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Some recent developments in spin glasses

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Abstract. I give some experimental and theoretical background to spin glasses, and then discuss the nature of the phase transition in spin glasses with *vector* spins. Results of Monte Carlo simulations of the Heisenberg spin glass model in three dimensions are presented. A finite-size scaling analysis of the correlation length of the spins and chiralities shows that there is a single, finite-temperature transition at which both spins and chiralities order.

Keywords. Spin glass; Monte Carlo; phase transition.

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1. Introduction

For a theorist such as myself, a spin glass is a system with disorder and frustration. A simple but useful example is shown in figure 1 in which there is a single square of Ising spins (which 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 and so there is competition or 'frustration'. Clearly, for a large system, it is non-trivial to find even the ground state of a system with frustration and disorder.

The simplest model which has the basic ingredients of disorder and frustration is the the Edwards–Anderson [1] (EA) model,

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

in which the spins $\mathbf{S}_i$ lie on the sites of a regular lattice, and the interactions J_{ij}, which we take to be between nearest neighbors only, are independent random variables with mean and standard deviations 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 J_{ij}. The $\mathbf{S}_i$ are of unit length and have m components:

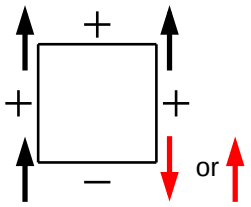

Figure 1. A toy model which shows frustration. If the interaction on the bond is a '+', the spins will be parallel and if it is a '−' they will be antiparallel. Clearly all these conditions cannot be met and so there is competition or 'frustration'.

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

Experimentally, there are different types of spin glasses.

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

$$J_{ij} \sim \frac{\cos(2k_{\mathrm{F}}R_{ij})}{R_{ij}^3}, \tag{4}$$

  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.*
- Other systems where spin glass ideas have proved useful are:
  – Protein folding.
  – Optimization problems in computer science.
  – Polymer glasses, foams, etc.

After considerable experimental and theoretical work, it became clear that a spin glass has a sharp thermodynamic phase transition at temperature $T = T_{\mathrm{SG}}$, such that for $T < T_{\mathrm{SG}}$ the spins freeze in some random-looking orientation. As $T \to T_{\mathrm{SG}}^+$, the spin glass correlation length ξ_{SG}, which we will discuss in detail below, diverges. Here we just note that the defining feature of the correlation length is that the *magnitude* of the correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ becomes significant for $R_{ij} < \xi_{\mathrm{SG}}$, though the *sign* is random. A quantity which diverges, therefore, is the *spin glass susceptibility*

$$\chi_{\rm SG} = \frac{1}{N} \sum_{\langle i,j \rangle} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2]_{\rm av} \tag{5}$$

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

$$m = \chi h - \chi_{\rm nl} h^3 + \cdots , \tag{6}$$

where h is the magnetic field. We expect that $\chi_{\rm nl}$ diverges at $T_{\rm SG}$ as

$$\chi_{\rm nl} \sim (T - T_{\rm SG})^{-\gamma}, \tag{7}$$

where γ is a critical exponent.

This divergent behavior has been seen in many experiments. Figure 2 shows the results of Omari *et al* [2] on 1% Mn in Cu. They define $m = a_1 h - a_3 c_3 h^3 + a_5 c_5 h^5$ and choose units (and constants $c_3 = 1/15, c_5 = 2/305$) such that $a_i = 1$ for independent Mn spins. It follows that a_3 is $\chi_{\rm nl}$ in dimensionless units. We see that $\chi_{\rm nl}$ becomes very large ($>10^3$), and presumably diverges. A fit gives $\gamma = 3.25$.

