Original Research Article

Numerical Simulation of Spin Glass State in Diluted Magnetic Materials Using Ising Spin Model in 2D with Distance Dependent interactions

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Abstract: In the present paper, existence of spin glass state using Ising spin model with Edwards-Anderson type of interactions has been investigated by employing numerical simulation (Monte Carlo) technique. The study shows a phase transition from paramagnetic state to spin glass state when far apart spins are included in addition to nearest neighbor ones using power law decaying interactions.

Keywords: phase transition, Edwards-Anderson Ising spin model, power law decaying interactions, exchange Monte Carlo, diluted magnetic materials.

1. Introduction

Spin glasses are random magnetic alloys resulting from frustration which is believed to be a consequence of quenched disorder (the randomness in the interactions).This state exists in the alloy of diluted magnetic atom and non magnetic metal such that the interaction between spins at each site is RKKY type of interaction which is an interaction due to conduction electrons. But such types of interactions decay with the distance between spins becoming longer and longer. Ground state of spin glass at low temperature is a frozen disordered state instead of an ordered one (the magnetization is zero). This implies that there is no long-range order in spin glasses. This is the result of competition in interaction between ferromagnetism and aniferromagnetism. According to previous studies of spin glass state, quenched disorder means that the interactions between spins and/or their locations have constrained disorder. Because of the conflict in the interaction between spins, the spin glass phase is an example of spontaneous cooperative freezing of the random spin orientations [1].In particular, when the coupling between spins are

ferromagnetic for some bonds and antiferromagnetic for the others, then the spin alignment cannot be uniform in space, unlike the ferromagnetic system, even at low temperatures [2-5]. Under such a situation the spins get randomly frozen in time. This is the phenomenon of the spin glass phase.

2. The Model

We assume that the Edwards-Anderson spin glass model [2-4], which is based on a set of N Ising spins $s_i = \pm 1$, the governing dynamics will be expressed as

$$H = \sum_{(ij)} J_{ij}\, s_i s_j. \qquad (2.1)$$

Where (ij) stands for a sum over nearest neighbors.

The exchange integral or bonds J_{ij} are independent random variables drawn from a given distribution with mean zero and variance one. This implies that each interaction coupling J_{ij} is expected to be distributed independently according to the probability distribution ($p(J_{ij})$). We can use the bimodal type of bond distribution $p(J_{ij})$ i.e.

$$P(J_{ij}) = p\delta(J_{ij} - J) + (1 - p)\delta(J_{ij} + J). \qquad (2.2)$$

In this equation J_{ij} may be either J (> 0) (with probability p) or -J(with probability 1-p)[5].

Here the spin variables are assumed to be of the Ising type ($s_i = \pm 1$) and fluctuate thermodynamically.

We focus on a generalization of the Edwards-Anderson Ising spin glass[6-7] model, i.e. the bonds take only two values $J_{ij} = \pm 1$, with probability of occurrence of this is equal and the probability of existence of interaction coupling depends on the distance between the two spins. A theoretical understanding of the spin-glass phase is relaying on the value of the overlap order parameter [8]. The spins that exist in one replica and those of the other are not affected thermodynamically each other. Nonetheless, we can expect that the spin configurations of the two replicas are similar to each other at low temperatures, if there is a single thermodynamic state into which the system is frozen else the overlap can take different values (including zero) if

many different states are present. Thus, we define the order parameter as the hamming distance of the spin configurations of the replicas [8]. For a given instance J of the quenched disorder the overlap is defined as:

$$q_J^{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i^{(1)}\rangle_\alpha \langle\sigma_i^{(2)}\rangle_\beta \qquad (2.4)$$

Here $\langle \dots \rangle_{\alpha,\beta}$ stands for thermal average (time average for Monte Carlo Calculations) in the state α,β and $N = L^d$ is the number of lattice sites. Where L is linear lattice size and d is dimension of the system. One may regard that the two identical copies represent the same system at two moments in time with infinite interval [9]. Spin glasses present a great challenge for numerical simulations. The effects of frustration and disorder lead to slow dynamics, with roughly logarithmic time dependence, so simulation must be run for many time steps. Furthermore, quenched in disorder gives rise to large sample to sample fluctuations making an average over many samples necessary to obtain accurate results.

