PHYSICAL REVIEW B VOLUME 19, NUMBER 5 1 MARCH 1979

Excitations in spin-glasses

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(Received 22 May 1978)

Starting from a ground state in which the spins have been frozen in random configurations we have analyzed the equations of motion for single-spin deviation excitations. The equations of motion involve two amplitudes at each site, just like an antiferromagnet. Making simple statistical assumptions about spin orientations in the ground state, we have analyzed the localization characteristics of these excitations. For a spin-glass model with short-ranged interactions, an explicit form of the localization function is derived. The local densities of states for spin deviation excitations have been calculated using a continued-fraction method for two models, namely (i) a small concentration of spins distributed randomly on a fcc lattice and interacting via a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, (ii) spins on each lattice site but interacting via a random exchange integral having a Gaussian distribution. In each case we find a finite density of states at zero energy, and thus explain the low-temperature behavior of the specific heat. For the RKKY model, the density of states at zero energy is found to increase with decreasing concentration, and thus we are able to show the approximate concentration independence of the linear term of the specific heat. Our density-of-states curves agree fairly with those obtained in Monte Carlo calculations on finite numbers of spins.

I. INTRODUCTION

This paper is concerned with developing a theoretical understanding of the low-temperature properties of dilute magnetic alloys which exhibit the so-scalled spin-glass behavior.[1] Among the low-temperature properties, the most striking one is the presence of a large contribution to the specific heat which is linearly proportional to the temperature and nearly independent of the concentration of the magnetic impurity.[2] The other low-temperature properties worth mentioning are (i) the low-temperature resistivity goes as $T^{3/2}$ in a large number of spin-glasses[3] and (ii) the recent measurements of neutron scattering cross sections show the possible existence of spin-wave-like excitations.[4]

A theoretical explanation for the specific-heat behavior was provided by Marshall[5] as long ago as 1960. Marshall's theory is based on the following two assumptions: (i) the spins on magnetic impurities interact according to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction; (ii) the spins may be treated as Ising spins. Marshall treated the problem within the molecular-field approximation. Since the magnetic impurities are randomly distributed, and interact via a long-range interaction, each impurity experiences a different molecular field given by

$$h_i = \sum_j J(R_{ij})\langle S_j\rangle . \tag{1.1}$$

Marshall, and later with greater refinement, Klein and Brout[6] and Klein[7] showed that the probability distribution of the molecular field $P(h)$ should be a cutoff Lorentzian, whose width Δ is proportional to the concentration of impurities. The two factors, i.e., (i) $P(0)$ finite and (ii) $P(0)$ proportional to the concentration, are sufficient to explain the specific-heat behavior.

A major criticism against Marshall's theory and its developments, which has also been a point of much confusion in the recent literature,[8] is the use of the Ising model for the spins. The actual spins are vectors and hence the random molecular field should also be a vectorial quantity. Anderson[9] by a simple phase-space argument, showed that for a vector $\vec{h}$, the probability of finding a given magnitude of h falls like h^2 as $h \to 0$. This makes the leading contribution to the specific heat proportional to T^3. Some authors[8] have argued that below the spin-freezing temperature, the distribution relevant for thermodynamic properties is the one-dimensional projection of the vector molecular field, in the direction in which the spin has frozen. This argument seems untenable to us because the field at site i, within the molecular-field approximation, is independent of site i, i.e.,

$$\vec{h}_i = \sum_{(j \neq i)} J_{ij}\vec{S}_j .$$

The confusion arises owing to the fact that the probability distribution of $|\vec{h}_i|$ and that of $\vec{h}_i \cdot \vec{e}_z(i)$ are quite different, and for the molecular-field argument it is the former distribution which is relevant.

Another difficulty of Marshall's theory is that the spin-hopping terms are completely ignored.[9]

It is well known that the molecular-field theory is wrong for the low-temperature properties of ferromagnets and antiferromagnets owing to the presence of spin-wave excitations. Clearly the spin-hopping terms which are responsible for spin waves would be of importance in determining the spectrum of the lowest-energy excitations in spin-glasses also. The purpose of the present paper is to determine the nature and density of states of such excitations.

Recently, Walker and Walstedt[10] have calculated by the Monte Carlo method the density of states of spin-flip excitations in a system of a finite number of spins ($N=96$) interacting via the RKKY interaction. They find that the density of states for such excitation is finite at zero energy and thus explain the specific-heat behavior in a far more convincing manner.

To determine the low-energy excitation spectrum, the first requisite is the knowledge of the ground-state wave function. The determination of the ground state of spin-glasses which are characterized by competing and random positive and negative exchange interactions is a well nigh impossible task. So a detailed calculation of the excitation spectrum is out of the question. However, questions like localization characteristics of excitations, averaged single-site density of states, etc., are amenable to treatment, as these involve only statistical properties of certain parameters of the ground state. The statistical properties of the ground state like the probability distribution of the local field, the average angle between two spins, etc., can be obtained by making simple assumptions. In treating coupled-spin systems in which all exchange interactions are not positive, one usually considers spin excitations from the classical ground state and works out the zero-point motion about the classical state from the spin-wave spectrum. In three dimensions the zero-point motion turns out to be small. The theory here is developed on the same assumptions.

The paper is organized as follows. In Sec. II, starting from a ground-state configuration in which various spins are frozen, in various directions, we derive equations of motion for spin-deviation excitations. These equations are analogous to those obtained for an antiferromagnet and thus require two amplitudes to be specified at each site. In Sec. III, we present a localization theory for such excitations which is a generalization of the arguments put forth by Anderson[11] and Economou and Cohen.[12] An explicit form of the localization function is derived for short-ranged exchange and some qualitative discussion is given for the RKKY interaction. In Sec. IV, we describe the method for calculating the local density of states by the continued-fraction method, as developed by Haydock *et al.*[13] A new procedure of self-consistent termination of the continued-fraction expansion is employed. The calculations are made for two models: (i) impurity spins coupled by the RKKY interaction and (ii) spins coupled by a short-ranged random exchange. The numerical results on density of states and specific heat are presented in Secs. V and VI. Our conclusions and the summary of the results are presented in Sec. VII.

