Phase transitions in spin glasses ☆

A.P. Young*

Physics Department, University of California Santa Cruz, CA 95064, USA

Available online 20 November 2006

Abstract

Whereas there has been a general consensus for some time that Ising spin glasses have a transition at finite temperature in zero field in three dimensions, there has *not* been general agreement on two other questions concerning phase transitions in spin glasses in three dimensions: (i) is there a transition at finite temperature in isotropic vector spin glasses (such as Heisenberg), and (ii) is there a phase transition (AT line) in a magnetic field in Ising spin glasses? By using Monte Carlo simulations, analyzed with finite-size scaling, I will argue that the answer to the first question is "yes", and to the second question is "no".
© 2006 Elsevier B.V. All rights reserved.

1. Introduction

In this paper, I will describe numerical results on the existence or not of phase transitions in spin glasses. In Section 2 I give some relevant background to spin glasses, followed, in Section 3, by a discussion of the finite-size scaling method used in the simulations. Sections 4 and 5 then discuss the results for the Heisenberg spin glass in zero field and the Ising spin glass in a field, respectively. The conclusions are summarized in Section 6.

2. Background

Spin glasses are systems with two key ingredients: *disorder*, and *frustration*, i.e. competition between different terms in the Hamiltonian so they cannot all be satisfied simultaneously. Most theoretical work therefore uses the simplest model with these features, the Edwards and

Anderson [1] (EA) model, whose Hamiltonian is

$$\mathscr{H} = -\sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i. \qquad (1)$$

The spins $\mathbf{S}_i$ are classical m-component vectors which lie on the sites i of a regular (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.

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

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 $\mathbf{h}_i$. We shall refer to the models with $m = 1, 2$ and 3 as follows:

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

A characteristic feature of spin glasses that is their dynamics is very slow at low temperature, due to the development of a complicated "energy landscape" with many valleys separated by barriers. In this paper, however,

we will focus on another important feature of spin glasses, namely that they can have a sharp thermodynamic *phase transition*.

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* ξ_{SG} which diverges. The significance of ξ_{SG} is that $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ is significant for $|\mathbf{R}_i - \mathbf{R}_j| < \xi_{SG}$ 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* χ_{SG} defined by

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

(note the square) which is accessible in simulations. It is also essentially the same as the *non-linear susceptibility*, χ_{nl}, defined by

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

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}, χ_{SG} and χ_{nl} are essentially the same: $T^3 \chi_{nl} = \chi_{SG} - \frac{2}{3}$.

Experimentally, it is found that χ_{nl} diverges:

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

with γ 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 a 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. 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 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 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 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, many properties of the spin glass phase are obtained. For our purposes we note just one of them: the *absence* of an AT line.

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 Eq. (4) to finite wavevector $\mathbf{k}$:

$$\chi_{SG}(\mathbf{k}) = \frac{1}{N} \sum_{i,j} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2]_{av} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \tag{7}$$

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

$$\chi_{SG}(\mathbf{k}) = \frac{\chi_{SG}(\mathbf{0})}{1 + \xi_L^2 \mathbf{k}^2 + \cdots}, \tag{8}$$

by fitting to $\mathbf{k} = 0$ and $\mathbf{k} = \mathbf{k}_{min} = 2\pi/L(1, 0, 0)$.

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

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

is the *bulk* (i.e. infinite-system size) correlation length. In particular, the correlation length ξ_L of the simulated

system, which has linear size L, varies as

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

Since ξ_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 Eq. (10), 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 χ_{SG}, rather than ξ_L as the quantity to analyze, there would have been an additional factor of L to an unknown power multiplying the scaling function in Eq. (10) which would have complicated the analysis.

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

4. 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 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 [9,10] did not find evidence for a transition and concluded that T_{SG}, is probably zero. Based in this, Kawamura [11–14] proposed that $T_{SG} = 0$ but there can be a transition involving "chiralities", $T_{CG} > 0$.

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 ground state*.

Following Kawamura, we define chirality by

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

see Fig. 1.

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
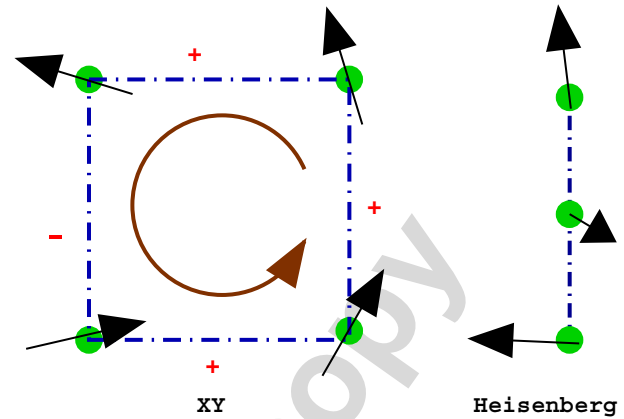

Fig. 1. Sketch illustrating chirality for the XY and Heisenberg models.

