Two- and three-spin cluster theory of spin-glasses

Kazuo Nakanishi*
Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 23 May 1980)

The cluster effect of spin-glasses is studied on the basis of the two- and three-spin cluster theory. In contrast to ordinary ferromagnets, the effective field containing the cluster effect is shown to be different from that containing no cluster effect, even at absolute zero. Numerical calculations are performed for the infinite-range model with 50 and 16 spins. It is shown that the solutions of the two-spin cluster equations at zero temperature are located at the bottom of deep valleys in the energy space. At finite temperatures the relationship between the local energy structure around the ground state and the existence of well behaved solutions is investigated. The Hessian matrix is examined also. The character of the lowest eigenvector of the Hessian matrix is found to be "localized" at low temperatures, while it is "extended" near the transition temperature. The effect of three-spin clusters is shown to play an important role in the temperature region where the three-spin cluster begins to be excited.

I. INTRODUCTION

Spin-glasses have recently attracted a great deal of interest,[1,2] because of the possibility of a new type of magnetic order which has not been found in pure systems. Typical systems of spin-glasses are dilute substitutional magnetic alloys, such as CuMn or AuFe, where the positive and negative values for the exchange interactions are produced by the oscillation of the so-called Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.[3] Due to the competition between positive and negative exchange interactions, spins at low temperatures are considered to be frozen in the sense that the thermal average of a spin takes a nonzero value, while its direction is random. Usually these states are highly degenerate and this kind of degeneracy causes anomalously long relaxation time phenomena.

Following Edwards and Anderson's pioneering work,[4] Sherrington and Kirkpatrick[5] (SK) proposed an infinite-range model of spin-glasses in which every spin is coupled with all others pairwise and the distributions of the exchange interaction is assumed to be Gaussian. This is an extension of the infinite-range model of ordinary ferromagnets, which we can treat exactly by the mean-field theory. SK studied this model using the replica method. Due to the pathology of the replica method, however, they obtained unphysical results, e.g., a negative entropy at sufficiently low temperatures. In order to remedy this difficulty, Thouless, Anderson, and Palmer[6] (TAP) developed a mean-field theory for this model. Making use of the Bethe approximation, they obtained a self-consistent equation and solved it in two limiting temperature regimes, i.e., in the vicinity of the critical temperature T_c and at very low temperatures. Their results near T_c agreed with those of SK, while at low temperatures they obtained a physically acceptable non-negative entropy. In addition, they suggested that the nontrivial solution of the self-consistent equation is located at the saddle point of the free energy as a function of the Edwards-Anderson order parameter. They showed the above fact explicitly immediately below T_c and speculated that it is true for the whole temperature region below T_c. This implies the existence of a critical line below T_c. As for the replica method, a recent idea[7] of the replica symmetry breaking has been successful.

The purpose of the present paper is to propose an effective mean-field theory and to study the cluster effect in spin-glasses. TAP found that in the infinite-range model there exists an extra field besides the conventional mean field. This extra field is due to the two-spin cluster effect, indicating the importance of the cluster effect in spin-glasses. In order to make a further investigation, we formulate a theory in which the effect of the two- and three-spin cluster is taken into account exactly. We apply it mainly to the infinite-range model.

The outline of this paper is as follows. In Sec. II the two-spin cluster theory is developed. In Sec. III, we apply the theory at zero temperature. It is shown that the two-spin cluster effect reduces the magnitude of the effective field calculated without considering the cluster effect. This should be compared with ordinary ferromagnets, in which the two-spin cluster effect disappears at zero temperature. Section IV is devoted to numerical treatments for the infinite-range model. It is demonstrated how the cluster theory works in spin-glasses. The low-lying modes of the

Hessian matrix are also examined numerically. The character of these modes is discussed in detail. In Sec. V we further examine the cluster effect by using the three-spin cluster theory. A brief summary is made in Sec. VI.

II. TWO-SPIN CLUSTER THEORY

We consider a system of interacting Ising spins which is described by the Hamiltonian

$$\mathcal{H} = -\sum_{(i,j)} J_{ij} S_i S_j ; \quad S_i = \pm 1 \ , \tag{2.1}$$

where we take the summation to be pairwise and we do not specify the interaction J_{ij} at this point. In order to study (2.1) we take out a two-spin cluster of sites i and j; we treat the term $J_{ij}S_iS_j$ exactly and make the mean-field approximation for other terms, i.e., we assume the effective fields $h_i^{(j)}$ and $h_j^{(i)}$ which act on sites i and j, respectively.[8] Then this local system can be expressed by the effective Hamiltonian $\mathcal{H}_{ij}$,

$$\mathcal{H}_{ij} = -J_{ij}S_iS_j - h_i^{(j)}S_i - h_j^{(i)}S_j + C \ , \tag{2.2}$$

where C is a constant, which we will determine later. From (2.2) we calculate the mean value for S_i at temperature T as

$$\langle S_i \rangle \equiv m_i = \tanh[\beta(h_i^{(j)} + k_i^{(j)})], \tag{2.3}$$

where $\langle A \rangle = \mathrm{Tr} A \exp(-\beta\mathcal{H}_{ij})/\mathrm{Tr}\exp(-\beta\mathcal{H}_{ij})$, $\beta = 1/T$ (we have set $k_B = 1$), and

$$k_i^{(j)} = T\tanh^{-1}(\tanh\beta J_{ij}\tanh\beta h_j^{(i)}) \ . \tag{2.4}$$

Equation (2.3) implies that $k_i^{(j)}$ is the effective field coming from site j to site i. This naturally requires the relation

$$h_i^{(j)} = \sum_{l \neq j} k_i^{(l)} \ . \tag{2.5}$$

Then from (2.4) and (2.5) we can determine $\{k_i^{(j)}\}$ self-consistently. With the solution one may calculate the effective field H_i at site i by the formula

$$H_i = \sum_l k_i^{(l)} \tag{2.6}$$

and

$$m_i = \tanh(\beta H_i) \ . \tag{2.7}$$

The next task is to calculate the free energy. First we determine the constant C in (2.2). Since $\langle\mathcal{H}_{ij}\rangle$ should give the same result as that obtained by the original Hamiltonian, we have the condition

$$\langle -J_{ij}S_iS_j \rangle = \langle \mathcal{H}_{ij} \rangle \ . \tag{2.8}$$