At low temperatures, the dynamics of spin glasses becomes very slow, such that below $T_{\rm SG}$ 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 $T_{\rm SG}$ and waits for a 'waiting time' $t_{\rm w}$. The system is then perturbed in some way, e.g. by applying a magnetic field,

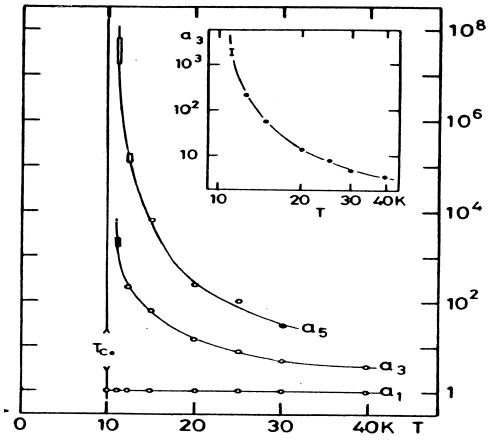

Figure 2. Results for the non-linear susceptibility of 1% Mn in Cu from Omari *et al* [2]. The quantity a_3 is the non-linear susceptibility in dimensionless units.

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.

More complicated temperature protocols are possible, which have led to surprising results. For example, one can cool smoothly below T_{SG} and wait at a temperature T_1, say, before cooling further, and then warming back up through T_{SG} this time without waiting at T_1. While waiting at T_1 during the cooling process, the data show a drift with time, and on warming, one finds a similar feature at T_1 even though the system did not wait there. This 'memory' effect [4] is still not well-understood, and neither is 'rejuvenation', the fact that aging at one temperature does not help equilibration at a lower temperature [4].

On the theoretical side, there is a mean field solution due to Parisi [5,6] which, following Sherrington and Kirkpatrick [7], is the exact solution of an EA-like model with infinite range interactions. One finds a finite spin glass transition temperature T_{SG}.

Most of what we know about short-range (EA) models in three dimensions has come from simulations on Ising systems, which also indicate a finite T_{SG}, as we will see below. However, less is known about vector spin glass models and these will be the main focus of the rest of the talk.

While the existence of a phase transition in three dimensions is not in serious dispute, at least for Ising spins, the nature of the equilibrium state below T_{SG} has been much more controversial. An experimental system is not in equilibrium below T_{SG}. So we ultimately need a theory for non-equilibrium behavior. However, to do this, we presumably need to know the equilibrium state towards which the system is trying to reach but never does. Two main proposals have been made for the nature of the equilibrium spin glass state:

- replica symmetry breaking (RSB), which is like the Parisi [5,6] mean field solution, and
- the 'droplet picture' (DP) of Fisher and Huse [8,9].

These differ in the nature of the large-scale, low-energy excitations, whose energy ΔE scales as

$$\Delta E \propto \ell^{\theta}, \tag{8}$$

where ℓ is the linear size of the excitation and θ is a 'stiffness' exponent. RSB and DP have different predictions for θ:

- RSB, $\theta = 0$ for some excitations.
- DP, $\theta > 0$ (but small, around 0.2 for 3d Ising).

Since in both scenarios θ is zero or very small, a lot of cancellation occurs in the energy to flip a cluster of spins. Hence, a characteristic feature of spin glasses is that there are excitations which involve a large number of spins but which cost very little energy.

In three dimensions, numerics, which are inevitably on small lattice sizes, seem to fit best an intermediate TNT (trivial–nontrivial) scenario [10,11]. In two dimensions, where $\theta < 0$ and consequently $T_{SG} = 0$, larger sizes can be studied and

it seems that the droplet theory works, though there are significant corrections to scaling for various quantities (see refs [12,13] for recent discussions).

A lot of attention in spin glasses has been given on (i) the nature of the phase transition and (ii) the nature of the spin glass phase below $T_{\rm SG}$. For both problems, most theory has been on Ising systems though the vector nature of the spins may be relevant. In the rest of this talk I will discuss the nature of the phase transition in *vector* spin glass models.

2. Vector spin glasses

Most theory has been done for the Ising ($S_i = \pm 1$) spin glass, where there is clear evidence for a finite $T_{\rm SG}$. The best evidence is from finite-size scaling (FSS) of the correlation length by Ballesteros *et al* [14]. This technique is discussed further below. However, many experimental systems, such as CuMn described above, are closer to an isotropic vector spin glass (in which $\mathbf{S}_i$ is a vector), where the theoretical situation is less clear.