II. EQUATIONS OF MOTION

The system is taken to be a set of exchange-coupled spins $\vec{S}_i$. The Hamiltonian is given as

$$H=-\tfrac{1}{2}\sum_{i\neq j} J(R_{ij})\vec{S}_i\cdot\vec{S}_j\ . \qquad (2.1)$$

The exchange interactions $J(R_{ij})$ is taken to be random. The specific models of randomness of $J(R_{ij})$ are discussed in later sections. The equation of motion for a given spin is

$$\frac{d}{dt}\vec{S}_i=\sum_{j=i} J(R_{ij})\vec{S}_i\times\vec{S}_j\ . \qquad (2.2)$$

Since we are interested in small deviations from the ground state, at each site we associate a set of three mutually orthogonal right-handed sets of vectors $\vec{e}_x(i)$, $\vec{e}_y(i)$, and $\vec{e}_z(i)$.[14] The vector $\vec{e}_z(i)$ is taken to be along the direction in which the spin $\vec{S}_i$ lies in the classical ground state. The zero-point motion about this state can be considered in the same manner as for an antiferromagnet. It is anticipated to be small in three dimensions.[15] Writing $\vec{S}_i=S\vec{e}_z(i)+\delta\vec{S}_i$, we can get a linearized equation for $\delta\vec{S}_i$. These equations are best expressed in terms of the usual boson operators

$$a_j=\frac{1}{\sqrt{2S}}\,(S_j^x+iS_j^y),\quad a_j^\dagger=\frac{1}{\sqrt{2S}}\,(S_j^x-iS_j^y)\ . \qquad (2.3)$$

Using Eq. (22), one finds the following equations for the a_j's:

$$i\frac{d}{dt}a_i=h_i a_i+\sum_{(j\neq i)}(A_{ij}a_j+B_{ij}a_j^\dagger)\ , \qquad (2.4a)$$

$$-i\frac{d}{dt}a_i^\dagger=h_i a_i^\dagger+\sum_{j(\neq i)}(A_{ij}^* a_j^\dagger+B_{ij}^* a_j)\ , \qquad (2.4b)$$

where

$$h_i=S\sum_j J(R_{ij})\vec{e}_z(i)\cdot\vec{e}_z(j)\ , \qquad (2.5)$$

$$A_{ij}=A_{ji}^*=-SJ(R_{ij})\vec{e}_+(i)\cdot\vec{e}_-(j)\ , \qquad (2.6)$$

$$B_{ij}=B_{ji}=-SJ(R_{ij})\vec{e}_+(i)\cdot\vec{e}_+(j) \qquad (2.7)$$

with

$$\vec{e}_\pm(j)=\vec{e}_x(j)\pm i\vec{e}_y(j)\ . \qquad (2.8)$$

h_i denotes the magnitude of the zero-temperature molecular field at site i due to all other spins. This follows because the direction of the spin at site i is along the direction of the molecular field, and the molecular field is given by

$$\vec{h}_i = S\sum_j J(R_{ij})\vec{e}_z(j)\,. \tag{2.9}$$

Below we shall impose explicit expressions for quantities h_i, A_{ij}, and B_{ij} which may be given in terms of angular coordinates of the spin at site i, referred to a fixed-coordinate system. These are

$$h_i = S\sum_{j(\neq i)} J(R_{ij})[\cos\theta_i\cos\theta_j + \sin\theta_i\sin\theta_j \times \cos(\phi_i - \phi_j)]\,, \tag{2.10}$$

$$A_{ij} = -\tfrac{1}{2}SJ(R_{ij})[(1+\cos\theta_i\cos\theta_j)\cos(\phi_i - \phi_j) + \sin\theta_i\sin\theta_j + i\sin(\phi_i - \phi_j) \times(\cos\theta_i + \cos\theta_j)]\,, \tag{2.11}$$

$$B_{ij} = -\tfrac{1}{2}SJ(R_{ij})[(1-\cos\theta_i\cos\theta_j)\cos(\phi_i - \phi_j) - \sin\theta_i\sin\theta_j + i\sin(\phi_i - \phi_j) \times(\cos\theta_i - \cos\theta_j)]\,. \tag{2.12}$$

The above equations show the detailed dependence of the coefficients occurring in equations of motion in the ground-state configuration. The task of determining the ground-state configuration for a given configuration of $J(R_{ij})$ is extremely difficult and perhaps fruitless, as finally one is interested only in certain statistical properties.

In order to consider questions of localization and density of states for spin excitations, the language of Green's functions is most appropriate. Accordingly, we define the following Green's functions:

$$G_{ij}^{aa} = -i\Theta(t)\langle 0|[a_i(t), a_j^\dagger(0)]|0\rangle\,, \tag{2.13a}$$

$$G_{ij}^{ba} = -i\Theta(t)\langle 0|[a_i^\dagger(t), a_j^\dagger(0)]|0\rangle\,, \tag{2.13b}$$

$$G_{ij}^{ab} = -i\Theta(t)\langle 0|[a_i(t), a_j(0)]|0\rangle\,, \tag{2.13c}$$

$$G_{ij}^{bb} = -i\Theta(t)\langle 0|[a_i^\dagger(t), a_j(0)]|0\rangle\,. \tag{2.13d}$$

The equations of motions for the frequency-transformed Green's functions may be written

$$\sum_l \begin{vmatrix} (E-h_i)\delta_{il} - A_{il} & -B_{il} \\ -B_{il}^* & -(E+h_i)\delta_{il} - A_{il}^* \end{vmatrix} \times \begin{vmatrix} G_{lj}^{aa}(E) & G_{lj}^{ab}(E) \\ G_{lj}^{ba}(E) & G_{lj}^{bb}(E) \end{vmatrix} = \delta_{ij}\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}\,, \tag{2.14}$$

where

$$G_{ij}^{ss'}(E) = \int_{-\infty}^{\infty} e^{iEt}G_{ij}^{ss'}(t)dt\,. \tag{2.15}$$

III. LOCALIZATION

The question of the localization of the excitations in disordered solids has received a tremendous amount of attention. But in all this work, only those excitations have been considered whose wave functions can be represented by a single complex amplitude at each site. For excitations in spin-glasses, we require the specification of two complex amplitudes at each site to describe the wave function. To consider the localization of such excitations, the presently available theory has to be extended.