This yields

$$C = h_i^{(j)}m_i + h_j^{(i)}m_j \ . \tag{2.9}$$

Let us consider

$$Z_{ij} = \mathrm{Tr}\exp(-\beta\mathcal{H}_{ij}) \ , \tag{2.10}$$

and then we have

$$-T\ln Z_{ij} = f_i^{(1)} + f_j^{(1)} + f_{ij}^{(2)} \ , \tag{2.11}$$

where

$$f_i^{(1)} = H_i m_i - T\ln(2\cosh\beta H_i)$$
$$= T\left[\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right] \ , \tag{2.12a}$$

and

$$f_{ij}^{(2)} = -k_i^{(j)}m_i - k_j^{(i)}m_j$$
$$- T\ln\left[\frac{\cosh\beta h_i^{(j)}\cosh\beta h_j^{(i)}}{\cosh\beta H_i\cosh\beta H_j}\right] - T\ln(\cosh\beta J_{ij})$$
$$- T\ln(1+\tanh\beta h_i^{(j)}\tanh\beta h_j^{(i)}\tanh\beta J_{ij}) \ . \tag{2.12b}$$

In the above we have separated $-T\ln Z_{ij}$ into the one-body parts $f_i^{(1)}$, $f_j^{(1)}$ and the two-body part $f_{ij}^{(2)}$. Finally we get the free energy in the form

$$F = \sum_i f_i^{(1)} + \sum_{(i,j)} f_{ij}^{(2)} \ . \tag{2.13}$$

It is instructive to apply the above method to the infinite-range model, in which every spin couples with each other and the distribution of J_{ij} is given by

$$P(J_{ij}) = \left[\frac{N}{2\pi\tilde{J}^2}\right]^{1/2}\exp\left[\frac{-J_{ij}^2N}{2\tilde{J}^2}\right] \ , \tag{2.14}$$

where N is the number of lattice sites. Equation (2.14) shows that J_{ij} is of the order of $N^{-1/2}$. Using this fact, we expand (2.4) with respect to J_{ij}. Then we have from (2.6) and (2.7)

$$k_i^{(j)} = J_{ij}m_j - \beta J_{ij}^2(1-m_j^2)m_i \ . \tag{2.15}$$

This reproduces TAP's self-consistent equation

$$T\tanh^{-1}m_i = \sum_j J_{ij}m_j - \beta\sum_j J_{ij}^2(1-m_j^2)m_i \ . \tag{2.16}$$

In this case unknown parameters are m_i. Incidentally it is not hard to show that the approximation made in the two-spin cluster theory is generally equivalent to the Bethe approximation, which TAP used; therefore it is quite natural that our method reproduces TAP's result. (See the Appendix for the equivalence between these approximations.) The same expansion yields the free energy in the form

$$F = -\sum_{(i,j)} J_{ij}m_im_j - \tfrac{1}{2}\beta\sum_{(i,j)} J_{ij}^2(1-m_i^2)(1-m_j^2)$$
$$+ T\sum_i[\tfrac{1}{2}(1+m_i)\ln\tfrac{1}{2}(1+m_i)$$
$$+ \tfrac{1}{2}(1-m_i)\ln\tfrac{1}{2}(1-m_i)] \ . \tag{2.17}$$

This is again identical to that considered by TAP. In TAP's work they obtained the free energy (2.17) by the diagrammatical method. Our method gives another way to get (2.17).

It is also interesting to investigate the infinite-range model by using a statistical approximation. That is, we ignore the correlations between $k_i^{(j)}$'s in (2.5) and have

$$\langle (h_i^{(j)})^2 \rangle_{\rm av} = (N-1)\langle (k_i^{(j)})^2 \rangle_{\rm av} \ , \tag{2.18}$$

where

$$\langle A_i^2 \rangle_{\rm av} = \frac{1}{N} \sum A_i^2 \ . \tag{2.19}$$

Since J_{ij} is small we have

$$\langle (k_i^{(j)})^2 \rangle_{\rm av} = \langle (J_{il} \tanh \beta h_l^{(j)})^2 \rangle_{\rm av} \ . \tag{2.20}$$

Using the above and $\langle J_{ij}^2 \rangle_{\rm av} = \tilde{J}^2/N$, one gets

$$\langle (h_i^{(j)})^2 \rangle_{\rm av} = \tilde{J}^2 \langle (\tanh \beta h_l^{(j)})^2 \rangle_{\rm av} \equiv \lambda^2 \ . \tag{2.21}$$

This leads to the self-consistent equation for λ

$$\lambda^2 = \frac{\tilde{J}^2}{(2\pi\lambda^2)^{1/2}} \int dh \exp(-h^2/2\lambda^2) \tanh^2 \beta h \ , \tag{2.22}$$

provided that $h_i^{(j)}$ obeys a Gaussian distribution. Equation (2.22) is essentially the same as that obtained by SK and by Klein *et al.*[9] It is known, however, that (2.22) yields unphysical results, e.g., a negative entropy at low temperatures. This suggests that the correlations between $k_i^{(j)}$'s are important.

