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Numerical study of the SK spin glass in a transverse field by the pair approximation

Terufumi Yokota
Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-11, Japan

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Abstract. The spin glass phase of the SK model in a transverse field is investigated by means of numerical solutions of the mean field equations that are obtained by the pair approximation. There exist many solutions that correspond to pure states. This is consistent with the concept of replica symmetry breaking. The solutions are shown to be marginally stable, as in the case of the classical SK model. From these results, the nature of the spin-glass phase may be considered as unchanged by the presence of a transverse field.

1. Introduction

In recent years a considerable number of investigations on quantum spin-glass models has appeared. In particular, much attention has been paid to the Sherrington–Kirkpatrick (SK) model with a transverse field.

The nature of the spin-glass phase for the SK model without a transverse field is rather well understood [1]. In this model, Parisi's replica symmetry breaking solution [2, 3] is believed to be exact. The order parameter becomes a function and the physical meaning of the order parameter function has been clarified. In the spin-glass phase, there is an infinite number of states separated by infinitely high barriers in the free energy. Each of these states is called a pure state. The order parameter function is expressed using the overlaps of pure states.

Thouless, Anderson and Palmer (TAP) developed a mean field theory for the SK model without relying on the replica technique [4]. It often happens that there is no numerical solution of the TAP equations for finite systems [5]. Nemoto and Takayama [6] discovered a clever method to find 'solutions' of the equations. They sought 'solutions' which minimize the norm of the gradient of the free energy, $|\nabla F|$. The 'solutions' become real solutions in the thermodynamic limit. All solutions of the equations are shown to be marginally stable. There is a number of solutions for the TAP equations, which increase exponentially with the number of sites [7]. All the features of solutions thus obtained are consistent with Parisi's scheme [7].

The question of how the above features of the spin-glass phase are influenced by the presence of a transverse field is interesting. Some earlier works suggested the existence of the replica symmetric spin glass phase for the SK model with a transverse field [9, 10]. However, more recent investigations seem to deny this possibility. The stability of the replica symmetric spin-glass phase was investigated numerically by Büttner and Usadel [11]. They showed that the stability line of the replica symmetry at non-zero temperature is the same as the transition line by investigating numerically the smallest eigenvalue of the Hessian matrix near the transition line. As a first step to the true solutions of the low temperature phase, first-stage replica symmetry breaking solutions have been obtained for the model [12, 13]. The replica symmetry breaking has also been studied by the Monte Carlo simulation by Lai and Goldschmidt [14]. They concluded that the overlap probability distribution $P(q)$ is similar to that for the classical case. Both numerical calculations are rather complicated due to the existence of quantum variables and it seems difficult to obtain full solutions. Furthermore it would be interesting to study other features of the spin glass phase, e.g. marginal stability and ultrametricity. Hence it would be worthwhile to make some approximate calculations.

In this paper, the nature of the spin-glass phase of the SK model in a transverse field is investigated by means of numerical solutions of the mean field equations that are obtained by the pair approximation. There exist many solutions, this being consistent with the replica symmetry breaking. Moreover, the solutions are shown to be marginally stable. From these results, it may be concluded that the effects of a transverse field on the nature of the spin-glass phase are qualitatively rather similar to the effects of temperature.

2. Mean field equations by the pair approximation

The pair approximation gives the TAP equations when it is applied to the SK model [15]. When there are quantum variables, account is only taken of the quantum effects within two-spin clusters in the pair approximation. Although the treatment is not sufficient even in the case of infinite-range quantum spin-glass systems, two-spin clusters seem to be important because the exchange coupling J_{ij} is a Gaussian random variable with zero mean and variance $1/N$.