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. [15–17], disagreed with Kawamura's claim that $T_{SG} = 0$. It therefore seemed useful [18] 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 scaled correlation length for spins and chiralities for a range of sizes is shown in Fig. 2. It is noteworthy that the results for the spins and chiralities are very similar; there is no evidence the chiral glass correlation length diverges while the spin glass correlation length does not. Furthermore, there are intersections for both sets of data at $T \simeq 0.15$ implying $T_{CG} = T_{SG} \simeq 0.15$.

Quite recently Campos et al. [19], have studied larger sizes, up to $L = 32$ and claimed that the data for the *largest* sizes indicates "marginal" behavior analogous to that in the KTB transition in the $d = 2$ XY ferromagnet. This means that there is a line of critical points terminating at T_{SG}, with no true long-range order for $T < T_{SG}$, so the data for ξ_L/L is *independent of size* in this region. Motivated by this work, Lee and APY (unpublished) have studied sizes up to $L = 32$ down to rather lower temperatures than in Ref. [19]. Our preliminary conclusion is that the claim by Campos et al. [19] of a line of critical points is probably correct. However, the line of critical points seems to be terminated at the *same* temperature for spins and chiralities, still indicating a common spin-glass and chiral-glass transition.
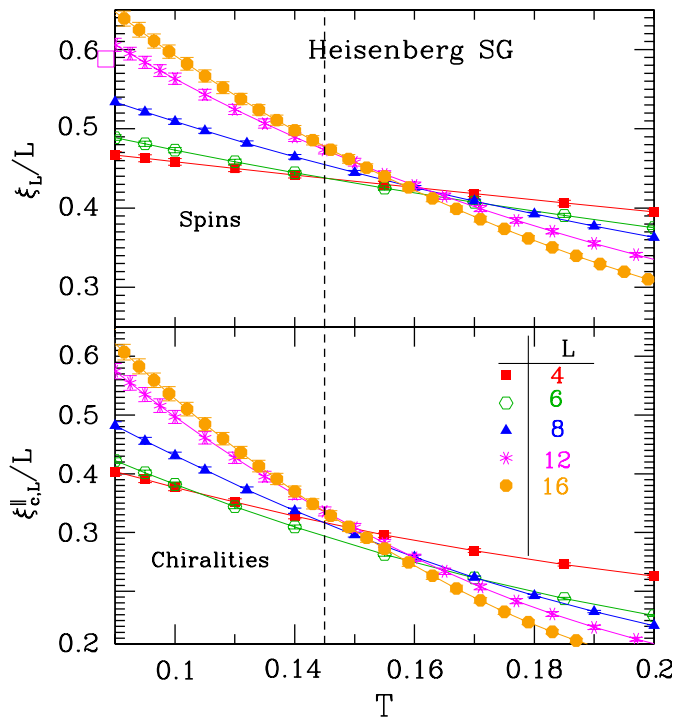
Fig. 2. The scaled spin glass and chiral glass correlation lengths for the Heisenberg spin glass for different sizes. (L.W. Lee and A.P. Young, unpublished.)

5. 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 and 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 Fig. 3. It is harder to determine experimentally whether there is an AT line than whether there is a transition in zero field, because, in zero field, χ_{nl} diverges and this provides a clear signatures of the transition. Unfortunately, however, χ_{nl} does *not* diverge on the AT line at non-zero field. Experiments therefore look for divergent relaxation times, and in what is probably the best experiment [20], *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: the spin glass susceptibility χ_{SG}. The zero field definition of χ_{SG} given in Eq. (7) is generalized in a field to

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

Eq. (12) is just the "replicon mode" of replica field theory. As discussed in Section 2, χ_{SG} and χ_{nl} are essentially equal in zero field, but this is not the case in a finite field where only χ_{SG} diverges. While χ_{SG} cannot be measured in

experiments in a field, it *can* be determined in simulations. More conveniently, one can obtain a correlation length ξ_L from $\chi_{SG}(\mathbf{k})$ using Eq. (8), and this can be analyzed by FSS according to Eq. (10) so the transition is indicated by intersection of the data for different sizes.