III. DISTRIBUTION OF EFFECTIVE FIELD AT $T=0$

Here we study the system at $T=0$. In this case (2.4) and (2.12) are rewritten in the form

$$k_i^{(j)} = \min(|J_{ij}|, |h_j^{(i)}|) \operatorname{sgn}(J_{ij} h_j^{(i)}) \ , \tag{3.1}$$

and

$$f_i^{(1)} = 0 \ ,$$

$$f_{ij}^{(2)} = -|J_{ij}| - 2|h_i^{(j)}| \Theta(-H_i h_i^{(j)}) - 2|h_j^{(i)}| \Theta(-H_j h_j^{(i)}) + 2\min(|J_{ij}|, |h_i^{(j)}|, |h_j^{(i)}|)\, \Theta(-J_{ij} h_i^{(j)} h_j^{(i)}) \ , \tag{3.2}$$

where $\Theta(x)$ is the theta function: $\Theta(x)=1$ for $x>0$ and $\Theta(x)=0$ for $x<0$.

A usual way to study the ground state at $T=0$ is as follows. First we calculate the energy as a function of state $\{S_i\}$. Then we have many local minima where the following condition is satisfied:

$$S_i = \operatorname{sgn}(B_i) \ , \tag{3.3}$$

with

$$B_i = \sum_j J_{ij} S_j \ . \tag{3.4}$$

The ground state is given by the state with the lowest energy. The parameter B_i can be regarded as the effective field acting on site i, since the excitation energy associated with flipping of S_i is given by $2|B_i|$. The distributions of B_i for various models have been investigated both analytically[10,11] and numerically.[6,12–16]

Since we have two effective fields B_i and H_i, it is interesting to compare these fields. First let us consider an ordinary ferromagnetic case, i.e., $J_{ij}=J$. For this case we have $h_i^{(j)} = (z-1)J$ in the ground state (z is the number of nearest-neighbor sites). This brings

$$k_i^{(j)} = J_{ij} \operatorname{sgn}(h_j^{(i)}) \ . \tag{3.5}$$

Equation (3.5) agrees with (3.4) so that we see $B_i = H_i$. For the case of spin-glasses, on the other hand, the situation is different: since $h_j^{(i)}$ is given as the summation of random fields, $|h_j^{(i)}|$ can be less than $|J_{ij}|$. Therefore the effective field due to (3.1) should be different from (3.4).

The difference between those fields is large in the following example. Suppose a one-dimensional system in which J_{ij} is nonzero only for the nearest-neighbor pair and obeys a Gaussian distribution with the width ΔJ. Since every bond is satisfied in the ground state of this particular model, we have

$$|B_i| = |J_{i-1,i}| + |J_{i,i+1}| \ . \tag{3.6}$$

From this one can calculate the distribution function $\tilde{P}_1(B_i)$ as follows:

$$P_1(B_i) = \int dJ_{i-1,i}\, dJ_{i,i+1}\, P'(J_{i-1,i}) P'(J_{i,i+1}) \delta(B_i - |J_{i-1,i}| - |J_{i,i+1}|)$$

$$= \frac{2}{\pi(\Delta J)^2} \exp[-B_i^2/4(\Delta J)^2] \int_0^{B_i} dx \exp[-(x - B_i/2)^2/(\Delta J)^2] \ , \tag{3.7}$$

where $P'(J_{ij})$ is the distribution function of J_{ij}. Next we examine the distribution of H_i. Here we note that the relation $k_i^{(i\pm1)} = h_i^{(i\mp1)}$ holds in this one-dimensional system. In order to solve the two-spin cluster equations self-consistently, we start from the site l where $|J_{l,l+1}|$ is the smallest ($|J_{l,l+1}| \equiv \epsilon$, for simplicity). Then one finds

that $|k_i^{(i-1)}| = \epsilon$ for all i because ϵ propagates the system in such a way that

$$|k_{l+1}^{(l)}| = |J_{l,l+1}| = \epsilon \ ,$$

$$|k_{l+2}^{(l+1)}| = \min(|J_{l+1,l+2}| \ , |k_{l+1}^{(l)}|) = \epsilon \ ,$$

and so on. (We have taken the periodic boundary condition.) Similarly, for the opposite direction, we get $|k_i^{(i+1)}| = \epsilon$ for all i. If we take account of the sign in (3.1) explicitly, we see that there exists a self-consistent solution for the case $\prod J_{i,i+1} > 0$, which gives $|H_i| = 2\epsilon$, while there is no solution for $\prod J_{i,i+1} < 0$. We consider only the relevant case $\prod J_{i,i+1} > 0$. Since the Gaussian distribution is assumed for J_{ij}, ϵ can take an arbitrarily small value. Consequently the distribution of H_i is to be

$$\tilde{P}_2(H_i) = \delta(H_i) \ , \tag{3.8}$$

which is apparently different from (3.7).

In contrast to this, the difference between B_i and H_i is small for the infinite-range model. The numerical results[6,15,16] show that the distribution function of B_i is proportional to B_i for small B_i. Therefore the number of sites where we have $|B_i| < |J_{ij}| \sim O(1/\sqrt{N})$ is given by $N(1/\sqrt{N})^2 \sim O(1)$. This leads to $B_i - H_i \sim O(1/\sqrt{N})$.

The origin of the difference between B_i and H_i is as follows. Recalling that $2|B_i|$ is the excitation energy due to a single-spin flipping, we see that B_i is related with the single-spin problem. On the other hand, since H_i is the result of the two-spin cluster theory, the correlation effect between two spins is included in the calculation of H_i. This explains the difference between B_i and H_i. Using the term Onsager's cavity and reaction fields, Kirkpatrick and Sherrington[15] and independently Cyrot[17] pointed out that the reaction field plays an important role in spin-glasses. Their arguments are essentially the same as ours. The difference between B_i and H_i was noticed also by Klein *et al.*[9]

At first sight one might feel curious about the expression (3.2) because (3.2) looks different from $-J_{ij}S_iS_j$. If we have a self-consistent solution of (2.5) and (3.1), however, we can show that (3.2) is consistent with $-J_{ij}S_iS_j$: with a self-consistent solution $\{k_i^{(j)}\}$ we can rewrite $f_{ij}^{(2)}$ in (3.2) in the form

$$f_{ij}^{(2)} = |J_{ij}| \ \text{ for } \begin{cases} J_{ij}h_i^{(j)}h_j^{(i)} < 0 \\ |J_{ij}| < |h_i^{(j)}|, |h_j^{(i)}| \end{cases}$$

$$= -|J_{ij}| \ \text{ otherwise} \ . \tag{3.9}$$

Equation (3.9) is equivalent to expressing

$$f_{ij}^{(2)} = -J_{ij}\,\mathrm{sgn}(H_i)\,\mathrm{sgn}(H_j) \ . \tag{3.10}$$

This gives the identical energy to that of the spin configuration $\{S_i\} = \{\mathrm{sgn}(H_i)\}$.