3. Distance dependent interaction coupling

Since such a kind of spin interaction is strongly dependent on distance between spins at the sites i and j, it is permissible to consider only spins at the nearest neighbors only. But in order to show a phase transition we explore distance dependent interaction coupling when couplings [10] between far away spins are permitted. Therefore we considered the following Hamiltonian for the Ising spins:

$$H = \sum_{(i<j)} J_{ij}\, s_i s_j. \qquad (3.1)$$

The exchange integral is a quenched random variable whose probability of being non- zero decays with distance between two spin sites[11] This implies that, if we consider two spins at the sites i and j, and then the distance between them is $d_{ij} = |d_i - d_j|$. The probability of the existence of coupling between them can be given as

$$p(J_{ij}) \propto d_{ij}^{-\rho} \qquad (3.2)$$

for $d_{ij} \geq 1$. The probability of existence of the none zero interaction coupling is equal and the distribution of interaction coupling is Gaussian type with zero mean and variance ($\overline{J_{ij}^2} \propto d_{ij}^{-\rho}$)[12-14]. Such a kind of method leads us to study long and short range regimes by changing the

exponent (ρ)[11]. The problem is that each spin interacts with all the others and numerical simulations are very computer time demanding, and it is hard to get clear experimental evidence supporting a specific spin-glass theory [12-13]. We, therefore, introduce a diluted version of the model, where the mean coordination number is fixed [15] i.e. for this work we use the coordination number ($z = 6$). The critical behavior is mean-field like ($\frac{3}{2}\rho - 2D = 0$) with critical exponents $\nu = \frac{1}{\rho - D}$ and $\eta = D - 2 - \rho$, according to finite size scaling approach. Where ν is the exponent of correlation length and η is the exponent of spin glass susceptibility. Here $\rho = \frac{8}{3} = 2.67$ is found in the renormalization [10] approach from the dimension of the coupling constant.

4. Computational technique

The general idea of parallel tempering is not limited to exchanges or swaps between systems at different temperatures. Investigators have developed a number of methods based on swapping alternative parameters in order to minimize barriers that inhibit correct sampling. Additionally, parallel tempering can be combined with a large number of alternative sampling methods, and its use has led to a great improvement in the sampling of many existing computational methods.

We have used replica exchange (parallel tempering)[17-21] Monte Carlo scheme because spin glass system has many local minima separated by entropic barriers at its ground state [22-23]. Just to implement a parallel tempering algorithm[10] one needs to make M replicas of the system (ensemble) to be analyzed, each of which characterized by different temperatures $T_1 > T_2 > \cdots > T_M$. The main idea of this method is to simulate independently the standard Monte Carlo[24] for each copy, all of them at different temperatures and to swap periodically the configurations of two randomly chosen temperatures [25-26]so that as to reduce the relaxation time of the simulation at each valley. We used the following details for the simulation:-

Rho($\frac{\text{gur}}{\rho}$)	Lattice size(L)	No. of samples(NJ)	No. of Monte Carlo steps (MCS)	No of temperatures(M)	Δ^{tion} (Ch$\frac{T}{\text{nge}}$ in T)
3	30, 40	200(for small L) &100 (for large L)	500000	10(for small L)&20(for large L)	0.2&0.1
4	30,40	200(for small L)	1000000	10(for small L)&20(for large	0.2&0.1

		&100 (for large L)		L)	

Table 1 Parameters that we used for the simulation.

5. Results and Discussion

The plots show the existence of phase transition from paramagnetic to spin glass state for larger system sizes. Basically, in this case the researches considered overlap order parameter in order to identify spin glass phase. Temperature varies with the concentration i.e. when concentration decreases, the transition temperature also decrease just like that of the experimental findings 30 years ago by Mydosh and Canella. The site density is directly proportional to the concentration of magnetic ions. It is easy to vary the concentration of spins and to find a spin density in zero molecular field which is independent of the composition.