Using a matrix notation for Green's functions, we may write a locator expansion as follows:

$$\underline{G}_{ij}(E) = \underline{g}_i(E)\delta_{ij} + \sum_l \underline{g}_i\underline{V}_{il}\underline{G}_{lj}\,, \tag{3.1}$$

where

$$\underline{g}_i(E) = \begin{vmatrix} (E-h_i)^{-1} & 0 \\ 0 & -(E+h_i)^{-1} \end{vmatrix} \tag{3.2}$$

and

$$\underline{V}_{ij} = \begin{vmatrix} A_{ij} & B_{ij} \\ B_{ij} & A_{ij} \end{vmatrix}\,. \tag{3.3}$$

With the help of Eq. (3.1) we define the local self-energy matrix $\underline{\Delta}_i$ as follows:

$$\begin{aligned}\underline{G}_{ii} &= \underline{g}_i + \underline{g}_i\underline{\Delta}_i\underline{g}_i + \underline{g}_i\underline{\Delta}_i\underline{g}_i\underline{\Delta}_i\underline{g}_i + \cdots \\ &= (1-\underline{g}_i\underline{\Delta}_i)^{-1}\underline{g}_i\,.\end{aligned} \tag{3.4}$$

The expression for $\underline{\Delta}_i$ follows from Eqs. (3.1) and (3.4):

$$\underline{\Delta}_i = \sum_{k(\neq i)} \underline{V}_{ik}\underline{g}_k\underline{V}_{ki} + \sum_{k,l(\neq i)} \underline{V}_{ik}\underline{g}_k\underline{V}_{kl}\underline{g}_l\underline{V}_{li} + \cdots \tag{3.5}$$

It is helpful to record some of these equations more explicitly, e.g.,

$$G_{ii}^{aa} = 1/(E - h_i - \Sigma_i^a) \tag{3.6}$$

with

$$\Sigma_i^a = \Delta_i^{aa} - \Delta_i^{ab}\Delta_i^{ba}/(E + h_i + \Delta_i^{bb})\,. \tag{3.7}$$

Similar expressions can be written for other components of Green's functions.

The problem of localization of spin excitation may now be formulated as follows. At time $t=0$, we create a spin excitation at site i, so that the initial wave function is

$$|\Psi(0)\rangle = a_i^\dagger|0\rangle\,. \tag{3.8}$$

At a later time t, the wave function will be of the form

$$|\Psi(t)\rangle = \sum_j [u_j(t)a_j^\dagger + v_j(t)a_j]|0\rangle . \tag{3.9}$$

The excitation will be localized if

$$p = |u_i(\infty)|^2 + |v_i(\infty)|^2 \neq 0 . \tag{3.10}$$

The quantity p may be written in terms of the Green's function as

$$\begin{aligned} p &= \lim_{s\to 0} \frac{s}{\pi} \int dE\,[G_{ii}^{aa}(E+is)G_{ii}^{aa}(E-is) \\ &\qquad + G_{ii}^{ba}(E+is)G_{ii}^{ba}(E-is)] \\ &= \int f(E)\,dE . \end{aligned} \tag{3.11}$$

The eigenstate at energy E is localized if $f(E)\neq 0$ and extended if $f(E)=0$. Following the development presented by Economou and Cohen,[12] the question of localization may now be related to the analytical properties of self-energies $\Delta_i^{\mu\nu}$ $(\mu,\nu = a,b)$. It should be noted that only two of the self-energies are independent. It is easily verified that

$$\Delta_i^{bb}(E) = [\Delta_i^{aa}(-E)]^*, \quad \Delta_i^{ab}(E) = [\Delta_i^{ba}(-E)]^* . \tag{3.12}$$

Further, from Eqs. (3.7) and (3.11) it is seen that in the energy region where the states are extended, either one or both of the independent self-energies (Δ_i^{aa} and Δ_i^{ab}) should have branch cuts. On the other hand, in the region where the states are localized, each of the $\Delta_i^{\mu\nu}$ should be analytic and it should be possible to have for each $\Delta_i^{\mu\nu}$ a convergent renormalized perturbation expansion.

The convergence of the perturbation expansion is considered by examining the behavior of higher-order terms. The terms in the respective series for Δ_i^{aa} and Δ_i^{bb} differ by only one factor, so it is expected that the two series will have same convergence properties. Thus we conclude that it is sufficient to examine the renormalized perturbation series for Δ_i^{aa} alone, which may be written

$$\Delta_i^{aa} = \sum_{L=1}^{\infty} T_L \tag{3.13}$$

and

$$T_L = \sum_{j=1}^{(2K)^L} X_j^L . \tag{3.14}$$

The sum j runs over all possible self-avoiding walks of length L. For large L, the number of such terms is $(2K)^L$, where K is the connectivity constant of the lattice. This is so because each of the K^L self-avoiding walks can be traversed in 2^L ways, corresponding to two possible hops (A hop or B hop) at each site. A typical term X_j^L has the following appearance:

$$\begin{aligned} X_j^L = {} & A_{0i}G_i^{a,0}B_{ij}G_j^{b,0,i} \\ & \times B_{jk}\,G_k^{a,0,i,j}\cdots G_m^{a,0,i,j}\cdots A_{m0} . \end{aligned} \tag{3.15}$$

Our next task is to find the probability distribution of X_j^L, which is a complicated exercise, as here, besides the well-known difficulties of the Anderson model, we have some additional complications: (i) the hopping integrals A_{ij} and B_{ij} are random and are correlated to the $\boldsymbol{h}_i$'s and among themselves and (ii) two kinds of hopping and two kinds of propagators are involved. In view of these complexities we shall be content with obtaining simple estimates. Following Anderson,[11] we shall ignore the self-energies of $G_n^{a,0,i,j\cdots}$, etc., while the random nature of the A_{ij}'s and B_{ij}'s can be taken into account reasonably by a simple approximation; their correlations with h_i have to be ignored except in some simple models of disorder. Employing these approximations Lyo[16] obtained a fair description of localization in antiferromagnets.