Old Monte Carlo simulations [15] found that $T_{\rm SG}$, if it occurs at all, must be very low, and this was interpreted as an evidence for $T_{\rm SG} = 0$. Motivated by this, Kawamura [16–19] argued that $T_{\rm SG} = 0$ but there can be a glass-like transition at $T = T_{\rm CG}$ in the 'chiralities' (i.e. vortices). This implies *spin–chirality decoupling*. However, the possibility of finite $T_{\rm SG}$ has been raised by various authors, e.g. Maucourt and Grempel [20], Akino and Kosterlitz [21], Granato [22], Matsubara *et al* [23,24], and Nakamura and Endoh [25]. Since the most successful approach for the Ising spin glass was the FSS scaling analysis of the correlation length, Lee and I decided to perform analogous calculations for vector spin glasses, investigating the correlation lengths of *both* the spins and chiralities.

There is an important difference between chiralities in frustrated and unfrustrated systems. In unfrustrated systems the ground state is collinear and so chirality needs to be *thermally excited*. Such thermally activated chiralities (vortices) are responsible for the Kosterlitz–Thouless–Berezinskii transition in the 2d XY ferromagnet. However, in spin glasses, chiralities are *quenched in* at low-T because the ground state is non-collinear as a result of the disorder and frustration.

To define chirality we follow Kawamura [17,18]:

$$\kappa_i^\mu = \begin{cases} \dfrac{1}{2\sqrt{2}} \sum\limits_{\langle l,m \rangle}{}' \operatorname{sgn}(J_{lm}) \sin(\theta_l - \theta_m), & \text{XY } (\mu \perp \text{square}), \\ \mathbf{S}_{i+\hat{\mu}} \cdot \mathbf{S}_i \times \mathbf{S}_{i-\hat{\mu}}, & \text{Heisenberg}, \end{cases} \tag{9}$$

see figure 3, where for the XY model i refers to the plaquette indicated, and for the Heisenberg model, i refers to the middle of the three sites.

To determine the correlation lengths of the spins and chiralities we need to Fourier transform the appropriate correlation functions:

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

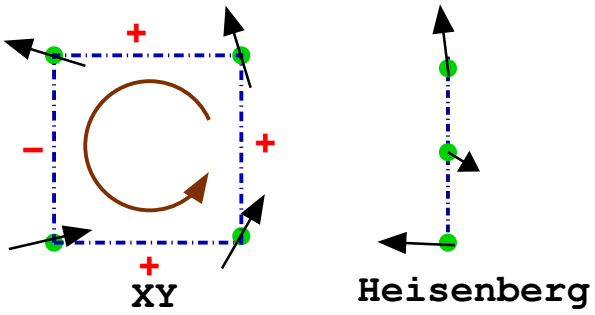

Figure 3. An illustration of chirality for XY and Heisenberg spin glasses.

$$\chi^{\mu}_{\rm CG}(\mathbf{k}) = \frac{1}{N}\sum_{i,j}[\langle \kappa^{\mu}_i \kappa^{\mu}_j\rangle^2]_{\rm av} {\rm e}^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \quad \text{(chiralities)}. \tag{10}$$

Note that $\chi_{\rm nl} \sim \chi_{\rm SG}(\mathbf{k}=0)$, which is essentially the 'correlation volume' of the spins.

We determine the spin glass correlation length of the finite-size system, ξ_L, from the Ornstein Zernicke equation:

$$\chi_{\rm SG}(\mathbf{k}) = \frac{\chi_{\rm SG}(\mathbf{0})}{1+\xi_L^2\mathbf{k}^2+\cdots}, \tag{11}$$

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

$$\xi_L = \frac{1}{2\sin(k_{\rm min}/2)}\left(\frac{\chi_{\rm SG}(0)}{\chi_{\rm SG}(\mathbf{k}_{\rm min})}-1\right)^{1/2}. \tag{12}$$

The chiral glass correlation length of the system, $\xi^{\mu}_{c,L}$, is determined in an analogous way.

