Phase Transition in Vector Spin Glasses

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Abstract

We first give an experimental and theoretical introduction 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 XY 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.

INTRODUCTION

It is a pleasure to present this paper on the occasion of Roger Elliott's 75th birthday and his induction as a "Miembro Correspondiente" of the "Academia Mexicana de Ciencias". Roger was both my undergraduate tutor and the supervisor for my D. Phil, so I had plenty of opportunity to learn from his great intuition for physics. In particular, I learned from his wonderfully clear lectures that the field of disordered systems is rich and interesting, and consequently disordered systems has been at the forefront of my research ever since. This talk will be about an area of disordered systems which has proved extremely challenging and where controversies continue: the *spin glass*.

A spin glass is a system with disorder and frustration. Figure 1 shows a toy example of frustration with 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 so there is competition or "frustration".

Most theoretical work uses 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

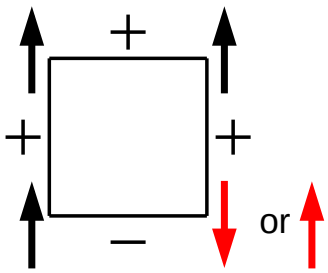

FIG. 1: A Toy model which shows frustration. If the interaction on the bond is a "+", the spins want to be parallel and if it is a "−" they want to be antiparallel. Clearly all these conditions can not be met so there is competition or "frustration".

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 we will follow common practice and take a Gaussian distribution for the J_{ij}. The $\mathbf{S}_i$ are of unit length and have m–components:

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

The Edwards Anderson model is the simplest one which includes the necessary ingredients of randomness and frustration.

Different types of experimental systems have these ingredients:

- Metals:

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

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

  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 $\cdots$

An important feature of spin glasses is that they undergo a sharp thermodynamic phase transition at temperature $T = T_{SG}$, such that for $T < T_{SG}$ the spin freeze in some random-looking orientation. As $T \to T_{SG}^+$, 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 correlation function $\langle S_i S_j \rangle$ becomes significant for $R_{ij} < \xi_{SG}$, though the *sign* is random. A quantity which diverges, therefore, is the *spin glass susceptibility*

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

(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,

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

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

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

where γ is a critical exponent.

This divergent behavior has been seen in many experiments. Fig. 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 χ_{nl} in dimensionless units. We see that χ_{nl} becomes very large, ($> 10^3$), and presumably diverges. A fit gives $\gamma = 3.25$.

An important feature of spin glasses at low temperature is that the dynamics becomes very slow, and 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.

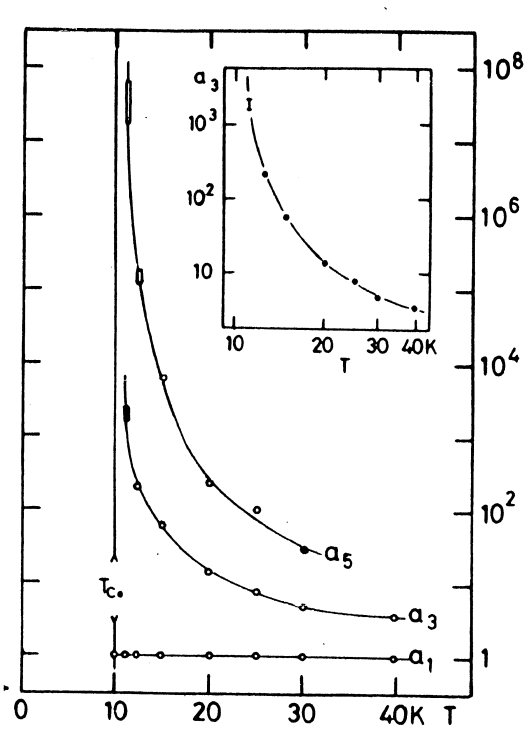

FIG. 2: Results for the non-linear susceptibility of 1% Mn in Cu from Omari et al.[2]. The quantity a_3 is the non-linear susceptibility in dimensionless units.

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 shows 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 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, the nature of the equilibrium state below T_{SG} has been much more controversial. While an experimental system is not in equilibrium below T_{SG}, to develop a theory for the non-equilibrium behavior we presumably need to know the equilibrium state towards which it is trying to get to but never reaches. There are two main scenarios:

- "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).

