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1992 J. Phys.: Condens. Matter 4 2615

(http://iopscience.iop.org/0953-8984/4/10/023)

J. Phys.: Condens. Matter 4 (1992) 2615–2622. Printed in the UK

First-order transitions in an infinite-range spin-glass model

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Received 13 August 1991, in final form 28 October 1991

Abstract. The spin-glass phase and the first-order spin-glass transitions are investigated for a generalized Sherrington–Kirkpatrick Ising spin-glass model with $S = 1$ in a crystal field. Mean field equations for the model are derived and they are solved numerically. The double peak structure in the distribution of $p_i = \langle S_i^2 \rangle$ is shown to be important near the first order transitions. The transitions are qualitatively similar to the ground state transition.

1. Introduction

The mean field theory of the Sherrington–Kirkpatrick (SK) spin-glass model is now rather well understood [1]. The concept of replica symmetry breaking appeared and its physical meaning has been clarified. There are many pure states in the spin-glass phase. The spin-glass transitions in this model are continuous.

Ghatak and Sherrington generalized the SK model to the case with integer-valued spins $S_i = 0, \pm 1, \pm 2, \ldots, \pm S$ and with a crystal field term $D(S_i)^2$ in the Hamiltonian [2]. They found both first order and continuous transitions within the replica symmetric approximation. The stability of the replica symmetric solutions has been analysed [3, 4], and the nature of the instability of the replica symmetric solutions along the first-order spin-glass transition lines remains to be clarified. Some eigenvalues of the Hessian matrix become complex and the free energy suffers discontinuity on the first-order transition line in the replica analysis. A full Parisi treatment would cure these inadequacies but it has not been performed yet.

Besides the replica method, there is an approach introduced by Thouless, Anderson and Palmer (TAP) which does not rely on the replica technique [5]. Although it is rather difficult to solve the TAP equations numerically, Nemoto and Takayama developed a method to find solutions [6]. This method was successfully applied to analyse the nature of the spin-glass phase for the SK model [7]. The SK model in a transverse field, which is a quantum spin-glass model, was also investigated by the same approach [8].

In this paper, we investigate the nature of the spin-glass phase and the first-order spin-glass transitions for the generalized SK model. The approach of Nemoto and Takayama to solve the mean field equations, which correspond to the TAP equations, is employed. A consistent description of the first-order transition is obtained. In particular, the free energy is continuous at the first-order transition, as it should be. In the spin-glass phase near the first-order transition, the distribution of $p_i = \langle S_i^2 \rangle$ is double peaked. One part of the system, with larger p_i, mainly contributes to the spin-glass order, this is similar to that for the SK model. Another part of the system with smaller p_i is almost paramagnetic. In the paramagnetic phase near the first-order transition, p_i is small. The nature of the first-order transitions is similar to the ground state first-order transition. It was pointed out by Lage and de Almeida that the ground state transition will occur at $D = U_{SG}$ where U_{SG} is the ground state energy for the usual ± 1 model [3]. In the spin-glass phase at $T = 0$, all p_i equal unity, and all p_i become zero in the paramagnetic phase.

2. Mean field equations

We consider an infinite-range spin-glass model with a crystal field described by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij} S_i S_j - \sum_i D S_i^2 \tag{1}$$

where the spin variable S_i takes the values 0 and ± 1. The exchange coupling J_{ij} has zero mean and variance $1/N$ and the sum $\Sigma_{\langle ij\rangle}$ is over all distinct pairs.