In this connection it is worthwhile to examine the relation between B_i and H_i. Let us consider a self-consistent solution $\{k_i^{(j)}\}$ and a spin configuration $\{S_i\} = \{\mathrm{sgn}(H_i)\}$. Using $\{S_i\}$ thus obtained, we calculate B_i. Then it turns out that $\mathrm{sgn}(H_i) = \mathrm{sgn}(B_i)$ and $|B_i| \geq |H_i|$. This can be seen if one notices the following:

$$\text{(i)} \quad J_{ij}S_j = k_i^{(j)} \ \text{ for } \begin{cases} J_{ij}h_i^{(j)}h_j^{(i)} < 0 \\ |J_{ij}| < |h_i^{(j)}|, |h_j^{(i)}| \end{cases} ,$$

$$\text{(ii)} \quad \mathrm{sgn}(H_i) = \mathrm{sgn}(J_{ij}S_j) = -\mathrm{sgn}(k_i^{(j)}) \ \text{ for } \begin{cases} J_{ij}h_i^{(j)}h_j^{(i)} < 0 \\ |h_j^{(i)}| < |J_{ij}|, |h_i^{(j)}| \end{cases} , \tag{3.11}$$

$$\text{(iii)} \quad \mathrm{sgn}(H_i) = \mathrm{sgn}(J_{ij}S_j) = \mathrm{sgn}(k_i^{(j)}) \ \text{ otherwise} \ .$$

IV. NUMERICAL RESULTS

In this section we make numerical calculations. Here we consider exclusively the infinite-range model with $N = 50$. Since $N = 50$ is not sufficiently large, we use the two-spin cluster equations (2.4) and (2.5) without making any expansion.

A. Metastable solutions

In order to solve the two-spin cluster equations we practically employ the following procedures: first we look for the states $\{S_i\}$ which satisfy the conditions (3.3) and (3.4) at $T = 0$; then taking $k_i^{(j)} = J_{ij}S_j$ as the initial state, we do an iterative calculation until all $k_i^{(j)}$ are consistent with each other. (Actually the interactions were terminated if five H_i's change their signs.) With the knowledge of the solution at $T = 0$, the calculation is extended to the case $T \neq 0$.

We have examined 25 systems and obtained the following results: (1) There are at least $300 \sim 500$ solutions of (3.3) and (3.4) for one system. These solutions have been found by the iteration of flipping the spin which unsatisfies (3.3). We have examined 1000 different initial states; about 20 new solutions have been found in the last 100 tries. The lowest-energy state, which we call the ground state, has been found within the first 30 tries. The ground-state energy is $(-0.7077 \pm 0.0244)N\tilde{J}$, which agrees with the previous works.[15,16] (2) For the two-spin cluster equations, on the other hand, 8 ± 4 solutions have been obtained at $T = 0$. Most of them come from the solutions of (3.3) and (3.4) which are found by early tries in the procedure mentioned above; at most two solutions come from the states found in the last 500 tries. (3) There are 9 systems in which the lowest-energy state at $T = 0$ is not a solution of the

two-spin cluster equations. (4) Most of the solutions do not continue to higher temperatures. In 11 systems we have obtained one solution for $T \geq 0.3\tilde{J}$; all of these start from the lowest-energy state at $T=0$. (5) Every solution disappears discontinuously at some temperature.

In Fig. 1 we present the numerical results obtained with three systems. The letters A, B, and C in the figure specify the system. For system A we have smooth temperature dependence of $q(=N^{-1}\sum m_i^2)$, while systems B and C have a discontinuity in q as a function of T; no solution has been obtained in the temperature region between dotted lines. In order to clarify the origin of the discontinuity, we have examined the local minima around the ground state in the energy space. For convenience we introduce symbols E_1 and E_2 to represent the closest and second-closest local minima to the ground state, respectively. After some careful calculations we have found that the number of the different spins between E_1 and the ground state is 2 in A and B, and is 3 in C; as for E_2 the difference from the ground state is four-, three-, four-spin cluster in A, B, C, respectively. The barrier height separating the state E_1 (or E_2) and the ground state has been found to be less than $\tilde{J}$. Since we take

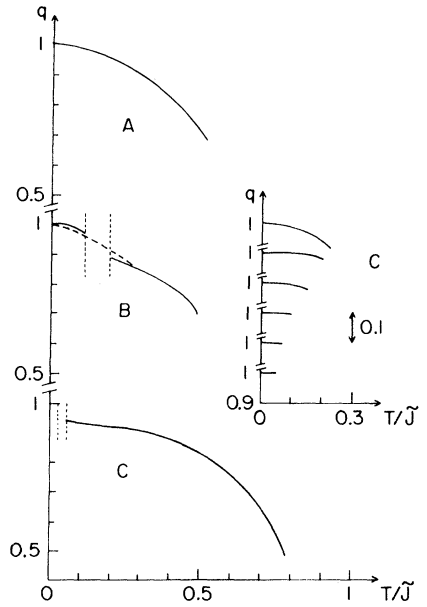

FIG. 1. Temperature dependence of the Edwards-Anderson order parameter $q(=N^{-1}\sum m_i^2)$ calculated from the two-spin cluster equations. Data are calculated for three systems of the infinite-range model with $N=50$. Letters A, B, and C, specify the system. In the temperature region between dotted lines in B and C, the two-spin cluster equations have no solution. A dashed line in B is the result from the mixture of the two- and three-spin cluster equations (see Sec. V for detail). In the inset the other solutions of the two-spin cluster equations in C are drawn.