Following approximations of Refs. 11, 12, and 16, the localization function is obtained as

$$L(E) = \left[\sum_j \exp(La_j)\right]^{1/L} , \tag{3.16}$$

where $La_j = \langle \ln X_j^L\rangle$. The sum T_L in Eq. (3.16) is evaluated in the following manner:

$$\begin{aligned} \langle T_L\rangle = {} & K^L \sum_{n=0}^{L} \exp[n\langle \ln|G_i^a|\rangle + (L-n)\langle \ln|G_i^b|\rangle] \\ & \times (-1)^{L-n} \sum_{j=1}^{L_{c_n}} \exp(p_j\langle \ln|A|\rangle - q_j\langle \ln|B|\rangle) , \end{aligned} \tag{3.17}$$

where $L_{c_n} = L!/n!(L-n)!$; p_j and q_j denote the number of A bonds and B bonds, respectively, in a walk configuration in which G^a's occur n times and G^b's occur $(L-n)$ times. Evaluation of this expression is again tedious, but a simple approximation is obtained if we require the localization function to give correct limits in case of zero disorder (for a pure antiferromagnet this kind of approximation cannot lead to correct answer, however, in this case the following approximation reduces to that of Ref. 16).

$$\begin{aligned} L(E) = {} & Z^2 \exp(-\langle \ln|E^2 - h_i^2|\rangle) \\ & \times (\exp\langle \ln|A|\rangle - \exp\langle \ln|B|\rangle)^2 . \end{aligned} \tag{3.18}$$

Here K has also been replaced by $\boldsymbol{Z}$ to produce the correct result for zero disorder. A feature worth pointing out about this formula is that the presence of two kinds of hoppings (A and B) in-

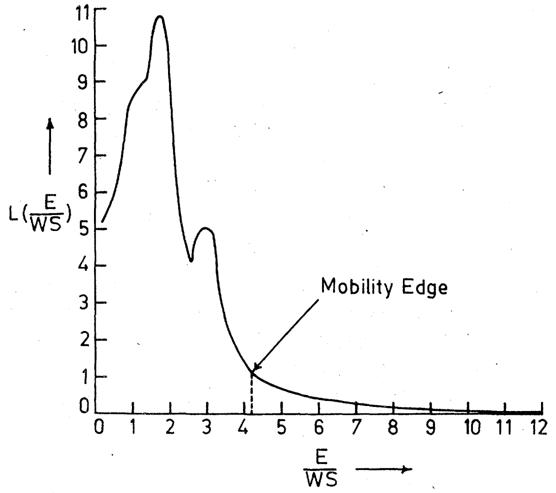

FIG. 1. Plot of the localization function according to Eq. (3.18).

creases the extent of localization in comparison to the cases of ferromagnets (only A hops) or antiferromagnets (only B hops). A calculation of the averages occurring in Eq. (3.18) has been performed as described in Secs. IV and V. The result is plotted in Fig. 1. The figure shows that the states of energy smaller than $4.2WS$ (see Sec. V for units) are extended and those with energies above this value are localized. It must be stressed that the approximation used here underestimates localization as has been discussed by Anderson.[11] Thus the true mobility edge should occur at considerably lower value of energy. The Monte Carlo studies[10,17] show a much greater extent of localization, which is quite understandable from our arguments.

The above type of theory may also be considered for RKKY interactions. Using Anderson's arguments for interaction falling off as r^{-3}, it would follow that all states in such systems should be extended. However, there are two factors which preclude such a conclusion. Firstly, the hopping matrix elements are random and secondly there are two kinds of hoppings which in some sense inhibit delocalization. The effect of the first factor is not qualitatively important; we have not been able to assess quantitatively the role of second factor for long-range interactions.

IV. DENSITY OF STATES

The local density of states for spin-deviation excitations is given in terms of the Green's functions by the following formula:

$$\rho_i(E)=\frac{1}{\pi}\lim_{\epsilon\to 0}\mathrm{Im}[G_{ii}^{aa}(E-i\epsilon)-G_{ii}^{bb}(E-i\epsilon)]\,. \tag{4.1}$$

We are interested in calculating the configurationally averaged density of states. The coherent-potential-approximation (CPA) and its cluster extensions have been extensively employed in recent years to calculate configurationally averaged Green's functions in disordered systems. However, this type of formalism is not quite applicable here for the following reasons. Firstly, for the realistic spin-glass systems like CuMn, the spins are coupled by the RKKY interaction, which means the spin excitations can hop over long range. Whereas CPA-type theories by virtue of their basic approximation are valid only for short-ranged hopping. Secondly, the hopping interaction is also random which makes the application of the above procedure very cumbersome. Finally, we expect the states to be localized over majority of the band and CPA-type theories are not applicable for calculation of density of states of localized states.

For these reasons we employ the continued-fraction method as developed by Haydock *et al.*[13] This method is particularly suitable for calculating local quantities and provides approximations which are amenable to configurational averaging. The method yields the Green's function in the form

$$\begin{aligned} G_{ii}^{aa}&=\cfrac{1}{\alpha_{1i}-\cfrac{\beta_{1i}}{\alpha_{2i}-\cfrac{\beta_{2i}}{\alpha_{3i}-\cdots}}}\\ G_{ii}^{bb}&=\cfrac{1}{\alpha'_{1i}-\cfrac{\beta'_{1i}}{\alpha'_{2i}-\cfrac{\beta'_{2i}}{\alpha'_{3i}-\cdots}}} \end{aligned} \tag{4.2}$$

As discussed by Haydock *et al.*,[13] the practical calculations are done by terminating the continued fraction in a self-consistent manner which yields a Herglotz function. Terminating the expansion at the nth stage gives a density of states whose first $2n$ moments are exact. In the present problem, since a configurational averaging is to follow the above calculation of density of states, we introduce the approximation at the second state. The usual procedure is

$$G_{ii}=\frac{1}{\alpha_{1i}-\beta_{1i}\mathcal{G}}\,, \tag{4.3a}$$

$$\mathcal{G}=\frac{1}{\alpha_2-\beta_2\mathcal{G}}\,. \tag{4.3b}$$

This procedure would have been satisfactory if we were dealing with one-component excitations like in a ferromagnet. For a two sublattice antiferromagnet, the more appropriate procedure is