The free energy and the mean field equations which are exact for the infinite-range model may be easily obtained either by a power expansion [9] or the two-spin cluster method [10], for example. The free energy becomes

$$\begin{aligned} F = \sum_{\langle ij\rangle} [-J_{ij} m_i m_j - (\beta J_{ij}^2/2)(p_i - m_i^2)(p_j - m_j^2)] - \sum_i D p_i \\ + (1/2\beta) \sum_i [(p_i + m_i)\ln(p_i + m_i) + (p_i - m_i)\ln(p_i - m_i) \\ + 2(1 - p_i)\ln 2(1 - p_i) - 2\ln 2] \end{aligned} \tag{2}$$

where m_i and p_i are thermal averages of S_i and S_i^2 respectively. From this free energy we obtain the following two sets of mean field equations:

$$(1/2\beta)\ln[(p_i + m_i)/(p_i - m_i)] - \sum_j J_{ij} m_j + \beta m_i \sum_j J_{ij}^2 (p_j - m_j^2) = \partial F/\partial m_i = 0 \tag{3}$$

$$(1/2\beta)\ln[(p_i^2 - m_i^2)/4(1 - p_i)^2] - D - \frac{\beta}{2}\sum_j J_{ij}^2 (p_j - m_j^2) = \partial F/\partial p_i = 0. \tag{4}$$

The free energy is not always convergent as in the case of the SK model. We use the method of Owen to discuss the convergence condition for the free energy [11]. The free energy can be written as

$$\beta F = -\ln \operatorname{Tr} \exp(-\beta H^{(0)}) - \ln\left\langle \prod_{\langle ij\rangle} \exp(-\beta (H - H^{(0)})_{ij}\right\rangle_{H^{(0)}} \tag{5}$$

where $\langle \ldots \rangle_{H^{(0)}}$ means the thermal average with respect to the Hamiltonian $H^{(0)}$. We chose $H^{(0)}$ as

$$H^{(0)} = \sum_i H_i^{(0)} \tag{6}$$

where

$$\begin{aligned} H_i^{(0)} = -\sum_j \Big\{ [J_{ij} m_j - \beta J_{ij}^2 m_i (p_j - m_j^2)] S_i - \sum_j \frac{\beta}{2} J_{ij}^2 (p_j - m_j^2) S_i^2 - D S_i^2 \\ + \frac{\beta}{2} \sum_j J_{ij} m_i m_j - \frac{\beta^2}{4} \sum_j (-p_i p_j - 3 m_i^2 m_j^2 + 2 m_i^2 p_j + 2 m_j^2 p_i). \end{aligned} \tag{7}$$

Then the first term in (5) will give the mean field free energy. The second term in (5) is calculated to be

$$\beta F_s = -\ln\Big\langle \prod_{(ij)} \Big\{ 1 + [\beta J_{ij} + 2m_i m_j(\beta J_{ij})^2](m_i - S_i)(m_j - S_j) + [(\beta J_{ij})^2/2](p_i - S_i^2)(p_j - S_j^2) - m_i(\beta J_{ij})^2(m_i - S_i)(p_j - S_j^2) - m_j(\beta J_{ij})^2(m_j - S_j)(p_i - S_i^2) \Big\} \Big\rangle_{H^{(0)}} \quad (8)$$

where we have expanded the exponential up to the second order in J_{ij}. Expanding the product in (8) around unity, we have tree diagrams which become zero with the choice of

$$m_i = \langle S_i \rangle_{H^{(0)}} \quad (9)$$

and

$$p_i = \langle S_i^2 \rangle_{H^{(0)}}. \quad (10)$$

It can be shown that (9) and (10) are equivalent to the mean field equations (3) and (4). Among various ring diagrams, we adopt the *ansatz* that the ring diagrams made of $[\beta J_{ij} + 2m_i m_j(\beta J_{ij})^2](m_i - S_i)(m_j - S_j)$ are most divergent. Then a series of double bond rings can be summed [11] to give

$$-\frac{1}{4}\ln\Big[1 - N^{-1}(\beta J)^2 \sum_i (p_i - m_i^2)^2\Big]. \quad (11)$$

This leads to the convergence condition

$$(\beta J)^2 N^{-1} \sum_i (p_i - m_i^2)^2 \leqq 1. \quad (12)$$

This condition will be used when the first-order transitions are investigated.