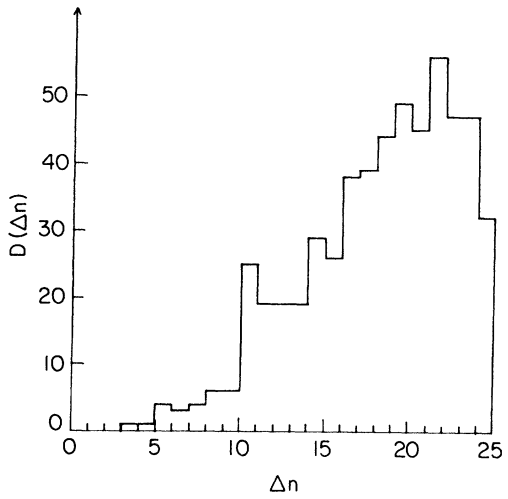

FIG. 2. Distribution $D(\Delta n)$ of the number of different spins Δn between two solutions of the two-spin cluster equations at $T=0$. Data are obtained from 25 systems of the infinite-range model with $N=50$. The largest Δn is $N/2=25$ because of the trivial degeneracy with respect to $S_i \rightarrow -S_i$.

into account the two-spin cluster effect exactly in (2.4) and (2.5), we expect that the irregular temperature dependence of q originates from cluster excitations which consist of more than three spins. In fact taking account of the three-spin cluster effect, we have examined system B and found that the discontinuity in q disappears (see the dashed line in Fig. 1; see also Sec. V for detail). In this connection we have investigated the systems where the solution starting from the lowest-energy state at $T=0$ does not continue over $T=0.3\tilde{J}$. We have confined ourselves to excitations whose energy is less than $\tilde{J}$ and found that E_1 and E_2 are different from the ground state by

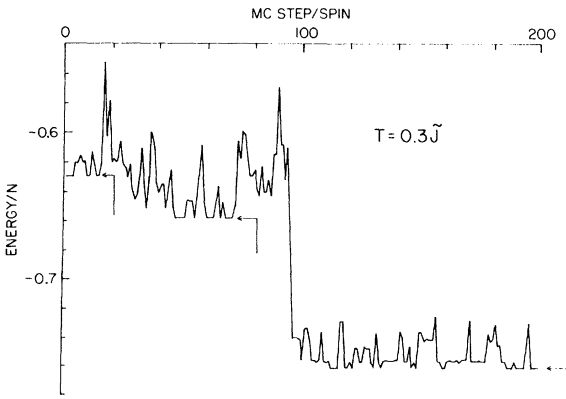

FIG. 3. Energy as a function of time obtained by the Monte Carlo calculation for system C. The states indicated by arrows correspond to the solutions of the two-spin cluster equations.

more than three spins. From these facts we conclude that if we obtain a discontinuity in $q(T)$ or the disappearance of the solution at unusually low temperature, then E_1 and/or E_2 differs from the ground state by more than three spins. (It should be noted that the converse is not always true; see system A for instance.)

Since we have several solutions at low temperatures (see the inset of Fig. 1), let us examine these solutions in detail. Figure 2 shows the distribution of the difference of spins between two solutions (for 25 systems). The figure indicates that they are separated with each other by a many-spin cluster. This means that the solutions are located at the bottom of deep valleys in the energy space. This agrees with the stable states in the usual sense. To demonstrate the stability of the solutions, we have done a Monte Carlo calculation. Figure 3 is the result, where the energy as a function of time is shown. There are three stable states in Fig. 3 (see arrows); we have found that these states are the solutions of the two-spin cluster equations.

B. Hessian matrix $\partial^2 F/\partial m_i \partial m_j$

The next task is to examine the matrix $A_{ij}=\partial^2 F/\partial m_i \partial m_j$. From (2.12) and (2.13) we have

$$A_{ij}=\begin{cases}\dfrac{T}{1-m_i^2}\left[1+\displaystyle\sum_k \dfrac{t^2(J_{ik})[1-t^2(h_k^{(i)})][1-t^2(h_i^{(k)})]}{[1-t^2(J_{ik})][1-t^2(h_k^{(i)})t^2(h_i^{(k)})t^2(J_{ik})]}\right] & \text{for } i=j \\ -\dfrac{t(J_{ij})[1+t(h_i^{(j)})t(h_j^{(i)})t(J_{ij})]}{[1-t^2(J_{ij})][1-t(h_i^{(j)})t(h_j^{(i)})t(J_{ij})]} & \text{for } i\neq j\ ,\end{cases} \tag{4.1}$$

where $t(x)=\tanh\beta x$. Putting the solution $\{k_i^{(j)}\}$ into (4.1), we diagonalize A_{ij} and then calculate a quantity V defined by

$$V=\left(\sum_i u_i^4\right)^{-1}\ , \tag{4.2}$$

in which u_i is the ith component of the normalized eigenvector $\vec{u}$ of the lowest mode of A_{ij}. One sees that the value of V is roughly equal to the number of nonvanishing components of $\vec{u}$.

In Fig. 4 we present the behavior of V as a function of T and several low eigenvalues of A_{ij} (system C). The solid line, which represents V, indicates that

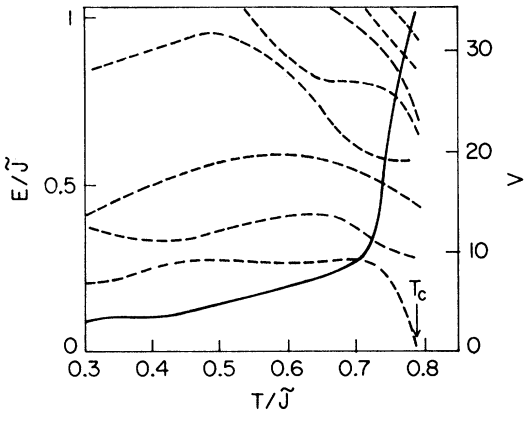

FIG. 4. Eigenvalues of the matrix $\partial F^2/\partial m_i \partial m_j$ (dashed line) and V (solid line) vs temperature for system C. The critical temperature T_c is given by the temperature at which the lowest eigenvalue vanishes.