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 $L/\xi_{\rm bulk}$ where

$$\xi_{\rm bulk} \sim (T-T_{\rm SG})^{-\nu} \tag{13}$$

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

$$\frac{\xi_L}{L} = X(L^{1/\nu}(T-T_{\rm SG})), \tag{14}$$

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 $T_{\rm SG}$ and splay out below $T_{\rm SG}$. Similarly, data for $\xi_{c,L}$ should intersect at $T_{\rm CG}$.

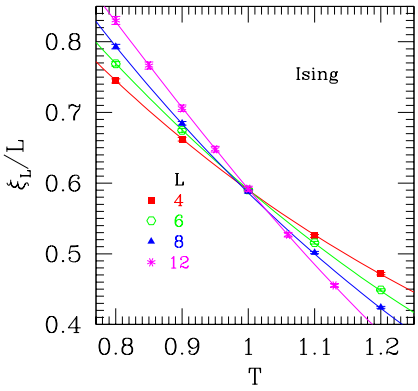

Figure 4. Data for the correlation length of the Ising spin glass showing clear evidence for a transition at $T_{\rm SG} \simeq 1.00$.

3. Results

Figure 4 shows that this works well for the Ising spin glass. These data, which is for the spin glass correlation length divided by L, show clear intersections and hence evidence for a transition, at $T_{\rm SG} \simeq 1.00$. Furthermore, the data splay out again on the low-T side demonstrating that there is spin glass order below $T_{\rm SG}$. This is data for the Gaussian distribution. The technique of determining $T_{\rm SG}$ by FSS of ξ_L was first used by Ballesteros *et al* [14] who took the '$\pm J$' distribution in which $J_{ij} = \pm 1$ with equal probability. This has a somewhat higher transition temperature, i.e., $T_{\rm SG} \simeq 1.14$.

Prior to the work of Ballesteros *et al*, determination of $T_{\rm SG}$ generally used the 'Binder ratio', a dimensionless ratio of the moments of the order parameter distribution which has a finite-size scaling of the same form as in eq. (14). However, this gives much less convincing demonstration of a transition; see figure 5 which shows data from Marinari *et al* [26] for the Gaussian distribution.

We have seen that the best method for studying the transition in the Ising spin glass is FSS of the correlation length. We now apply this to the spin glass with vector spins. Similar results were obtained [27] for both the XY and Heisenberg models. Here, for conciseness, we just present results for the Heisenberg case.

Figure 6 shows data for ξ_L/L. It has some additional data beyond that given in Lee and Young [27]. The data intersect and splay out again at low temperatures indicating a finite-temperature spin glass transition. The inset shows that the data can be collapsed reasonably according the FSS form in eq. (14) with $T_{\rm SG} \simeq 0.16$, $\nu \simeq 1.2$.

Figure 7 shows data for the chiral correlation length. There are actually two such lengths depending upon whether the wavevector $\mathbf{k}_{\rm min}$ in eq. (12) is parallel or perpendicular to the line of spins shown in figure 3 for the Heisenberg case. The main figure in figure 7 shows the parallel correlation length and the inset the

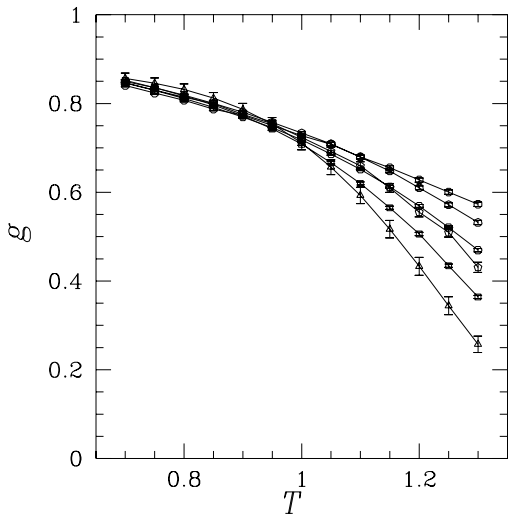

Figure 5. Data for the Binder ratio length of the Ising spin glass with Gaussian interactions, from Marinari *et al* [26]. The data merge but do not splay out strongly on the low-T side, unlike the results for the correlation length shown in figure 4.