Next we will consider the instability line of the paramagnetic phase (the continuous transition line) by using (3) and (4) to compare it with the result obtained by the replica method. This line is obtained from the first-order terms of (3) in magnetization and they are given by

$$\frac{1}{\beta_c} \times \frac{1}{p_i} m_i - \sum_j J_{ij} m_j + \beta m_i \sum_j J_{ij}^2 p_j. \quad (13)$$

To the zeroth order in m_i, (4) becomes

$$\frac{1}{\beta}\ln[p_i/2(1-p_i)] - D - \frac{\beta}{2}\sum_j J_{ij}^2 p_j = 0. \quad (14)$$

To carry out an analytic calculation, we will make an approximation of $p_i = p$. Then (14) becomes

$$(1/\beta)\ln[p/2(1-p)] - D - (\beta/2)\, p = 0. \quad (15)$$

Terms in (13) are rewritten using the maximum eigenvalue of the random matrix J_{ij} and they become zero on the transition line as follows:

$$-2 + p(1/T_c) + (1/p)T_c = 0. \quad (16)$$

From (15) and (16), we obtain

$$T_c \ln(T_c/2(1 - T_c)) = D + \tfrac{1}{2} \quad (17)$$

which is just the same second order transition line as the one in the replica method [4].

It does not seem clear whether (17) is exact because we have used the approximation of $p_i = p$. Numerical results obtained by solving (3) and (4) show that p_i depends on position.

We mention the paramagnetic phase using (15). This equation has three solutions or one solution depending on the region of parameters. The line separating these regions is

$$D = -(1/4T)(1 \pm (1 - 8T^2)^{1/2}) + 2T \ln\{[1 \pm (1 - 8T^2)^{1/2}]/4T\} \qquad (18)$$

which has also been used in [4]. The first-order transition line locates in the region with three solutions. In the following section, these three solutions will be used as initial conditions to obtain numerical solutions for (3) and (4) in the paramagnetic phase.

3. Numerical solutions of the mean field equations

In order to discuss the nature of the first-order spin-glass transitions and the spin-glass phase, we solve the mean field equations (3) and (4) numerically. We adopt the method of Nemoto and Takayama [6], in which $|\nabla F|$ is minimized.

The system size we use is $N = 40$ and 15 samples of random bond configurations are prepared. Here we simply expect that the size of the system is enough to describe the system satisfactorily. In fact, the nature of the spin-glass phase has been described rather well by using a finite size system for the SK model [7]. Because spin-glass transitions for $T < 1/3$ are expected to be first order [2], the numerical study is performed at $T = 0.2$ in this paper. The numerical procedure to obtain solutions for the spin-glass phase is as follows. First, 500 initial configurations for $\{S_i\}$ are tried for each sample at $T = D = 0$. Among many solutions thus obtained, the minimum energy is denoted by $E_{\min}$ for each sample. We let survive only solutions which satisfy the following energy condition:

$$10^{-5} < \exp[-5.0(E - E_{\min})] \qquad (19)$$

because only a small number of solutions are statistically important. Next, the temperature is raised to 0.2. Solutions are updated by iterations to minimize $|\nabla F|$. The adopted convergence condition is

$$|m_i^{(n+1)} - m_i^{(n)}| < 10^{-5} \qquad (20)$$

for all sites and n is the number of iterations. Some solutions join each other in this process. We calculate the smallest eigenvalue of the Hessian matrix $\partial^2 F/\partial X \partial Y$ where X and Y are selected from $\{m_i, m_j, p_i, p_j\}$. We accept only solutions with the non-negative smallest eigenvalue. This procedure to seek solutions is repeated to decrease the value of D by the step of -0.02.