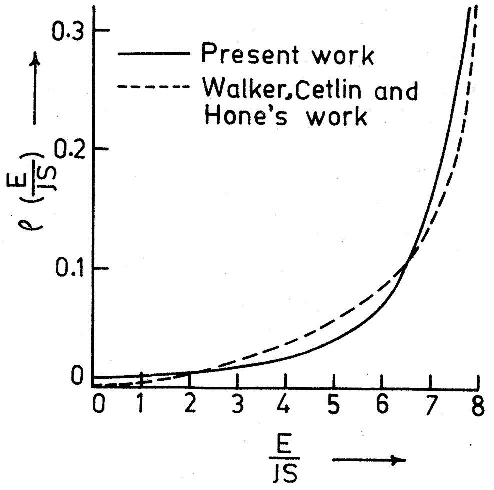

FIG. 2. Comparison of the density of states calculated according to Eqs. (4.9) and the exact calculation of Ref. 25, Eq. (4.4), yields the formula

$$\rho(E)=\frac{304}{\pi}(\epsilon^2+12)^{1/2} \times\left(\frac{[(8-\epsilon)/(8+\epsilon)]^{1/2}}{[30(\epsilon-8)]^2+64(\epsilon^2+12)(8-\epsilon)/(\delta+\epsilon)} + \frac{[(\epsilon+8)/(8-\epsilon)]^{1/2}}{[30(\epsilon-8)]^2+64(\epsilon^2+12)(8+\epsilon)/(\delta-\epsilon)}\right).$$

$$G_{ii}^{aa}=\frac{1}{\alpha_1-\beta_1 g_b}, \quad G_{ii}^{bb}=\frac{1}{\alpha_1'-\beta_1' g_a}; \tag{4.4a}$$

$$g_b=\frac{1}{\alpha_2-\beta_2 g_a}, \quad g_a=\frac{1}{\alpha_2-\beta_2' g_b}. \tag{4.4b}$$

This procedure, while being exact for a one-dimensional antiferromagnet, gives a fairly good account of density of states for a bcc antiferromagnet for which detailed comparisons with the numerically calculated exact density of states[18] is shown in Fig. 2. For other lattices, similar comparisons are obtained. In all cases, the upper-band limit is correctly obtained. The equations of motion in the spin-glass case are neither like an antiferromagnet nor like a ferromagnet. So we tried both of the procedures given in Eqs. (4.3) and (4.4), respectively. We found that the procedure of Eq. (4.4) is found to be more satisfactory, though the general form of the density-of-states curves is somewhat similar.

For the random problem, the coefficients α_n and β_n are dependent upon i and are random quantities. Their explicit values are listed below:

$$\alpha_{1i}=E-h_i, \quad \alpha_{1i}'=-E-h_i, \tag{4.5}$$

$$\beta_{1i}=\beta_{1i}'=\sum_j(|A_{ij}|^2+|B_{ij}|^2), \tag{4.6}$$

$$\alpha_{2i}=\frac{1}{\beta_{1i}}\left(\sum_j[(E-h_j)|A_{ij}|^2-(E+h_j)|B_{ij}|^2] +\sum_{j,k}[A_{ij}(A_{ik}^*A_{jk}^*+B_{ik}^*B_{kj}) +B_{ij}(A_{ik}^*B_{kj}^*+B_{ik}^*A_{kj})]\right), \tag{4.7a}$$

$$\alpha_{2i}'=\frac{1}{\beta_{1i}}\left(\sum_j[-(E+h_j)|A_{ij}|^2+(E-h_i)|B_{ij}|^2] +\sum_{j,k}[A_{ij}^*(A_{ik}+B_{ik}B_{kj}^*) +B_{ij}^*(A_{ik}B_{kj}+B_{ik}A_{kj}^*)]\right). \tag{4.7b}$$

The expressions for β_2 and β_2' are very long and will be given elsewhere.[19] For performing the configurational averaging the following approximation is introduced. The quantities g_a and g_b are obtained from averaged values of α_{2i}, β_{2i}, α_{2i}', and β_{2i}', i.e., g_a is obtained from the equation:

$$g_a=\frac{1}{\alpha_2'-\dfrac{\beta_2'}{\alpha_2-\beta_2 g_a}}, \tag{4.8}$$

where $\alpha_2'=\langle\alpha_{2i}'\rangle$, etc.

Thus the configurationally averaged expression G is obtained as

$$G_{ii}^{aa}=\int P(\beta,h)\frac{1}{E-h-\beta g_b}\,d\beta\,dh \tag{4.9a}$$

and

$$G_{ii}^{bb}=\int P(\beta,h)\frac{1}{-E-h-\beta g_a}\,d\beta\,dh, \tag{4.9b}$$

where $P(\beta,h)$ is the joint probability distribution function of β_{1i} and h_i. In practice, it is quite intractable to obtain the joint probability distribution of β and h. So, we have obtained the distributions of β and h separately and then taken into account the correlations of β and h by means of a simple constraint. The most important aspect of correlations between β and h comes from considerations of stability. Clearly the energy of all the excitations must be non-negative. For this to be true each eigenvalue of the matrix $(h\delta_{ij}+A_{ij})$ should be positive and be greater than the corresponding eigenvalue of the matrix (B_{ij}).[14] This restriction is rather difficult to impose mathematically, because both the matrices are random. However, it is easier to think about this restriction in terms of quantities h and β. The above restriction may be roughly written in the form

$$\beta<\mu h^2, \tag{4.10}$$

where μ is a constant whose value may lie between Z^{-1} and unity. For random systems, a precise value of μ cannot be estimated. In most of the calculations we have taken $\mu = 1$. Thus we take the probability distribution $P(\beta, h)$:

$$P(\beta, h) = P(\beta)P(h)\Theta(\beta - \mu h^2) . \tag{4.11}$$

We have done explicit calculations for these probability distributions and density of states for two cases: (i) Nc spins are distributed randomly on a fcc lattice of N sites and interact via the RKKY exchange interaction and (ii) the spins are present on each lattice site but the exchange integral obeys a Gaussian distribution. The calculation and results are discussed in Sec. V.