$\vec{u}$ is described by cluster excitations consisting of a small number of spins at low temperatures, while many-spin cluster excitations dominate $\vec{u}$ in the vicinity of T_c. If we use the terms "localized" and "extended," we can say that the lowest mode is localized at low temperatures and extended near T_c. The character of the localized mode has been found to be a mixture of three- and four-spin cluster excitations; the nonvanishing components of $\vec{u}$ are located at the same sites as we specify the local minimum states E_1 and E_2. In this sense $\vec{u}$ at low temperatures reflects the local structure around the ground state in the energy space. As for $T\lesssim T_c$, $\vec{u}$ is related with the state vector $\vec{m}=(m_1,m_2,\ldots,m_N)$, because $\vec{u}$ is almost parallel to $\vec{m}$ (e.g., $\vec{u}\cdot\vec{m}/|\vec{m}|\sim 0.84$ for system C). The critical temperature T_c is given by the temperature at which the eigenvalue of $\vec{u}$ vanishes. We have examined the other two systems A and B and obtained qualitatively the same results.

Since the result mentioned above has been obtained in the systems $N=50$, we need to extend our consideration to the large N limit in order to see whether the above result is correct for the infinite-range model. In this limit the matrix A_{ij} has the form

$$A_{ij}=\left[\beta\sum_k J_{ik}^2(1-m_k^2)+\frac{T}{1-m_i^2}\right]\delta_{ij} -J_{ij}-2\beta J_{ij}^2 m_i m_j\ . \tag{4.3}$$

At $T=T_c=\tilde{J}$ we see that $A_{ij}=-J_{ij}+2\tilde{J}\delta_{ij}$, and therefore $\vec{u}\propto\vec{M}$, where $\vec{M}=(M_1,M_2,\ldots,M_N)$ is the

eigenvector belonging to the largest eigenvalue of the matrix J_{ij}. Since M_i is a Gaussian variable,[6] $\vec{u}$ is extended. This indicates that the numerical results near T_c are reliable. To examine the low-temperature region, we calculate the distribution function of the diagonal elements of A_{ij} as follows:

$$W(y) = \int dH_i\, \rho(H_i,T) \times \delta(y - T\cosh^2\beta H_i - \beta\tilde{J}^2(1-q)) \cong \tfrac{1}{2}\rho(0,T)[T/(y-y_0)]^{1/2} \quad \text{for } y \gtrsim y_0 \ , \tag{4.4}$$

where $\rho(H_i,T)$ is the temperature-dependent distribution function of the effective field H_i and $y_0 = \beta\tilde{J}^2(1-q) + T$. Following TAP's speculation, on the other hand, we consider that the lowest eigenvalue of A_{ij} is zero. This requires that the mixing effect due to the off-diagonal element broadens the sharp peak in $W(y)$ around y_0 so that the levels existing in the region $y_0 < y < cy_0$ [c is a constant of $O(1)$] contribute to the lowest mode. Therefore, roughly speaking, the number of nonvanishing components of $\vec{u}$ is given by

$$N\int_{y_0}^{cy_0} W(y)\, dy \sim \frac{NT^2}{\tilde{J}^2} \ , \tag{4.5}$$

in which we have used $y_0 \propto T$ (see Ref. 6) and assumed $\rho(0,T) \propto T/\tilde{J}^2$. Equation (4.5) shows that the lowest mode is extended as far as we consider $T > \tilde{J}/\sqrt{N}$.

In this way we have seen that $\vec{u}$ of the infinite-range model is extended for $T \leqq T_c$ except at unusually low temperature. This means that the localized eigenvector $\vec{u}$ in the system $N = 50$ comes from the size effect. However, the picture obtained by the numerical result is still applicable to a model with finite-range interaction: using a two-dimensional Ising model with the Gaussian random nearest-neighbor interaction, Dasgupta *et al.*[18] calculated the distribution of barrier height between the ground state and the local minima. Their result shows that the distribution of barrier height has a maximum around $n\Delta J$, where n is the number of different spins between the local minimum and the ground state, and ΔJ is the width of the distribution of J_{ij}. Although their calculation was made only for $n = 2, 3$ in the two-dimensional case, this suggests that the characteristic magnitude for the barrier height concerned with n-spin cluster is given by $n\Delta J$ in general, i.e., for general dimensions as well as general n. On the other hand the Monte Carlo data[13] indicate that the critical temperature is given by $T_c \sim \Delta J$ (for two $\sim$ six dimensions). Therefore if we consider a temperature which is low compared with T_c, we have cluster excitations consisting of a small number of spins besides single-spin excitations; this implies that the lowest mode of A_{ij} is localized at low temperatures. As for the region $T \lesssim T_c$ we refer to Anderson's argument[19]; that is, the necessary condition for a sharp transition is that the eigenvector belonging to zero eigenvalue of A_{ij} is extended at $T = T_c$. The above results are what we have obtained by our numerical calculation.