We need also paramagnetic solutions to discuss the first-order transitions. These solutions are obtained numerically as follows. For given T and D, uniform p is obtained by solving (15). The first order transitions seem to occur in the region with three solutions for (15) [4]. Adopting these three solutions as initial values of p_i, the mean field equations (3) and (4) are solved numerically. Then, the obtained p_i depends on position. We find the following results. The solution with the largest initial value of p is situated out of the range of the convergence condition of (12). The solution with the middle value of p becomes locally unstable because the smallest eigenvalue of the Hessian matrix becomes negative. Only the solution with the smallest initial value of p survives.

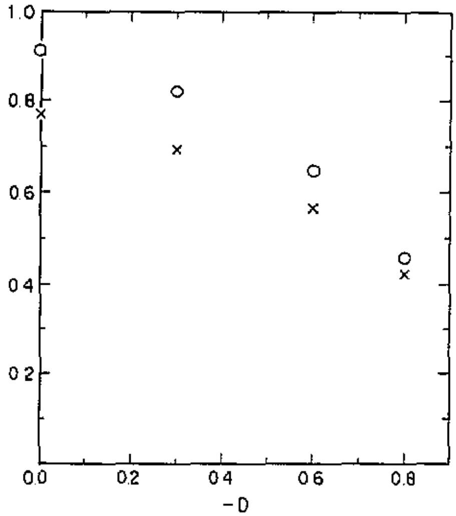

Figure 1. The Edwards–Anderson order parameter and an order parameter $\tilde{q}$, defined in the text, at $T=0.2$. The circles and the crosses represent $q_{\rm EA}$ and $\tilde{q}$ respectively.

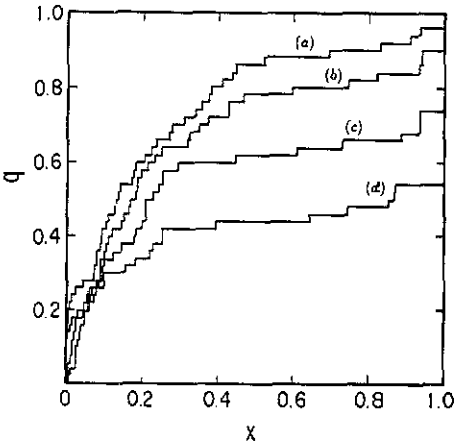

Figure 2. The order parameter function $q(x)$ for D equal to (*a*) 0.0, (*b*) −0.3, (*c*) −0.6 and (*d*) −0.8 at $T=0.2$.

We obtain the first-order transition point by comparing the free energy of the paramagnetic and the spin-glass phases. We identify the right thermodynamic phase as the one with smaller free energy. The transition occurs at

$$D = -0.85 \pm 0.05 \tag{21}$$

for $T = 0.2$. There is no discontinuity in the free energy and a consistent description of the first-order spin-glass transition is obtained.

Next we will discuss the order parameters. The Edwards–Anderson order parameter and the averaged spin-glass order parameter defined by

$$q_{\rm EA} = \left\langle \sum_a P_a q_{aa} \right\rangle_J = \left\langle \sum_a P_a (1/N) \sum_i \langle S_i \rangle_a^2 \right\rangle_J \tag{22}$$

and

$$\tilde{q} = \left\langle \sum_{ab} P_a P_b |q_{ab}| \right\rangle_J = \left\langle (1/N) \sum_i \langle S_i \rangle^2 \right\rangle_J \tag{23}$$

are shown in figure 1. Here the overlap of magnetization between two pure states

$$q_{ab} = \frac{1}{N} \boldsymbol{m}_a \cdot \boldsymbol{m}_b \tag{24}$$

and the statistical weight of a pure state

$$P_a = \mathrm{e}^{-\beta F_a} \Big/ \sum_b \mathrm{e}^{-\beta F_b} \tag{25}$$

are used. At the first order transitions they are discontinuous. The spin-glass order parameter function $q(x)$ obtained by