The Hamiltonian of the SK model in a transverse field is given by

$$\mathcal{H} = -\sum_{(ij)} J_{ij}\sigma_i^z\sigma_j^z - \sum_i \Gamma\sigma_i^x. \tag{1}$$

By using the pair approximation, mean field equations can be obtained which reduce to the TAP equations when the transverse field is absent. The derivation of the equations has been reported [16] and are reproduced here. The equations are obtained by the extremum conditions of the free energy with respect to the magnetization and are given by

$$\sum_j (h_i' - h_i) + h_i = \sum_j J_{ij} h_i'^{(1)} + \sum_j J_{ij}^2 h_i'^{(2)} + h_i = 0 \tag{2}$$

where h_i and h_i' are effective fields in the one-body Hamiltonian and the pair

Hamiltonian respectively. They are expressed by using the magnetization m_i and the transverse field Γ. The one-body effective field is related to the magnetization as

$$m_i = (h_i/E_i)\tanh(\beta E_i) \tag{3}$$

where

$$E_i = (h_i^2 + \Gamma^2)^{1/2}. \tag{4}$$

Expressions for h_i' are given by

$$h_i'^{(1)} = -m_j \tag{5}$$

and

$$\begin{aligned}
\chi_i h_i'^{(2)} = {} & -\Gamma^2(3h_i h_j^2/2E_i^5E_j^2)\tanh\beta E_i \tanh^2\beta E_j + \Gamma^4(h_i/E_i^4E_j^3) \\
& \times \tanh^2\beta E_i \tanh\beta E_j - \beta\Gamma^2[(h_i h_j^2/E_i^4E_j^2)(1 - \tfrac{3}{2}\tanh^2\beta E_j) \\
& - (h_i^3/E_i^3E_j^3)\tanh\beta E_i \tanh\beta E_j)](1 - \tanh^2\beta E_i) \\
& + \beta^2(h_i^3h_j^2/E_i^3E_j^2)\tanh\beta E_i(1-\tanh^2\beta E_i)(1-\tanh^2\beta E_j) \\
& - \Gamma^2(h_i(\Gamma^2 - 3h_j^2)/2E_i^5E_j^2)\tanh\beta E_i + \Gamma^4(h_i/2E_i^4E_j^3)\tanh\beta E_j \\
& + \Gamma^4[h_i/2(h_i^2-h_j^2)^2][(\tanh\beta E_i/E_iE_j^2) + (\tan\beta E_i/E_i^3) \\
& - (2\tanh\beta E_j/E_i^2E_j)] - \Gamma^4[h_i/2(h_i^2-h_j^2)][(-3\tanh\beta E_i/E_i^3E_j^2) \\
& + (\tanh\beta E_i/E_i^5) + (2\tanh\beta E_j/E_i^2E_j^3) - (\tanh\beta E_j/E_i^4E_j)] \\
& - \beta\Gamma^2(h_i/2E_i^4)(1 - \tanh^2\beta E_i) - \beta\Gamma^4[h_i/2(h_i^2-h_j^2)E_i^4] \\
& \times (1 - \tanh^2\beta E_i).
\end{aligned} \tag{6}$$

Here χ_i is the susceptibility for the one-body effective field and is given by

$$\chi_i = \frac{\partial m_i}{\partial h_i} = \frac{\tanh\beta E_i}{E_i} - \frac{h_i^2}{E_i^3}\tanh\beta E_i + \frac{\beta h_i^2}{E_i^2}(1-\tanh^2\beta E_i). \tag{7}$$

The expression for $h_i'^{(1)}$ is the same as the expression for the classical model and this is a problem in the pair approximation. The reaction field which is given by $-h_i'^{(2)}$ contains quantum effects.

3. Numerical solutions of the mean field equations

The nature of the spin glass phase is now discussed by solving equations (2) numerically. These equations do not always have a solution [5]. The method considered by Nemoto and Takayama [6] is adopted. In this method, quasisolutions which minimize $|\nabla F|$ are picked up. Solutions with vanishing $|\nabla F|$ are real solutions. In the thermodynamic limit, $|\nabla F|$ is expected to vanish and quasisolutions become real solutions.

Numerical calculations are now described more closely. Taking $N = 40$ and 80 as the system size, calculations are performed for 15 samples of random bond configurations. Several solutions are obtained for each sample. First, 100 initial conditions are tried for each sample at $T = \Gamma = 0$ and many solutions are obtained. This is easily performed numerically because the reaction field is not necessary at $T = \Gamma = 0$. In fact, the number

Table 1. Number of solutions. These numbers are sums of 15 samples.

