Heisenberg Spin Glass on a Hypercubic Cell

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Abstract

We present results of a Monte Carlo simulation of an Heisenberg Spin Glass model on a hipercubic cell of size 2 in D dimensions. Each spin interacts with D nearest neighbors and the lattice is expected to recover the completely connected (mean field) limit as $D \to \infty$. An analysis of the Binder parameter for $D = 8, 9$ and 10 shows clear evidence of the presence of a spin glass phase at low temperatures. We found that in the high temperature regime the inverse spin glass susceptibility grows linearly with T^2 as in the mean field case. Estimates of T_c from the high temperature data are in very good agreement with the results of a Bethe-Peierls approximation for an Heisenberg Spin Glass with coordination number D.

1 Introduction

Despite the fact that many real spin glasses, like $\mathrm{Eu_xSr_{1-x}S}$, CuMn, AgMn , are Heisenberg like systems, the very existence of a finite temperature transition in three dimensions seems to be ruled out for systems with short range interactions [1]. Simulations of a model with long range RKKY interactions are compatible with the system being at its lower critical dimension [2]. A possible way out of the puzzle has been the consideration of anisotropy. Matsubara et al. [3] have shown that even a small amount of anisotropy in the Hamiltonian is enough for having a spin glass phase at low temperatures. The previous models [1, 2, 3] are of the class with *bond disorder*. A finite temperature transition was also found in an isotropic *site diluted* model with RKKY interactions [4]. More recently, Coluzzi [5] have found evidence for a finite temperature transition in the four dimensional bond disordered lattice with nearest neighbour interactions (nni). Consequently the lower critical dimension for the model with nni would be between three and four.

In this letter we address the problem of the spin glass transition in Heisenberg systems putting enphasis in the connectivy structure of the lattice rather than the dimension. In fact, the coordination number in the real three dimensional space may not be six for an amorphous system, as forced by the hypercubic lattice geometry. Instead, we have studied a model in which N spins are placed in the vertices of a D dimensional *hipercubic cell* of side 2 so that the size of the system is $N = 2^D$ and where each spin interacts with its D nearest neighbors. This model has been introduced by Parisi *et al.* [6] who studied the static properties of Ising spin glasses and the approach to mean field behaviour that is expected when $D \to \infty$. Note that in this geometry D is not the dimension of real space but defines the connectivity structure of the system. From the point of view of the connectivity the behaviour of the *hipercubic cell* in dimension D has to be compared with that of the *hipercubic lattice* in *D/2* dimensions. For an Heisenberg system the spins interact through the Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{<ij>}^{N} J_{ij}\ \mathbf{s_i} \cdot \mathbf{s_j} \tag{1}$$

The vector spins $\{\mathbf{s_i}, i = 1 \dots N\}$ have components $\{s_i^\alpha, \alpha = 1 \dots 3\}$ and are normalized in the unit sphere. The random interactions are chosen from a Gaussian distribution with $\overline{J_{ij}} = 0$ and $\overline{J_{ij}^2} = 1/D$. It is important to note that in this geometry the size N and the "dimension" D are constrained so it is not possible to do the usual finite size scaling analysis by fixing D and let N grow to the thermodynamic limit. A real phase transition can only occur in the limit $D \to \infty$ which corresponds to mean field. Nevertheless clear evidences of a phase transition can already be seen at finite size N (or equivalently, finite "dimension" D). We will see that the present model is very well suited for studying the approach to mean field behaviour and the effects of finite connectivity.