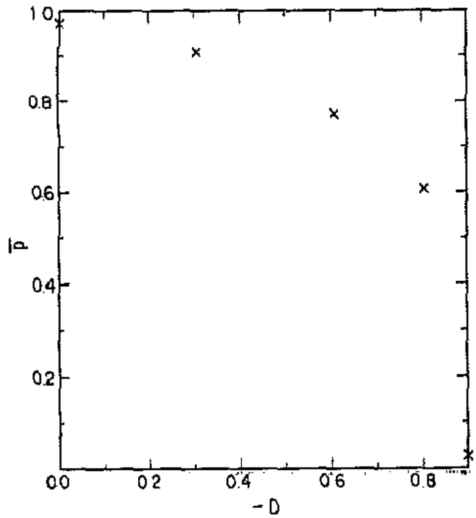

Figure 3. The statistical average of p_i at $T = 0.2$.

$$x(q) = \left\langle \sum_{ab} P_a P_b \theta(q - q_{ab}) \right\rangle_J \tag{26}$$

is shown in figure 2. The replica symmetry is obviously broken near the first-order transition.

The statistical average of p_i defined by

$$\bar{p} = \left\langle \frac{1}{N} \sum_i \langle S_i^2 \rangle \right\rangle_J = \left\langle \sum_a P_a \frac{1}{N} \sum_i \langle S_i^2 \rangle_a \right\rangle_J \tag{27}$$

is shown in figure 3. This is also discontinuous at the first order transition. To discuss the nature of the spin-glass phase and transition, the distributions of p_i are shown in figure 4. As D is decreased, a second peak with smaller values for p_i grows. About half the sites with larger p_i contribute mainly to developing the spin-glass order near the transition. In the paramagnetic phase near the first order transition, there is no site with larger p_i and a single peak distribution is observed.

We mention the replica symmetry in p. If the replica symmetry in p is also broken, we would obtain a non-trivial distribution for p_a defined by

$$p_a = \frac{1}{N} \sum_i \langle S_i^2 \rangle_a, \tag{28}$$

where the index a denotes a pure state. The probability distribution of p_a is defined by

$$P(p) = \langle P_J(p) \rangle_J = \left\langle \sum_a P_a \delta(p - p_a) \right\rangle_J. \tag{29}$$

The order parameter $p(x)$ may be defined by

$$x(p) = \int_0^p \mathrm{d}p' P(p') = \left\langle \sum_a P_a \theta(p - p_a) \right\rangle_J. \tag{30}$$

In figure 5, $p(x)$ obtained numerically by using (30) is shown. It seems that $p(x)$ is non-trivial especially when D is small. To make a definite conclusion for the replica symmetry breaking in p, it is necessary to study the size dependence of $p(x)$.