Hence, a lot of cancellation occurs in the calculation of the energy to flip a cluster of spins. A characteristic feature of spin glasses, then, is the presence of excitations which involve a large number of spins but which cost very little energy.

There are two main sets of issues in spin glasses:

- The nature of the phase transition.
- The nature of the spin glass phase below T_{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.

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_{SG}. The best evidence is from finite size scaling (FSS) of correlation length by Ballesteros et al.[10] This technique is discussed further below. However, many experimental systems, such as CuMn described above, are closer to an isotropic vector spin glass ($\mathbf{S}_i$ is a vector), where the theoretical situation is less clear.

Old Monte Carlo simulations[11] found that T_{SG}, if it occurs at all, must be very low, and this was interpreted as being evidence for $T_{SG} = 0$. Motivated by this, Kawamura[12–15] argued that $T_{SG} = 0$ but there can be a glass-like transition at $T = T_{CG}$ in the "chiralities" (i.e. vortices). This implies *spin–chirality decoupling*. However, the possibility of finite T_{SG} has been raised by various authors, e.g. Maucourt and Grempel[16], Akino and Kosterlitz[17], Granato[18], Matsubara et al.[19, 20], and Nakamura et al.[21].

The situation seemed confusing and so we decided to try to clarify it by a FSS analysis of the correlation lengths of *both* the spins and chiralities for the XY and Heisenberg spin glasses. We expected this to be useful because:

- It was the most successful approach for the Ising spin glass[10].
- It probes directly *divergent* quantities.
- If spin-chirality decoupling occurs then eventually the spin glass correlation length must exceed the chiral glass correlation length. Can we see this?

Next we discuss how to define chirality in spin glasses. 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, an important difference is that chiralities are *quenched in* at low-T because the ground state is non-collinear as a result of the disorder and frustration. Following Kawamura[13, 14] we define chirality by:

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

see Fig. 3.

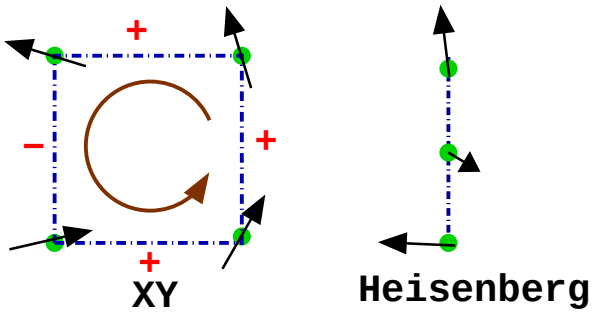

FIG. 3: An illustration of chirality for XY and Heisenberg spin glasses.

Next we discuss the various quantities that will be calculated in the simulations. To determine the correlation lengths of the spins and chiralities we need to Fourier transform the appropriate correlation functions:

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

Note that $\chi_{nl} \sim \chi_{SG}(\mathbf{k}=0)$, 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:

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

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

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

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

The results for the correlation lengths will be analyzed according to finite-size scaling (FSS). The basic assumption of FSS is that the size dependence comes from the ratio $L/\xi_{\rm bulk}$ where

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

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

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

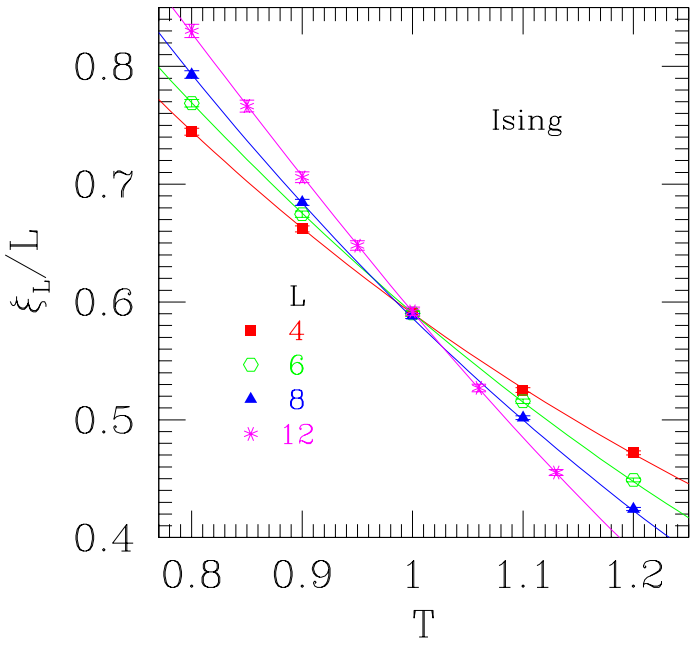

FIG. 4: Data for the correlation length of the Ising spin glass showing clear evidence for a transition at $T_{SG} \simeq 1.00$.