	Γ					
N	0.0	0.2	0.4	0.6	0.8	1.0
40	173	153	91	53	29	17
80	82	85	65	51	36	23

of initial conditions does not seem to be enough for $N = 80$ and consequently important solutions with large statistical weight are missing, as will be seen below. The minimum energy of solutions is denoted by E_{min} for each sample. Because solutions with negligible statistical weight may be abandoned to save computational time, solutions are retained for which the energy satisfies the following condition:

$$10^{-5} < \exp[-5.0(E - E_{min})]. \tag{8}$$

Here it is assumed that a solution with negligible statistical weight remains negligible when parameters T and Γ vary. Considering the numerical results, this assumption holds true in most cases we have examined explicitly. Next, the temperature is raised to 0.2. Solutions are updated by iterations to minimize $|\nabla F|$. Convergence is considered to be accomplished if the condition

$$|m_i^{(n+1)} - m_i^{(n)}| < 10^{-5} \tag{9}$$

is satisfied for all sites i. For a solution which satisfies the condition (9), the smallest eigenvalue of the Hessian matrix composed by the element $\partial^2 F/\partial m_i \partial m_j$ is calculated. When the eigenvalue is positive, the solution is accepted and when it is negative, further iterations are made to obtain an acceptable solution. In addition, when $|\nabla F|$ becomes smaller than about 10^{-4}, F itself is minimized to seek a real solution. These procedures are repeated to raise the value of Γ by steps of 0.1.

Some numerical results to investigate the nature of the spin glass phase within the pair approximation are now shown. First, the number of solutions is shown in table 1. The number is the sum over 15 samples. Hereafter all the results are for $T = 0.2$. Although the number for $\Gamma = 0.0$ is smaller than the number for $\Gamma = 0.2$ in the case of $N = 80$, this may be an artefact of the numerical method. Confluence of some solutions can occur in the course of the iterations to ensure that the smallest eigenvalue of the Hessian matrix remains positive. Most solutions (c., 95%) are with non-zero $|\nabla F|$ for $\Gamma = 0$. The ratio of solutions with non-zero $|\nabla F|$ decreases as the transverse field increases. This ratio is about 40% for $\Gamma = 0.6$. For $\Gamma \geqq 1.0$, most solutions are at the minimum of the free energy.

The smallest eigenvalue of the Hessian matrix is shown in figure 1. Because the smallest eigenvalue is identically zero for non-zero minimum $|\nabla F|$, account is only taken of solutions which minimize the free energy. The value in the figure is obtained by first averaging within a sample and then taking an average over samples. Since the $N^{-2/3}$ scaling is considered to hold good for the classical case, the same scaling is assumed to hold for the quantum case. The broken lines are only a guide for the eye. The scaling seems to be good even for the quantum case and this ensures the marginal stability of the solutions.

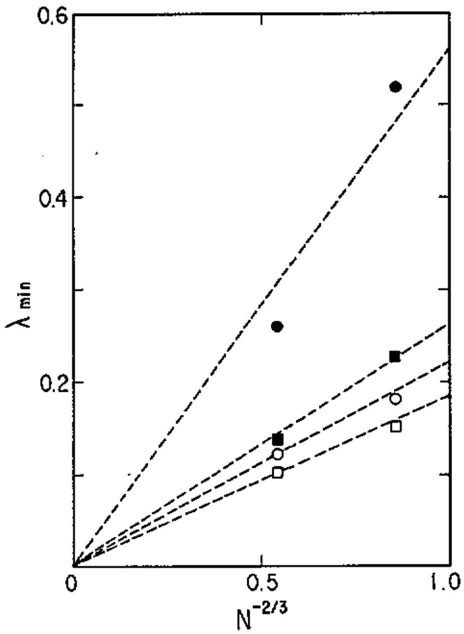


Figure 1. The smallest eigenvalues of the Hessian matrix at $T = 0.2$: ● for $\Gamma = 0.0$; ■ for $\Gamma = 0.3$; ○ for $\Gamma = 0.6$; □ for $\Gamma = 0.9$. To obtain the eigenvalues, account is only taken of solutions which minimize the free energy. The values are obtained by first averaging within a sample and then taking averages over samples. The broken lines are only a guide for the eye and represent the $N^{-2/3}$ scaling which is considered to be good for the classical case.

To see that quasisolutions with non-zero minimum $|\nabla F|$ become real solutions, $|\nabla F|$ must be shown to vanish in the thermodynamic limit. Unfortunately the size of the system examined seems to be too small to verify this statement. Therefore quasisolutions are simply assumed to become real solutions in the thermodynamic limit.