In the simulations [21] 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 Fig. 4. 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 [22], which studied a one-dimensional model in which the interactions fall of 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 $d > 6$.
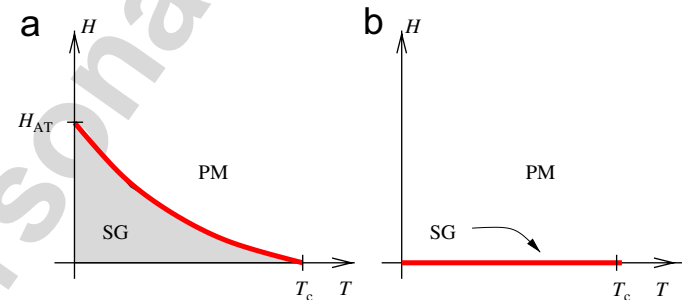

Fig. 3. The magnetic field-temperature phase diagram according: (a) to the RSB picture, and (b) the droplet picture. The transition line in (a) is known as the Almeida–Thouless (AT) line.
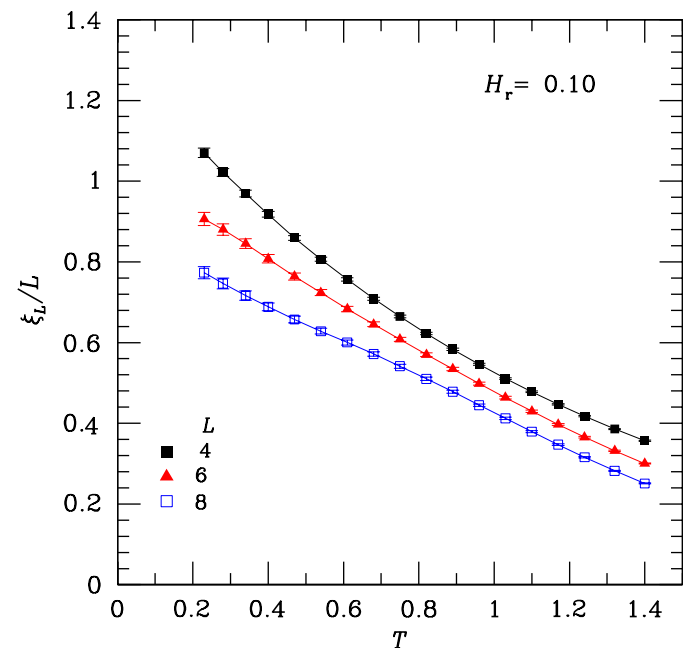

Fig. 4. The scaled correlation length for the Ising spin glass with (random) field strength $H_r = 0.1$ (H.G. Katzgraber and A.P. Young, unpublished).

6. 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.

References

[1] S.F. Edwards, P.W. Anderson, J. Phys. F 5 (1975) 965.
[2] D. Sherrington, S. Kirkpatrick, Phys. Rev. Lett. 35 (1975) 1792.
[3] G. Parisi, Phys. Rev. Lett. 43 (1979) 1754.
[4] H.G. Ballesteros, et al., Phys. Rev. B 62 (2000) 14237.
[5] D.S. Fisher, D.A. Huse, Phys. Rev. Lett. 56 (1985) 1601.
[6] H.G. Katzgraber, M. Körner, A.P. Young, Phys. Rev. B 73 (2006) 224432.
[7] N. Kawashima, A.P. Young, Phys. Rev. B 53 (1996) R484.
[8] E. Marinari, G. Parisi, J.J. Ruiz-Lorenzo, Phys. Rev. B 58 (1998) 14852.
[9] S. Jain, A.P. Young, J. Phys. C 19 (1986) 3913.
[10] J.A. Olive, A.P. Young, D. Sherrington, Phys. Rev. B 34 (1986) 6341.
[11] H. Kawamura, M. Tanemura, Phys. Rev. B 36 (1987) 7177.
[12] H. Kawamura, M.S. Li, Phys. Rev. Lett. 87 (2001) 187204.
[13] H. Kawamura, Phys. Rev. Lett. 80 (1998) 5421.
[14] K. Hukushima, H. Kawamura, Phys. Rev. E 61 (2000) R1008.
[15] F. Matsubara, T. Shirakura, S. Endoh, Phys. Rev. B 64 (2001) 092412.
[16] S. Endoh, F. Matsubara, T. Shirakura, J. Phys. Soc. Japan 70 (2001) 1543.
[17] T. Nakamura, S. Endoh, J. Phys. Soc. Japan 71 (2002) 2113.
[18] L.W. Lee, A.P. Young, Phys. Rev. Lett. 90 (2003) 227203.
[19] I. Campos, M. Cotallo-Aban, V. Martin-Mayor, S. Perez-Gaviro, A. Tarancon, cond-mat/0605327.
[20] J. Mattsson, T. Jonsson, P. Nordblad, H.A. Katori, A. Ito, Phys. Rev. Lett. 74 (1995) 4305.
[21] A.P. Young, H.G. Katzgraber, Phys. Rev. Lett. 93 (2004) 207203.
[22] H.G. Katzgraber, A.P. Young, Phys. Rev. B 72 (2005) 184416.