V. GAUSSIAN MODEL

To proceed further with the calculation, we shall have to make specific assumptions about certain statistical properties of ground-state configurations. The simplest assumption which has been often employed is that of complete randomness in spin orientation, i.e.,

$$p(\theta_i, \phi_i)\, d\Omega_i = d\Omega_i / 4\pi . \tag{5.1}$$

We use a slightly generalized form of Eq. (5.1), namely,

$$p(\theta_i, \phi_i) = \begin{cases} (1/4\pi)(1+\sigma), & 0 < \theta_i \leqslant \frac{1}{2}\pi \\ (1/4\pi)(1-\sigma), & \frac{1}{2}\pi < \theta_i < \pi \end{cases} \tag{5.2}$$

where σ may be chosen to be a small number (0.01 to 0.2 in our case). $\sigma = 0$ corresponds to complete randomness. In the Gaussian model, the J_{ij}'s distribution is

$$P(J) = (1/\sqrt{2\pi}\, W)\, e^{-J^2/2W^2} . \tag{5.3}$$

The quantities of main interest are h and β. Assuming complete randomness of spin orientation, the distribution of h has been shown to be Gaussian,[20]

$$P(h) = \sqrt{2/\pi}\, (h^2/\Delta^3) e^{-h^2/2\Delta^2} , \tag{5.4}$$

where

$$\Delta = \tfrac{1}{3}\sqrt{Z}\, WS . \tag{5.5}$$

In calculating the probability distribution for β, we find that it makes little quantitative difference if we average over azimuthal angles to begin with, but the algebra is simplified considerably. The following expression for β_i is used:

$$\beta_i = \tfrac{1}{2} \sum_j |SJ(R_{ij})|^2 [1 + \cos^2(\theta_i - \theta_j)] . \tag{5.6}$$

Using standard methods [(5)–(7)], we find

$$P(\beta) = \int_{-\infty}^{\infty} \frac{d\rho}{2\pi}\, e^{i\rho\beta} \left(\frac{1}{\sqrt{i\rho}\, W^2 S^2} \ln \frac{(i\rho W^2 S^2)^{1/2} + (1 + 2i\rho W^2 S^2)^{1/2}}{(1 + i\rho W^2 S^2)^{1/2}} \right)^Z . \tag{5.7}$$

For $Z = 12$, $P(\beta) \propto \beta^5$ for small β and $P(\beta) \propto \beta^{-3/2}$ for large β. Keeping in view the constraint (4.10), we replace this complicated distribution by

$$P(\beta) = \tfrac{1}{16} , \quad 0 \leqslant \beta \leqslant 16 . \tag{5.8}$$

The specific choice is made to yield the correct value for the average. In first-order approximation, the effect of a nonzero value of σ is neglected in obtaining distributions $P(\beta)$ and $P(h)$. The average values of the other continued-fraction coefficients are easily evaluated with the help of Eqs. (5.2) and (5.3). These are given as

$$\langle \alpha_2 \rangle = \tfrac{3}{2} E\sigma - \langle h \rangle , \quad \langle \alpha_2' \rangle = \tfrac{3}{2} E\sigma - \langle h \rangle \tag{5.9}$$

with

$$h = (8Z/9\pi)^{1/2} WS . \tag{5.10}$$

The expressions for $\langle \beta_2 \rangle$ and $\langle \beta_2' \rangle$ are given in Ref. 19.

The results for the density of states are shown in Figs. 3 and 4. The energy unit is taken to be WS. Figure 3 shows the plot for density of states when $\mu = 1$. Curves of a similar nature are obtained for other values of μ. Also shown is the plot when no restriction is imposed on the values of β. In Fig. 4 we exhibit the density-of-states curves for different value of σ parameter. We find that curves are not too sensitive to values of σ, in the range of small values of σ. The general shape of these curves is quite like those obtained in Monte Carlo calculations.[10,17] The significant point is the nonzero density of states at zero energy. The question of interest is what may be the nature of these low-energy collective excitations. Clearly the low-energy excitations involve a large number of spins. Monte Carlo calculations[10] have shown that the ground-state energy is a rather insensitive function of spin configurations close to ground-state configurations. This means that there are a large number of configurations differing much in spin orientations but little in energy, and the lowest-energy excitations may consist of tunneling among these configurations. The excitations calculated here may well correspond to this picture.

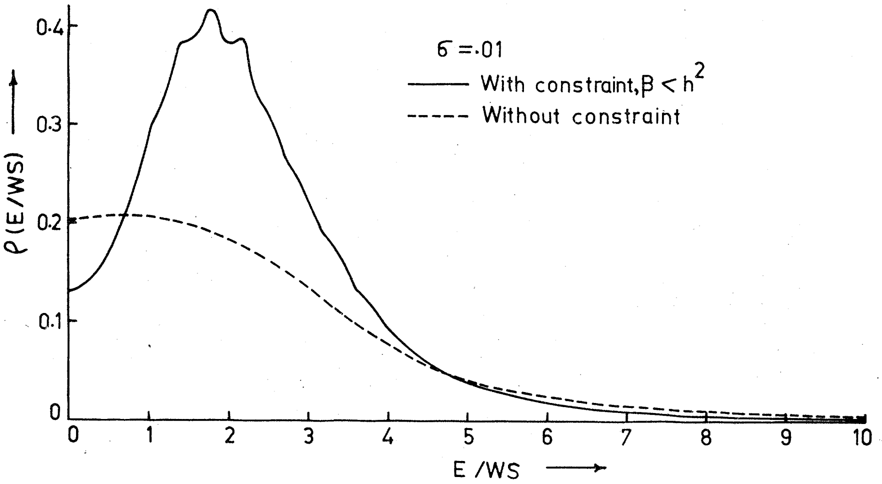

FIG. 3. Plots of the density of states for the Gaussian model in two approximations.