Consider next the spin glass order parameters. In figure 2, the Edwards–Anderson order parameter and the averaged order parameter defined by

$$q_{\mathrm{EA}} = \left\langle \sum_a P_a q_{aa} \right\rangle_J = \left\langle \sum_a P_a \frac{1}{N} \sum_i \langle \sigma_i^z \rangle_a^2 \right\rangle_J \tag{10}$$

and

$$\bar{q} = \left\langle \sum_{ab} P_a P_b |q_{ab}| \right\rangle_J = \left\langle \frac{1}{N} \sum_i \langle \sigma_i^z \rangle^2 \right\rangle_J \tag{11}$$

respectively are shown. In this expression, the overlap of magnetization between two pure states

$$q_{ab} = \frac{1}{N} \boldsymbol{m}_a \cdot \boldsymbol{m}_b \tag{12}$$

and the statistical weight of a pure state

$$P_a = \exp(-\beta F_a) \Big/ \sum_b \exp(-\beta F_b) \tag{13}$$

are used. Although the size dependence of the results is rather weak, the value for $N =$

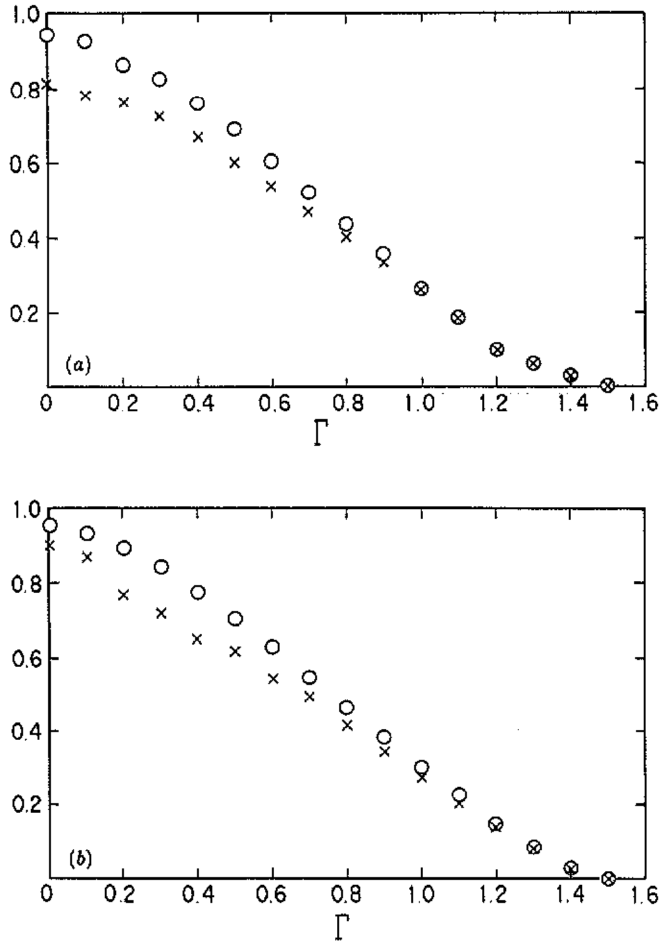
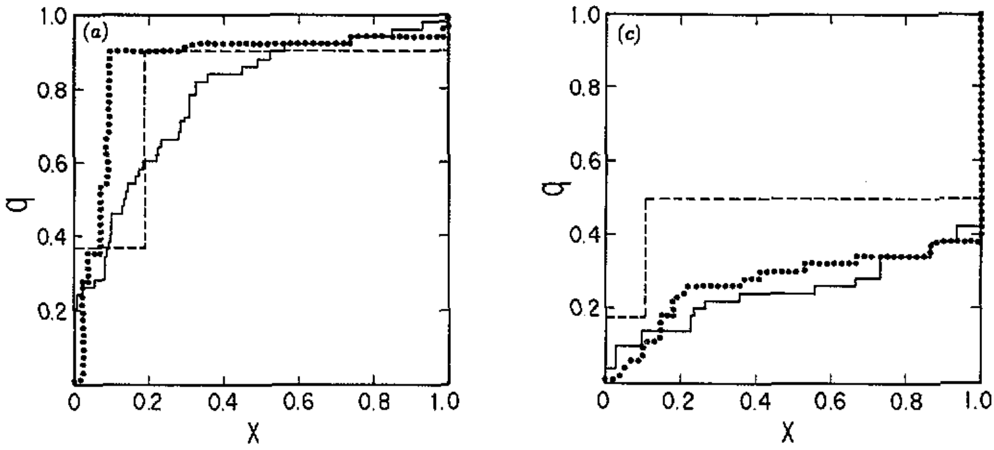