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}. Similarly, data for $\xi_{c,L}$ should intersect at T_{CG}.

RESULTS

Let's first see how FSS scaling of the correlation length works for the Ising SG. The data in Fig. 4 shows clear intersections, and hence evidence for a transition, at $T_{SG} \simeq 1.00$, and the data splay out again on the low-T side demonstrating that there is spin glass order below T_{SG}. This is data for the Gaussian distribution. The technique of determining T_{SG} by FSS of ξ_L was first used by Ballesteros et al.[10] who took the "$\pm J$" distribution in which $J_{ij} = \pm 1$ with equal probability. This has a somewhat higher transition temperature, $T_{SG} \simeq 1.14$.

Prior to the work of Ballesteros et al., determination of T_{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 Fig. 5 which shows data from Marinari et al.[22] for the

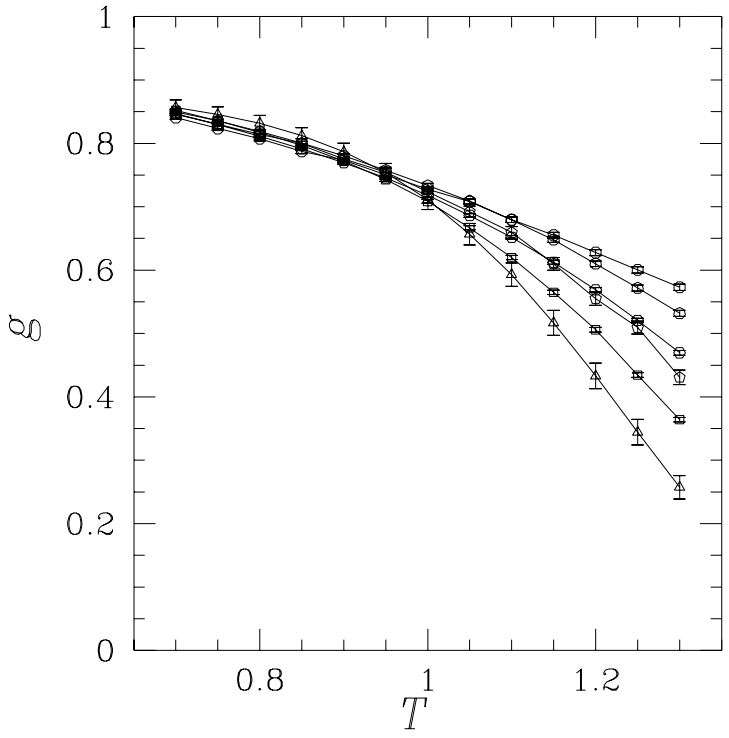

FIG. 5: Data for the Binder ratio length of the Ising spin glass with Gaussian interactions, from Marinari et al.[22]. The data merge but do not clearly splay out on the low-T side, unlike the results for the correlation length shown in Fig. 4.

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[23] for both the XY and Heisenberg models. Here, for conciseness, we just present results for the XY case.

Figure 6 shows data for ξ_L/L. While the intersections are not quite as clean as those for the Ising model, the data does 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 the FSS form in Eq. (14) with $T_{SG} \simeq 0.33, \nu \simeq 1.2$.

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 normal to the plaquettes. The main figure shows the perpendicular correlation length and the inset the parallel correlation length. Apart from the smallest size, the data intersect