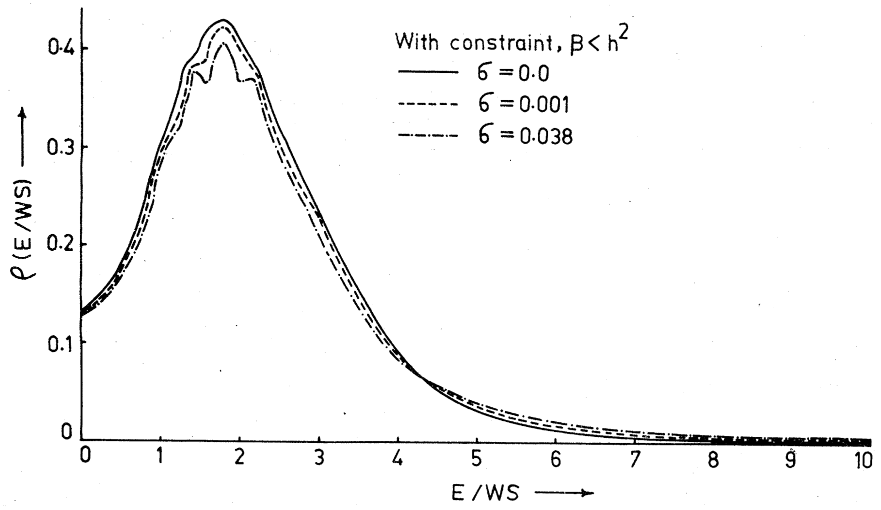

FIG. 4. Plots of the density of states for the Gaussian model with three values of σ.

We have used this excitation density to calculate the specific heat, which is shown in Fig. 5. C_m is fairly linear up to $0.1T_c$.

VI. RUDERMAN-KITTEL-KASUYA-YOSIDA MODEL

In this model we use the long-range form of the RKKY interaction, i.e.,

$$J(R_{ij}) = (A/|\bar{R}_{ij}|^3)\cos 2k_F R_{ij}\,. \tag{6.1}$$

Here again the probability distribution of h is available in the literature,[21] and is given by (assuming complete randomness in orientation of spins)

$$P(h) = (4/\pi)[\Delta h^2/(\Delta^2 + h^2)^{3/2}]\,, \tag{6.2}$$

where

$$\Delta = \tfrac{4}{3}\pi^2 c(AS/a^3)\,, \tag{6.3}$$

where a is the lattice parameter and c the concentration of magnetic atoms. In the present case the calculation of $P(\beta)$ can also be done exactly, in fact, a result for a similar quantity was obtained by Anderson.[11] Using his expression, essentially, we find,

$$P(\tilde{\beta}) = \frac{0.563\pi c}{\tilde{\beta}^{3/2}} \exp[-(0.271\pi^{3/2}c)^2/\tilde{\beta}]\,, \tag{6.4}$$

where $\tilde{\beta} = \beta/(AS/a^3)^2$. Using the probability distributions of Eq. (5.2), we obtain the various averages as

$$\langle\alpha_2\rangle = \tfrac{3}{2}E\sigma - \langle h\rangle + 36\pi c(3\ln 3 - \tfrac{14}{3}\ln 2)(\tfrac{10}{9} + \tfrac{4}{9}\sigma^2)\,, \tag{6.5a}$$

$$\langle\alpha_2'\rangle = -\tfrac{3}{2}E\sigma - \langle h\rangle + 36\pi c(3\ln 3 - \tfrac{14}{3}\ln 2)(\tfrac{10}{9} + \tfrac{4}{9}\sigma^2)\,, \tag{6.5b}$$

where

$$\langle h\rangle = \frac{16\pi c}{3}\left(\ln\frac{(1+\Delta^2)^{1/2}}{\Delta} - \frac{1}{2} + \frac{\Delta^2}{2(1+\Delta^2)}\right)\,. \tag{6.6}$$

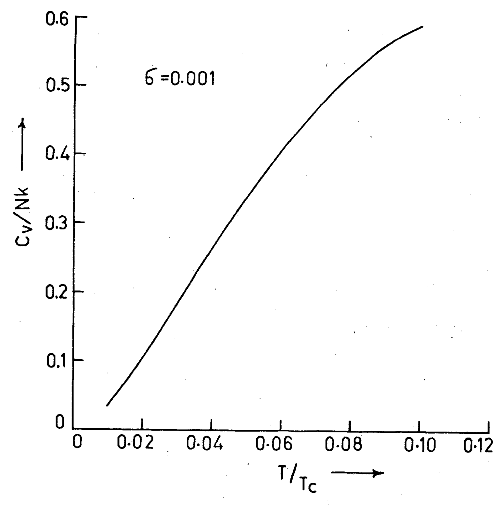

FIG. 5. Calculated specific heat as function of temperature for the Gaussian model. (N is the total number of sites, k is the Boltzmann constant.)

The calculation of $\langle h\rangle$ has been made with the help of the distributions given in Eq. (6.2) with a further provision that the maximum value of h is AS/a^3, which is of the order of the field experienced by a spin due to its nearest neighbor. The averages have been carried out correct to order c^2. The expressions for $\langle\beta_2\rangle$ and $\langle\beta_2'\rangle$ are recorded in Ref. 19.

For the long-ranged interaction we could not find a satisfactory expression for the constraint arising due to stability requirements. The calculations without incorporating any constraint have been shown for three concentrations in Fig. 6. Several points about this calculation are worth noting. The density of states at zero energy is finite and decreases with the increasing concentrations. Most of the excitations have energies below AS/a^3—which is the exchange energy between two spins in the nearest-neighbor positions.

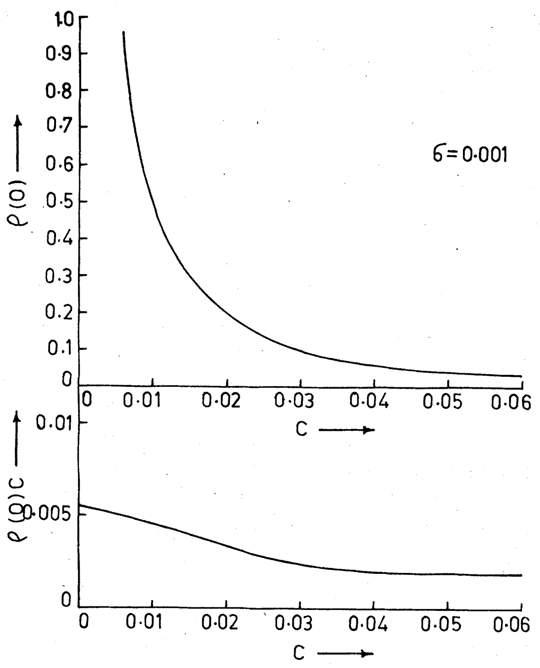

FIG. 7. (a) Plot of the density of state at zero energy $\rho(0)$ as function of concentration. (b) Plot of $\rho(0)c$ as function of concentration.