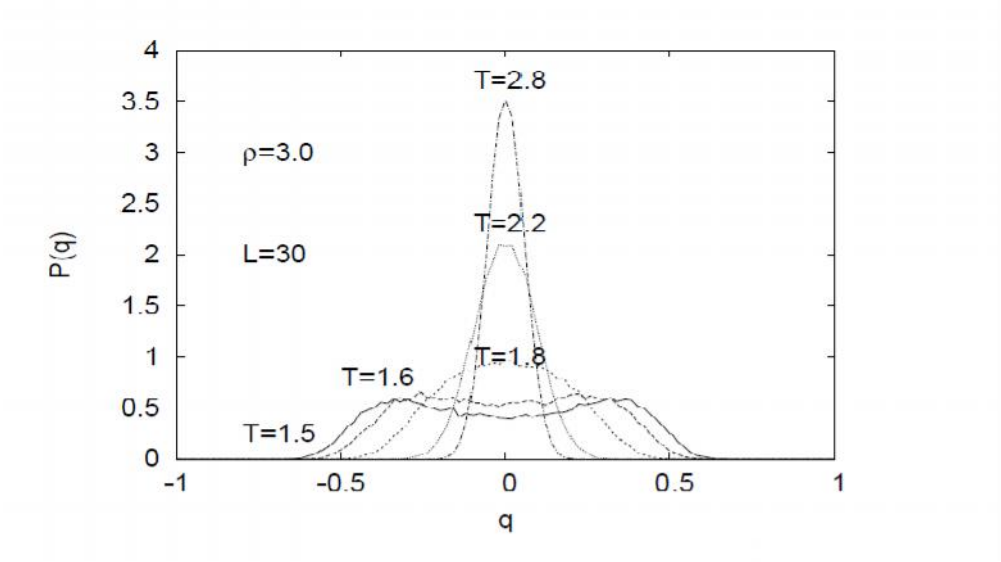

Fig.1 The plot of Probability distribution of overlap parameter (P(q)) versus order parameter (q) for different temperatures T =1.0; 1.4; 1.8; 2.2; 2.8 and ρ = 3.0, = 30. This plot illustrates how pure paramagnetic phase at high temperature is translated to spin glass phase at low temperature.

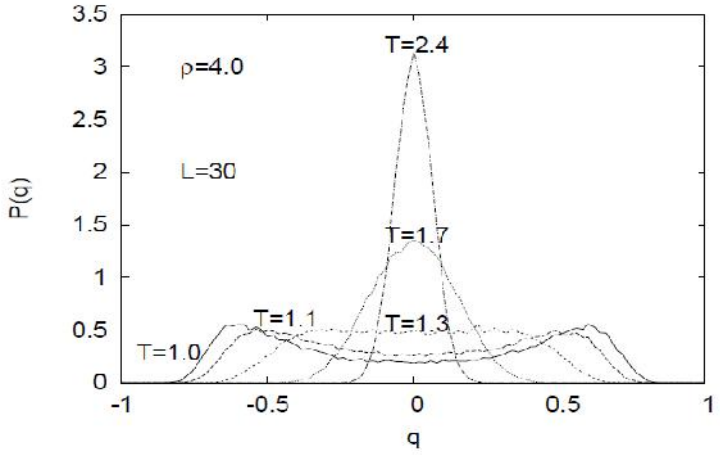

Fig.2: This figure explains the probability distribution of order parameter verses overlap parameter just like the above figure but for L =30, ρ = 4.0, and T = 1.5,1.6,1.8,2.2,2.8. In this case, the figure shows how the peaks of p(q) depend on the value of ρ and temperature.

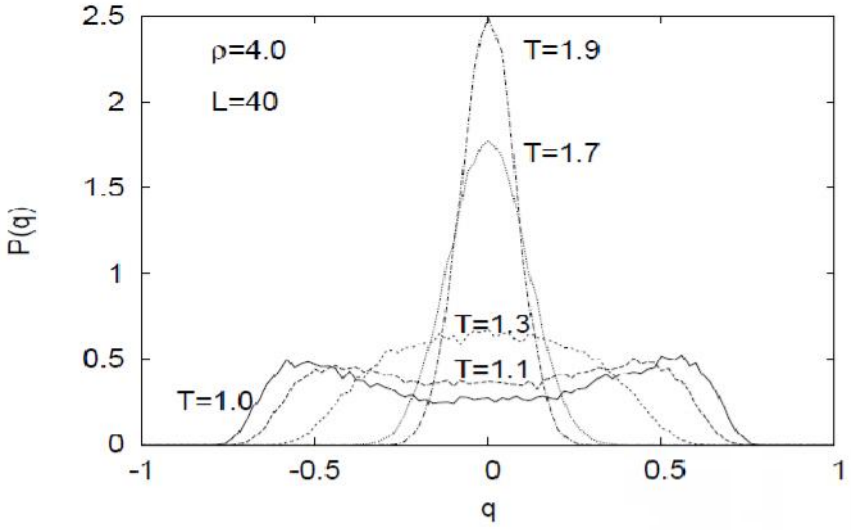

Fig.3: Schematic representation of p(q) versus for $L = 40, \rho = 4.0$, T = 1.0,1.1,1.3,1.7,1.9. This figure helps for comparison i.e. the effect of rho (ρ) on the phase transition temperature and the role of lattice on the existence of overlap order parameter.

6. Conclusion

Some of the physical quantities that we used diverge at the critical point. In order to avoid this complication in the simulation time we introduced finite size scaling approach. We have simulated different systems with different geometrical organization of random interactions. For each system we have simulated two replicas in order to study the overlap order parameter. We have taken a simulation for the probability of overlap distribution function for $\rho = 3, 4$. In both cases we found evidence for the existence of a phase transition from the paramagnetic to the spin glass phase. Specially for $\rho = 4$, double peaked distributions, typical of the spin glass phase are displayed at low T for small sizes. These results are in agreement with previous studies.

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