2 The Binder Parameter and Spin Glass Susceptibility

In vector models the usual spin glass order parameter becomes a matrix in the spin components. It is possible to define the set of overlaps

$$q^{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} s_i^\alpha s_i^\beta \,, \tag{2}$$

where for the Heisenberg case $\alpha = 1\ldots 3$ denotes spin components and $i = 1\ldots N$ the sites on the lattice. As the system presents a global rotational symmetry it is useful to define a rotationally invariant order parameter Q whose moments are

$$Q^k = \left[\sqrt{\frac{1}{3}\sum_{\alpha\beta}(q^{\alpha\beta})^2}\,.\right]^k \tag{3}$$

A useful quantity for determining the existence of a phase transition is the so called Binder parameter defined, for the Heisenberg system [5], as

$$g = \frac{1}{2}\left[11 - 9\,\frac{\overline{< Q^4 >}}{\left(\overline{< Q^2 >}\right)^2}\right] , \tag{4}$$

where $< \ldots >$ means a thermal average and the overbar an average over disorder realizations of the bonds. From the scaling properties of this adimensional quantity it turns out that at the critical point the value of g is independent of the system size and consequently the curves for different sizes must cross each other at T_c. This fact permits a rather accurate determination of the critical temperature. Considering two replicas of the system σ and τ it can be defined the spin glass susceptibility as

$$\chi_{SG} = \beta^2 \frac{3}{N}\overline{\left\langle\left(\sum_{i=1}^{N}\sigma_{\mathbf{i}}\cdot\tau_{\mathbf{i}}\right)^2\right\rangle}\,. \tag{5}$$

The factor 3 has been introduced in order to have $\chi_{SG}/\beta^2 = 1$ for $T \to \infty$ as in the SK model [8]. With our definition of the parameter Q the spin glass susceptibility can be expressed

$$\chi_{SG} = 3\,N\,\beta^2\,\overline{< Q^2 >}\,. \tag{6}$$

The spin glass susceptibility is expected to diverge at and below the spin glass transition temperature T_c.

We have done Monte Carlo simulations of the Heisenberg spin glass previously defined and measured the moments Q^2 and Q^4 and also the Binder parameter and spin glass susceptibility. The dynamics used has been a standard heat bath algorithm [1]. As we are here interested in static properties we have checked that the system was thermalized before measuring physical quantities by looking at the coincidence of the susceptibilities calculated by two different methods, replicas and auto-overlaps as in [9]. We have simulated systems of $N = 256$, 512 and 1024 spins corresponding to $D = 8$, 9 and 10 respectively.

3 Results

At high thermal noise $T \to \infty$ the spins become independent variables and the limiting values of the moments $< Q^2 >$ and $< Q^4 >$ can be determined exactly [10]. It is found that

$$\lim_{T\to\infty} \langle Q^2 \rangle = 1/3N\,, \tag{7}$$

and

$$\lim_{T\to\infty} \langle Q^4 \rangle = \frac{11 - 2/N}{81N^2}\,. \tag{8}$$

Figure 1 shows a plot of $\log\langle Q^k \rangle$ vs $\log N = D \log 2$ for $T = 5$. The solid lines show the exact predicted behaviour. The agreement between both results, simulations and analytic, is very impressive given credit to both our data and the analytic result. As at this temperature the spins are uncorrelated it is not necessary to perform the average over disorder samples. At lower temperatures we have averaged over 50 to 100 samples.

In Figure 2 we can see the spin glass susceptibility rescaled with T^2 vs temperature in the range $0.15 \leq T \leq 0.5$. The behaviour suggests a finite temperature phase transition in this range of temperatures. From Eqs.(6) and (7) it can be seen that the curves must go to 1 as the temperature increases. Further evidence is obtained from the Binder parameter shown in Figure 3. Normally the transition temperature is evidenced by the point where the curves for different sizes intersect. Our results are consistent with a transition at $T_c \approx 0.3$. But the behaviour is quite peculiar; in the high T regime $g \approx 0$ for the three sizes studied. A possible explanation for this fact may be that the geometry of the lattice is not fixed and also the use of free boundary conditions [11]. In this lattice all spins are also in the boundary, so using free boundary conditions make the spins less constrained than, for example, using periodic boundary conditions. We also recall that in this model N and D grow together, it is not possible to fix D and let N grow to the thermodynamic limit. In this sense, the three sizes studied correspond also to three different "dimensions" of the cell, or coordination values D. The effect of increasing D is to move the corresponding curve slightly to the right, and this is why we do not see a clear crossing of the succesive D curves.

