}{2\sqrt{2}} \sum_{(l,m)} \text{sgn}(J_{lm}) \sin(\theta_l - \theta_m), & \text{XY(\mu square)} \\
S_{i+\mu} \cdot S_i \times S_{i-\mu}, & \text{Heisenberg}
\end{cases}
\]  

(13)

See figure 5.

Kawamura’s idea is that there can be a “chiral-glass” transition at \( T = T_{CG} \) where the chiralities freeze in random directions, without spin glass order occurring at this temperature.
The chiral glass correlation length diverges as $T \to T_{CG}^+$ while the spin glass correlation length stays finite in this limit. This implies “spin–chirality decoupling”, at least at large length scales.

However, several authors, e.g. Refs. [16, 17, 18], disagreed with Kawamura’s claim that $T_{SG} = 0$. It therefore seemed useful [19] to study the XY and Heisenberg spin glass models using FSS of the correlation length for the following reasons. Firstly, by focusing on spin glass and chiral glass correlation lengths one can potentially see directly if the chiral glass correlation length diverges while the spin glass correlation length correlation length stays finite, as predicted in the spin-chirality decoupling scenario. Secondly, as discussed above, FSS of the correlation length was the most successful technique to show the transition in the Ising spin glass, so it is natural to try it for the vector case.

Here, for reasons of space, we just describe some results for the Heisenberg case. The work of Lee and myself [19], which used only modest computer resources and was for sizes only up to $L = 12$, indicated a transition at the same temperature for spins and chiralities, with spin-glass and chiral-glass ordering below the transition. However, subsequently, Hukushima and Kawamura [20], Campos et al. [21], and Lee and I [22], have found that the situation becomes rather less clear when results of larger sizes are included. Hukushima and Kawamura studied sizes up to $L = 20$ while Campos et al., and Lee and I, went up to $L = 32$. The latter two papers argued that the data fitted most naturally a scenario in which $d = 3$ is close to (and possibly equal to) the lower critical dimension (the dimension below which fluctuations destroy the finite temperature transition) for both spins and chiralities. However, Hukushima and Kawamura interpreted their results as indicating a transition in the chiralities but not the spins.

More work is needed to clarify this situation, and is currently in progress.

6. Ising Spin Glass in a Magnetic Field

As discussed in section 2, in MFT there’s a line of phase transitions in a magnetic field for an Ising spin glass, known as the Almeida Thouless (AT) line, which separates a spin glass phase, with divergent relaxation times and “replica symmetry breaking”, from a paramagnetic “replica symmetric” phase with finite relaxation times, see figure 3. Experimentally, it is harder to determine whether there is an AT line than whether there is a transition in zero field. The reason is that $\chi_{nl}$ diverges in zero field, providing a clear signatures of the transition, whereas $\chi_{nl}$ does not diverge on the AT line at non-zero field. Experiments therefore look for another signature of the transition, a divergent relaxation time. In what is probably the best such experiment [23], no such divergence in a field was found, implying the absence of an AT line.

Although there is no static divergent quantity measurable in experiments, there is such a quantity which is accessible in simulations, namely the spin glass susceptibility $\chi_{SG}$. The zero
The scaled correlation length for the Ising spin glass with (random) field strength $H_r = 0.1$ (H. G. Katzgraber and A. P. Young, unpublished).

Figure 6. The scaled correlation length for the Ising spin glass with (random) field strength $H_r = 0.1$ (H. G. Katzgraber and A. P. Young, unpublished).

Equation (14) is just the “replicon mode” of replica field theory, which diverges for the SK model along the AT line. As discussed in section 2, $\chi_{SG}$ and $\chi_{nl}$ are essentially equal in zero field, but this is not the case in a finite field where only $\chi_{SG}$ diverges. While $\chi_{SG}$ can not be measured in experiments in a field, it can be determined in simulations. More conveniently, one can obtain from the simulations a correlation length $\xi_L$ from $\chi_{SG}(k)$ using equation (9), and this can be analyzed by FSS according to equation (11), so the transition is indicated by intersection of the data for different sizes.

In the simulations [24] we actually used a Gaussian random field, rather than a uniform field, for technical reasons, but MFT predicts an AT line for this case too, just as for a uniform field. Some results are shown in figure 6. The strength of the (random) field is $H_r = 0.1$ which is very small compared with the zero field transition temperature [6] $T_{SG} \simeq 0.96$. There is no sign of an intersection indicating the absence of an AT line.

Subsequent work [25], which studied a one-dimensional model in which the interactions fall off with a power of the distance, found that an AT line does occur in the region where the zero field exponents are mean field like. For the short range case this would be $d > 6$.

7. Conclusions
In this paper I have argued that results of numerical simulations in spin glasses can be conveniently analyzed by a FSS of the scaled correlation length. I have presented results for models in three dimensions which indicate that (i) there is a single transition, involving both
spins and chiralities, for the Heisenberg spin glass, and (ii) there is no Almeida Thouless line for an Ising spin glass in a magnetic field. Of course, it would desirable to perform calculations on larger lattice sizes to confirm these conclusions.

Acknowledgments
I acknowledge support from the National Science Foundation under grant DMR 0337049. I am also very grateful to the Hierarchical Systems Research Foundation for a generous allocation of computer time on its Mac G5 cluster. I thank my collaborators in the work described here, Helmut Katzgraber, and Lik Wee Lee, for many stimulating interactions, and Victor Martin-Mayor for most helpful correspondence. I’m also grateful for comments from Ian Campbell.

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