V. THREE-SPIN CLUSTER THEORY

The three-spin cluster theory is just the extension of the two-spin cluster theory. In the same way as we formulate the two-spin cluster theory, we take out a three-spin cluster of sites i,j,k and have the local Hamiltonian[8]

$$\mathcal{H}_{ijk} = -J_{ij}S_iS_j - J_{jk}S_jS_k - J_{ki}S_kS_i - h_i^{(jk)}S_i - h_j^{(ki)}S_j - h_k^{(ij)}S_k \ , \tag{5.1}$$

where $h_i^{(jk)}$ is the effective field acting on site i. With this Hamiltonian we calculate the mean value for S_i and obtain

$$m_i = \tanh[\beta(h_i^{(jk)} + r_i^{(jk)})] \ , \tag{5.2}$$

where

$$\beta r_i^{(jk)} = \tanh^{-1}[t(J_{ij})t(h_j^{(ki)})] + \tanh^{-1}[t(J_{ik})t(h_k^{(ij)})] + \tfrac{1}{2}\ln\left[\frac{1+t(J_{ij}+h_j^{(ki)})t(J_{ik}+h_k^{(ij)})t(J_{jk})}{1+t(J_{ij}-h_j^{(ki)})t(J_{ik}-h_k^{(ij)})t(J_{jk})}\right] \ , \tag{5.3}$$

with $t(x) = \tanh(\beta x)$. Since $r_i^{(jk)}$ includes the effect of two-spin cluster, we extract the field $k_i^{(jk)}$ due to the three-spin cluster by the formula

$$k_i^{(jk)} = r_i^{(jk)} - k_i^{(j)} - k_i^{(k)} \ , \tag{5.4}$$

where $k_k^{(j)}$ is given by (2.4). Introducing the effective field on site i

$$H_i = \sum_i k_i^{(j)} + \sum_{(j,k)} k_i^{(jk)} \ , \tag{5.5}$$

we obtain

$$h_i^{(j)} = H_i - k_i^{(j)} \ , \qquad h_i^{(jk)} = H_i - r_i^{(jk)} \ . \tag{5.6}$$

Equations (5.4)–(5.6) together with (2.4) are the self-consistent equations which determine $\{k_i^{(j)}\}$ and $\{k_i^{(jk)}\}$. We call them the three-spin cluster equations in the following.

Now let us solve the three-spin cluster equations numerically. Again we consider the infinite-range model; here we take $N=16$. In order to demonstrate how the three-spin cluster theory works, we choose the system in which the difference between the state E_1 (see Sec. IV A) and the ground state is a three-spin cluster. Using the same procedure as mentioned in Sec. IV A, we solve the three-spin cluster equations numerically.[20] The result is shown in Fig. 5, in which the solution of the three-spin cluster equations is drawn by a solid line. For comparison we have plotted the solution of the two-spin cluster equations (dashed line) and the solution of the ordinary mean-field equation $m_i=\tanh(\beta\sum J_{ij}m_j)$ (dotted line). The solid line in Fig. 5 shows a sharp drop in q around $T\sim 0.15\tilde{J}$ and takes a nearly constant value $q\sim 0.8$ for $0.3\tilde{J}\lesssim T\lesssim 0.6\tilde{J}$. This means that the state E_1 begins to be thermally excited around $T\sim 0.15\tilde{J}$ and is almost completely excited for $T>0.3\tilde{J}$; notice $(16-3)/16\sim 0.8$, which agrees with the value for q for $0.3\tilde{J}\lesssim T\lesssim 0.6\tilde{J}$. The difference between the solid and dashed lines is large around $T\sim 0.15\tilde{J}$. This implies that the three-spin cluster theory is vital for the temperature region where the state E_1 begins to be excited. Open circles show the solution of the mixture of the two- and three-spin cluster equations in which we take account of the three-spin cluster effect only for the relevant three-spin cluster and apply the two-spin cluster theory to the other spins. From the figure one realizes that this treatment is practically sufficient to consider the three-spin cluster excitation. The dashed line for system B in Fig. 1 has been calculated by this method.

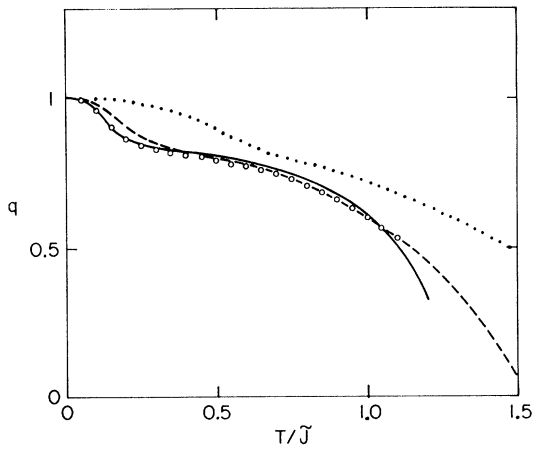

FIG. 5. Temperature dependence of the Edwards-Anderson order parameter $q(=N^{-1}\sum m_i^2)$ calculated by the following equations: the three-spin cluster equations (solid line), the two-spin cluster equations (dashed line), the ordinary mean-field equation (dotted line), and the mixture of the two- and three-spin cluster equations (open circles). Calculation is made for a system of the infinite-range model with $N=16$.

As for the dashed line in Fig. 5, it vanishes around $T\sim 1.55\tilde{J}$. This high critical temperature is due to the large fluctuation of J_{ij}. This kind of fluctuation is small for large N; we have not obtained such a result for $N=50$.

In the large-N limit, the three-spin cluster equations are written in the form

$$T\tanh^{-1}m_i=\sum_i J_{ij}m_j-\sum_j J_{ij}^2\chi_j m_i-\sum_{(j,k)}J_{ij}J_{jk}J_{ki}\chi_j\chi_k m_i\ , \tag{5.7}$$

where $\chi_i=\beta(1-m_i^2)$. One sees that the last term in (5.7) comes from the three-spin cluster effect and it is order of $N^{-1/2}$. This indicates that the effect of the three-spin cluster gives no contribution in the $N\to\infty$ limit. This may be understood by the following arguments. We first consider an energy barrier separating the ground state and the local minimum which differs from the ground state by an n-spin cluster, and then we introduce a parameter R_n to represent the barrier height measured from the ground state. Next we recall that the three-spin cluster theory plays an important role for the temperature region $T\sim O(R_{n=3})$; e.g., $R_3\sim 0.6\tilde{J}$ for the case of Fig. 5. This explains the unimportance of the three-spin cluster effect in the large-N limit because we see $R_3\sim O(\tilde{J}/\sqrt{N})$ and we have used $\tilde{J}/\sqrt{N}\ll T$ to obtain (5.7).