Figure 2. The Edwards–Anderson order parameter q_{EA} and an order parameter $\bar{q}$ defined in the text for (*a*) $N = 40$ and (*b*) $N = 80$ at $T = 0.2$. The circles and the crosses represent q_{EA} and $\bar{q}$, respectively.

80 seems to be a little larger than the value for $N = 40$ especially for $0.5 \leqq \Gamma \leqq 1.2$. The order parameter function $q(x)$ is obtained by using the formula

$$x(q) = \left\langle \sum_{ab} P_a P_b \theta(q - q_{ab}) \right\rangle_J . \tag{14}$$

In figure 3, $q(x)$ is shown for $\Gamma = 0.1$, 0.5 and 1.0 together with the first-step replica symmetry breaking results [13]. The full lines and the dotted lines represent the results for $N = 40$ and 80, respectively, while the results by the replica method are indicated by the broken lines. The curve for $N = 80$ is rather steep. This may be due to the fact that statistically important solutions are missing in this case as mentioned above. The curves for $\Gamma = 1.0$ in the pair approximation are considerably below the curve of the replica method. Whether this is due mainly to the inadequacy of the approximation or to the size dependence mentioned above cannot be concluded definitely.



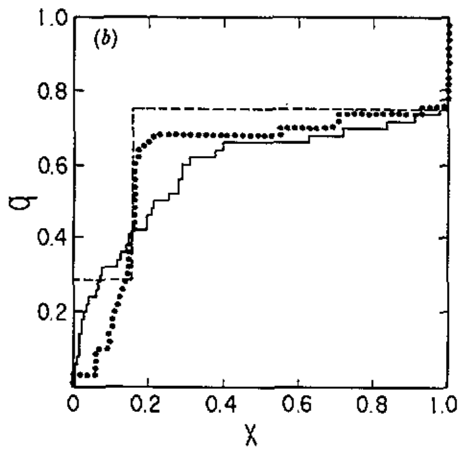


Figure 3. The order parameter function $q(x)$ for $\Gamma = 0.1, 0.5$ and 1.0 at $T = 0.2$ are shown in (*a*), (*b*) and (*c*) respectively. The full lines and the dotted lines represent results for $N = 40$ and 80, respectively, while the results for the first-step replica symmetry breaking [10] are shown by the broken lines.

These numerical results suggest that the qualitative nature of the spin-glass phase is similar to that of the classical case. Solutions join together by the effect of quantum tunnelling represented by the transverse field. This situation is rather similar to the confluence of solutions by thermal effects in the classical SK model. Quantum fluctuations are not expected to be important qualitatively for the critical behaviour at non-zero temperature in this model [17]. The same kind of effective Hamiltonian as in the classical case would then describe the system qualitatively near the second order transition line. In particular, the nature of the replica symmetry breaking is expected to be the same as the classical case near the second-order transition line at non-zero temperature.

Quantum effects are most essential at zero temperature. The ground state of the model is described by a classical Ising system with an extra dimension [17]. In this case, equivalent classical Ising spin glass systems with Γ playing the role of temperature are stacked infinitely along the extra direction with ferromagnetic interactions between layers. Although such ferromagnetic interactions are not expected to change the nature of the spin-glass phase, it is a problem that remains.

In order to check ultrametricity, the numerical solutions have been analysed. Unfortunately the number of pure states as well as the size of the system are too small to derive a definite conclusion.

To summarize, the nature of the spin-glass phase for the SK model with a transverse field has been investigated within the pair approximation. There are many pure states as in the classical case. Marginal stability of solutions persists also for the quantum system. Consequently, the same qualitative picture exists of the spin-glass phase for the model as for the classical SK model. The effects of a transverse field are rather similar to the effects of the temperature in the classical model.

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