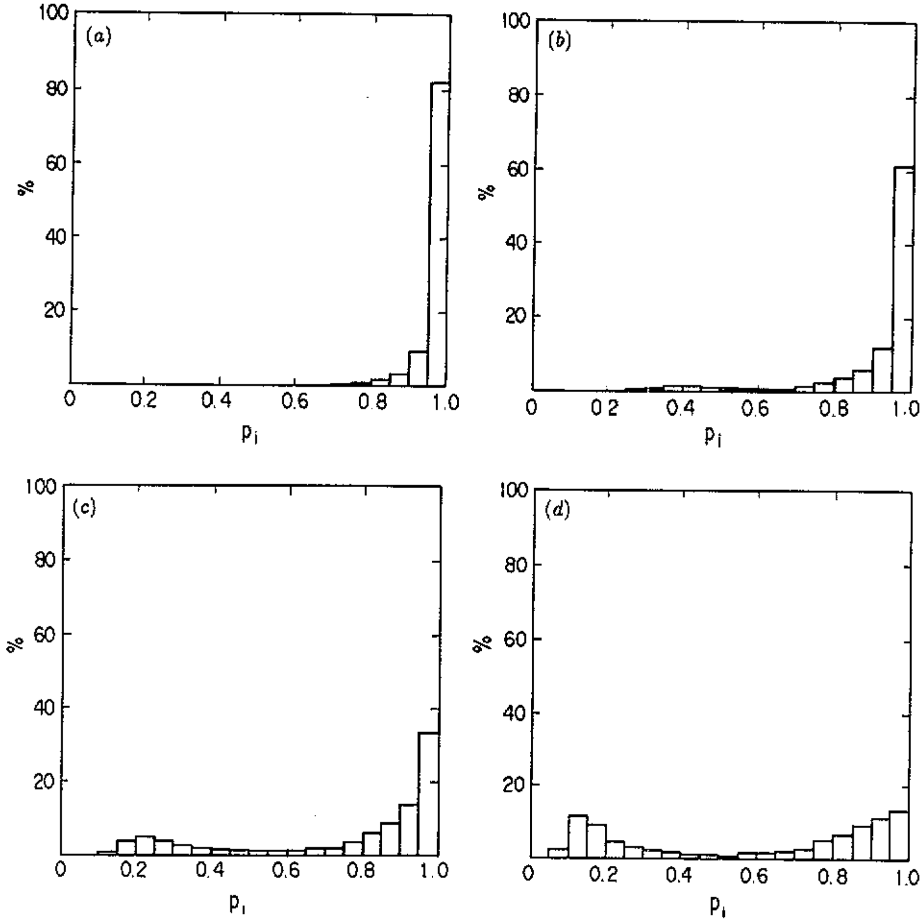

Figure 4. The distribution of p_i for $D = 0.0$, -0.3, -0.6, and -0.8 at $T = 0.2$ are shown in (*a*), (*b*), (*c*), and (*d*) respectively.

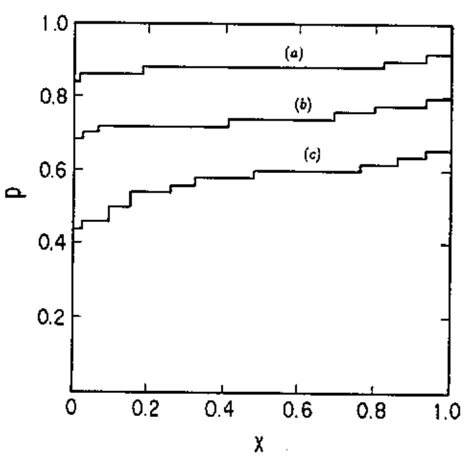

Figure 5. The order parameter function $p(x)$, defined in the text, for D equal to (*a*) -0.3, (*b*) -0.6 and (*c*) -0.8 at $T = 0.2$.

4. Summary and discussion

In this paper we have studied the nature of the first-order spin-glass transition and the spin-glass phase of an infinite-range Ising spin-glass model.

Mean field free energy and mean field equations have been obtained. The convergence condition for the free energy has been discussed. We have shown that the continuous transition line obtained by the replica method can be reproduced when the fluctuation in p_i is neglected. Whether this is justified or the locus of the transition line should be modified remains to be clarified.

The first-order spin-glass transition is described consistently in this method. There is no discontinuity in the free energy. The order parameters are obtained numerically. The spin-glass order parameters are consistent with the concept of the replica symmetry breaking. In particular, the replica symmetry is broken on the first-order transition line. The distributions of p_i show that the nature of the spin-glass transition is similar to the ground state spin-glass transition at $D = U_{SG}$ [3]. In this transition, a finite fraction of spins contribute mainly to the energy in the spin-glass phase. In the paramagnetic phase, all spins have smaller values of p_i and the transition is of first order with a discontinuity in m_i and p_i. The nature of the continuous transition is different. In this case, a single peak distribution of p_i is observed and most p_i are large at the transition and only m_i becomes small because of thermal fluctuations.

The replica symmetry breaking of q is related to the existence of many pure states. Whether all pure states have the same average of p_i should be clarified to make a definite conclusion for the replica symmetry breaking in p.

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