VI. SUMMARY

In this paper we have formulated the two- and three-spin cluster theory and applied it to the spin-glass problem.

(1) At $T=0$ we have shown that the effective field calculated by the two-spin cluster theory is different from the result obtained by the formula $B_i=\sum_j J_{ij}S_j$, in which no cluster effect is considered. This presents a striking contrast to ordinary ferromagnets, where these results are the same at $T=0$.

(2) The numerical calculation has been made for the infinite-range model with $N=16$ and 50. At $T=0$ we have obtained several solutions of the two-spin cluster equations. These solutions are located at the bottom of deep valleys in the energy space, implying that the solutions are stable. This result is remarkably different from that of the ordinary mean-field equation, where we have a large number of solutions, but most of them are not so stable. For finite temperatures we have examined the relationship between the local energy structure around the ground state and the existence of well behaved solutions. It has been shown that the irregular temperature dependence of the solution originates from the presence of the local minima which differ from the ground state by more than three spins. We have diagonalized the matrix $\partial^2F/\partial m_i\partial m_j$ and found that the

lowest mode is localized at low temperatures, while it is extended near T_c. Although this is the consequence of the finite size in the case of the infinite-range model, this picture is applicable to a model with finite-range interaction. We have also shown that the three-spin cluster theory is vital for the temperature region where the thermal agitation begins to excite local minima which are different from the ground state by a three-spin cluster.

ACKNOWLEDGMENTS

The author would like to express his sincere thanks to W. L. McMillan for helpful discussions and for suggesting the basic idea of this work. Y. A. Ono and M. Ma read and criticized the manuscript, which the author appreciates. This research was supported by NSF-MRL Grant No. DMR-77-23999 and in part by Yamada Science Foundation.

APPENDIX

Here we show that the approximation made in the two-spin cluster theory is equivalent to the Bethe approximation. In the Bethe approximation we consider a cluster in which we have a central site 0 and all its neighbors i; we assume mean fields h_i on sites i. Then we start from

$$\mathcal{H} = -\sum_i J_{0i} S_0 S_i - \sum_i S_i h_i \quad . \tag{A1}$$

The mean value for S_0 is given by

$$m_0 = \tanh\left(\sum_i \tanh^{-1}(\tanh\beta J_{0i} \tanh\beta h_i)\right) \quad . \tag{A2}$$

To obtain m_1 (i.e., the mean value for $S_{i=1}$), we calculate

$$\frac{Z_+}{Z_-} = \exp(2\beta h_1)\left(\frac{\exp(\beta J_{01} + 2Y) + \exp(-\beta J_{01})}{\exp(-\beta J_{01} + 2Y) + \exp(\beta J_{01})}\right) , \tag{A3}$$

where $Z_\pm$ is the partition function for $S_1 = \pm 1$, and $Y = \sum_{i \neq 1} \tanh^{-1}(\tanh\beta J_{0i} \tanh\beta h_i)$. Then it is easy to arrive at

$$m_1 = \tanh[\beta h_1 + \tanh^{-1}(\tanh\beta J_{01} \tanh Y)] \quad . \tag{A4}$$

Equations (A2) and (A4) agree with (2.4) and (2.5) in the text.

---

*On leave of absence from the Institute for Solid State Physics, University of Tokyo, Tokyo, Japan.

[1]For recent review on the theory of spin-glasses, see for example, A. Blandin, J. Phys. (Paris) 39, C6-1499 (1978).

[2]For recent review on the experimental work on spin-glasses, see for example, J. A. Mydosh, J. Magn. Magn. Mater. 7, 237 (1978).

[3]See for example, A. Narath, in *Magnetism*, edited by H. Suhl (Academic, New York, 1973), Vol. V.

[4]S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).

[5]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 35, 1792 (1975).

[6]D. J. Thouless, P. W. Anderson, and P. G. Palmer, Philos. Mag. 35, 593 (1977).

[7]G. Parisi, Phys. Lett. A73, 203 (1979); Phys. Rev. Lett. 43, 1754 (1979).

[8]Although our method has been developed independently, the same treatment was made several decades ago: see T. Oguchi, Prog. Theor. Phys. (Kyoto) 13, 148 (1955); P. W. Kasteleijn and J. Van Kranendonk, Physica (Utrecht) 22, 317 (1956); R. Kikuchi, Phys. Rev. 81, 988 (1951).

[9]M. W. Klein, L. J. Schowalter, and P. Shukla, Phys. Rev. B 19, 1492 (1979).

[10]M. W. Klein, Phys. Rev. B 14, 5008 (1976).

[11]C. Held and M. W. Klein, Phys. Rev. Lett. 35, 1783 (1975).

[12]K. Binder, Z. Phys. B 26, 339 (1977).

[13]D. Stauffer and K. Binder, Z. Phys. B 34, 97 (1979).

[14]L. R. Walker and R. E. Walstedt, Phys. Rev. Lett. 38, 514 (1977).

[15]S. Kirkpatrick and D. Sherrington, Phys. Rev. B 17, 4384 (1978).

[16]R. G. Palmer and C. M. Pond, J. Phys. F 9, 1451 (1979).

[17]M. Cyrot, Phys. Rev. Lett. 43, 173 (1979).

[18]C. Dasgupta, S. -k. Ma, and C. -K. Hu, Phys. Rev. B 20, 3837 (1979).

[19]P. W. Anderson, in *Ill-Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, Amsterdam, 1979).

[20]For $N = 16$ it is easy to determine the ground state by inspecting all configuration of the spins. The ground state thus obtained is found to coincide with that determined by the method mentioned in Sec. IV.