In Fig. 7, we have plotted $\rho(0)$ and the product $\rho(0)c$ versus concentration c. It is seen that $\rho(0)c$ is nearly constant with concentration which implies that the linear (in temperature) contribution to specific heat is nearly independent of the concentration. All the above points are in accord with the experiments and the Monte Carlo calculations.[10,17] Our calculations also show some resonance structure at higher energies. The positions of the resonance peaks do not depend upon the concentration. We have not been able to find any physical interpretation for these peaks.

We have also performed the calculations with the constraint $\beta < h^2$. These are shown in Fig. 8.

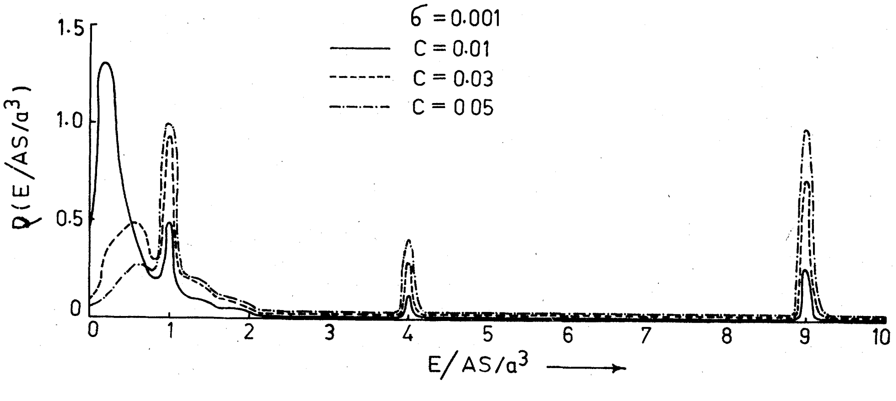

FIG. 6. Plots of the density of states for the RKKY model for three concentrations. No restriction on values of β is imposed.

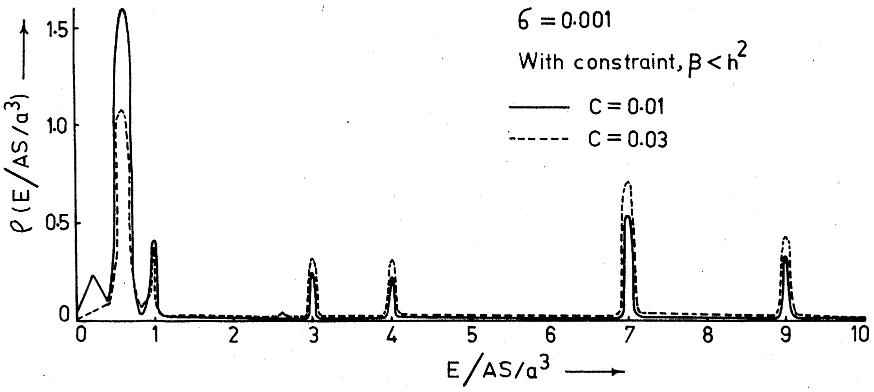

FIG. 8. Plots of density of states for the RKKY model for two concentrations. In this calculation the constraint $\beta < h^2$ has been used.

The general nature of the curves is similar. But the density of states at zero energy gets reduced by a factor of the order of 5 to 10. The numerical agreement for specific-heat calculation gets worse. In fact, in this calculation any constraint of the form $\beta < \mu h^2$ leads to a similar large reduction in the density of states at zero energy. It is quite possible that there is an energy gap in the excitations at fact which is consistent with the measurements of Wenger and Keesom.[4,10]

VII. CONCLUSIONS

In this paper we have obtained a description of the low-temperature excitations in spin-glasses. Our description is in good accord with that obtained in Monte Carlo studies of finite numbers of spins.[10,17] In terms of the low-temperature excitations discussed in our paper and in Refs. 10 and 17, one is able to obtain a better understanding of low-temperature properties, particularly specific heat. The present understanding seems to us far more convincing than that obtained on the basis of molecular-field theory. As far as we know, ours is a first analytical calculation of the density of states of excitations in spin-glasses. Thus it is complementary to the Monte Carlo calculations done earlier. The specific results obtained in this paper are the following:

(i) The localization characteristics of spin-glass excitations are studied and an explicit form of the localization function is obtained for short-ranged exchange. The low-energy excitations up to one-third of the bandwidth are found to be extended and the higher-energy excitations are found to be localized. Our approximation underestimates localization.

(ii) For the RKKY interactions, we have not been able to reach any quantitative conclusions regarding localization. A simplistic application of Anderson's arguments for interactions falling off as r^{-3} suggests that in this case all the excitations must be extended. We point out some arguments as to why this may not be so.

(iii) We have extended the application of the continued-fraction method to excitations described by two complex amplitudes at each site. A procedure for the self-consistent termination of a continued fraction is given. This procedure gives a good description of the density of states of pure antiferromagnets.

(iv) The above method is applied to (a) the Gaussian model and (b) the RKKY model. In both models one finds a finite density of states at zero energy. The density of states in the Gaussian model is quite featureless and has the same general shape as found in Monte Carlo calculations. The density of states for the RKKY model shows considerable structure with resonancelike modes at high energies. Most of the states occur with energies below the exchange energy corresponding to two spins at nearest-neighbor sites. Our calculation for the RKKY model is not as reliable as that for the Gaussian model.

(v) The zero-energy density of states for the RKKY model is found to decrease with the increasing concentration. The product $\rho(0)c$ is seen to be nearly constant. The contribution to the magnetic specific heat which is linear in temperature involves $\rho(0)c$. Thus, it is seen that this coefficient is approximately independent of concentration is in accord with experiments.

Finally, it should be mentioned that the further correctness of our calculational method can only be established if we can provide an explanation of the other low-temperature properties, namely, (i) the $T^{3/2}$ law for the resistivity and (ii) the presence of spin-wave-like excitations through a calculation of the dynamic structure factor $S(q,\omega)$. Work is in progress on both these calculations.

ACKNOWLEDGMENTS

We have benefited from discussions with Dr. M. Barma and Dr. B. S. Shastry. One of us (R. B.) wishes to acknowledge the financial support of the Council of Scientific and Industrial Research, India.

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