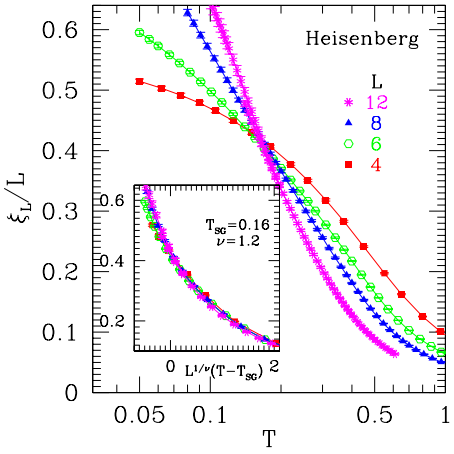

Figure 6. Data for the spin glass correlation length of the Heisenberg spin glass divided by L (based on ref. [27] with some additional data).

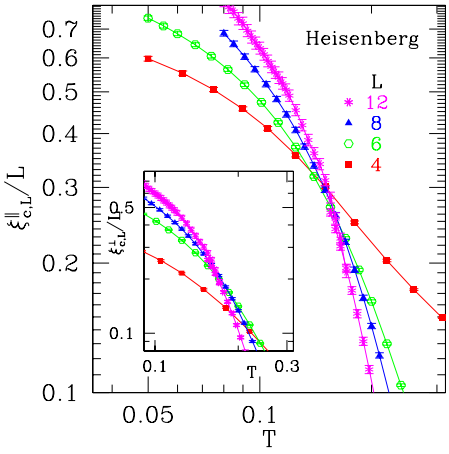

Figure 7. Data for the chiral glass correlation length of the Heisenberg spin glass divided by L (based on ref. [27] with some additional data).

perpendicular correlation length. Apart from the smallest size, the data intersect pretty well. Furthermore, the transition temperature $T_{\rm CG}$ seems to be equal to $T_{\rm SG}$, namely about 0.16.

Table 1. Values for $T_{\rm SG}/T_{\rm SG}^{\rm MF}$ determined from the numerics.

m	Model	$T_{\rm SG}^{\rm MF}$	$T_{\rm SG}$	$T_{\rm SG}/T_{\rm SG}^{\rm MF}$
1	Ising	2.45	1.00	0.41
2	XY	1.22	0.34	0.28
3	Heisenberg	0.82	0.16	0.20

We conclude that a *direct* study of the correlation lengths indicates that there is a single phase transition at which both spins and chiralities order in vector spin glasses.

4. Conclusions

It is interesting to see how the spin glass transition temperature varies with the number of spin components m. To compare different values of m it is necessary to note that there is an m dependence for $T_{\rm SG}$ even in mean field theory: $T_{\rm SG}^{\rm MF} = \sqrt{z}/m$ where z ($= 6$ here) is the number of neighbors. Hence we show values for $T_{\rm SG}/T_{\rm SG}^{\rm MF}$ determined from the numerics in table 1.

We see that $T_{\rm SG}/T_{\rm SG}^{\rm MF}$ is small and decreases further with increasing m. Physically, this means that fluctuation effects are large and get larger with increasing m. The data suggest that perhaps $T_{\rm SG} = 0$ for $m = \infty$. Preliminary results by Dhar, Lee and the author [28], indicate that this is the case.

To conclude, I believe that one important question, whether or not an isotropic Heisenberg spin glass has a finite-temperature spin glass transition, has been answered in the affirmative. However, the nature of the putative equilibrium state below $T_{\rm SG}$, towards which the system evolves but never reaches, as well as non-equilibrium phenomena such as aging and rejuvenation, remain to be fully understood.

Acknowledgments

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