A sensible analysis can be made of the approach to the thermodynamic limit, *i.e.* the infinite dimension or completely connected model, where mean field is exact. In the simulations we expect to see corrections to mean field behaviour coming from the finite connectivity D. It is known that the Heisenberg spin glass in the mean field limit presents a transition at a critical temperature $T_c = 1/3$ (for spins normalized in the unit sphere) below which there is a continuous breaking of the replica symmetry [7]. Our results from the Binder parameter suggest a slightly lower value that can be explained in part as a finite D correction. In fact, a Bethe-Peierls approximation for the Heisenberg spin glass with coordination D predicts a tranisition at a critical temperature given by the equation [1]:

$$(D-1)\ \overline{[\coth(J_{ij}/T_c) - T_c/J_{ij}]^2} = 1 \tag{9}$$

In Table 1 we show the solutions of this equation for different D values. Note that the results will depend strongly on the normalization chosen for the $J_{ij}'s$, for example if we had chosen $\overline{J_{ij}^2} = 1$ as usual for short range models, the T_c predicted for $D = 8$ would

D	T_c
6	0.2117
7	0.2288
8	0.2413
9	0.2514
10	0.2594
100	0.3259

Table 1: The critical temperatures predicted by the Bethe-Peierls approximation

D	T_c
8	0.2576
9	0.2641
10	0.2730
mean field	0.3333

Table 2: The critical temperatures from a linear fit of the high temperature data

be $T_c = 0.6825$ instead of $T_c = 0.2413$, a considerable difference. As can be seen the T_c predicted for the range of D studied in our simulations are considerably lower than the mean field value 0.333 which shows that the approach to the mean field limit is slow.

The mean field spin glass susceptibility for an Heisenberg system in the paramagnetic phase can be shown to be:

$$\chi_{SG} = \frac{\beta^2}{1-(\beta/3)^2} = \frac{1}{T^2 - 1/9} \tag{10}$$

so that the inverse susceptibility is expected to behave linearly with T^2. We show in Figure 4 a plot of χ_{SG}^{-1} vs T^2 for the mean field result together with the results of our simulations in the range of temperatures 0.35 - 0.5. The solid lines are linear fits to the data points. In this range a perfect linear behaviour is observed in agreement with mean field but with slope slightly different from one. If we consider values of $T < 0.35$ the behaviour is no longer linear suggesting that we are departing from the high T regime.

From the linear fits we were able to estimate by extrapolation the critical temperatures for the different D studied and compare with the results of the Bethe-Peierls approximation. The results are summarized in Table 2 and show a very good agreement with the analytic ones of Table 1.

4 Conclusions

We have presented evidence that isotropic Heisenberg spin glasses with finite connectivities present, at low temperatures, a spin glass transition for not too small connectivities. The overal behaviour of the system is in qualitative agreement with mean field predictions. At high temperatures finite size effects seem to be very weak and the main corrections come from the finite connectivity D. The critical temperatures for $D = 8$, 9 and 10 depart considerably from the mean field ($D = \infty$) result. An improved estimation with a Bethe-Peierls approximation, which takes into account finite connectivity effects, is in very good agreement with the numerical results from extrapolations of the high temperatura data.

We think that the hipercubic cell can be a useful model for studying the robustness of mean field predictions in the more realistic case of short range interactions, while keeping the possibility (specially from a computational point of view) of going to considerbly larger values of the connectivity than those which can be attained in ordinary hipercubic lattices. For the Heisenberg model it would be of particular interest the calculation of the distribution of overlaps $P(Q)$ which gives information of the structure of phase space and whose non trivial character for short range interactions is still in debate.

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