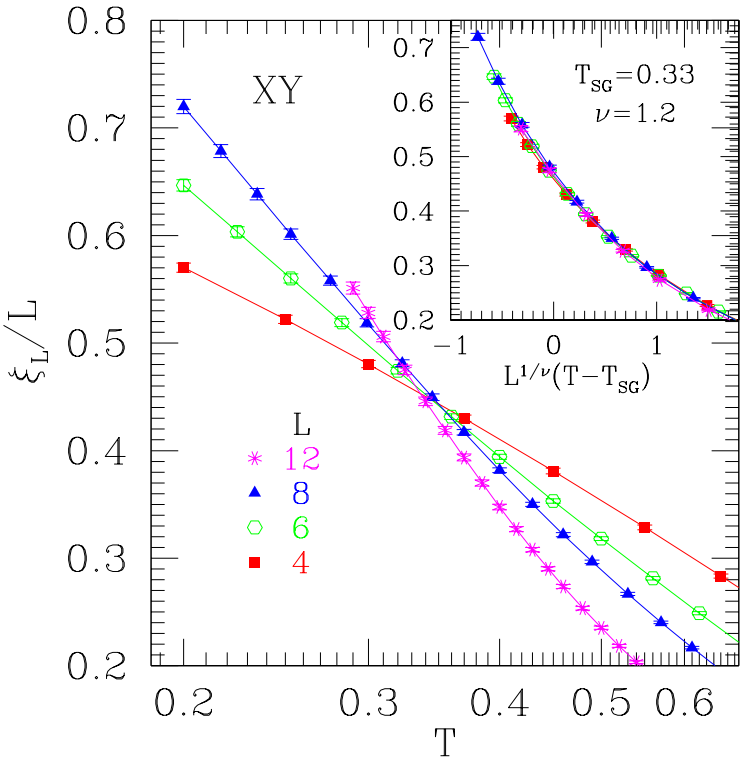

FIG. 6: Data for the spin glass correlation length of the XY spin glass (from Ref. [23]).

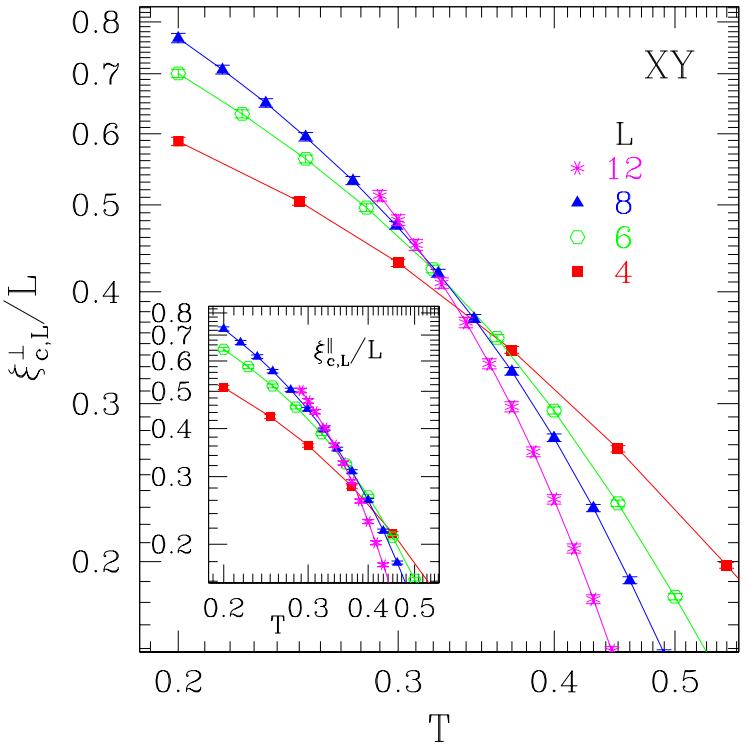

FIG. 7: Data for the chiral glass correlation length of the XY spin glass (from Ref. [23]).

pretty well. Furthermore, the transition temperature T_{CG} seems to be equal to T_{SG}, namely about 0.33.

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.

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_{SG} even in mean field theory: $T_{SG}^{MF} = \sqrt{z}/m$ where z (= 6 here) is the number of neighbors. Hence we show below values for T_{SG}/T_{SG}^{MF} determined from the numerics:

m	model	T_{SG}^{MF}	T_{SG}	T_{SG}/T_{SG}^{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 see that T_{SG}/T_{SG}^{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 $T_{SG} = 0$ for $m = \infty$. This is currently under investigation.

To conclude, spin glasses continue to present serious challenges. In this talk, I have presented results which, in my view, resolve one of the controversies, whether there is a finite temperature spin glass transition in a vector spin glass without anisotropy. The answer appears to be "yes". However, the nature of the putative equilibrium state below T_{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.

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