

Ground state and excitation spectrum of disordered Heisenberg magnets

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A systematic method is proposed for evaluating the configuration-averaged Green functions $\langle \hat{G} \rangle$ of a disordered Heisenberg magnet with randomly distributed competing exchange interactions. A prescription is given for constructing the zeroth approximation \hat{G}_0 with the aid of the local-field distribution function $P(\varepsilon)$, which reflects the type and energy structure of the ground state. The excitation spectrum of a disordered ferromagnet is analyzed in the zeroth approximation. An effective translational medium, described by a matrix \hat{H}_0 , and a scattering matrix are introduced, and fluctuations are also incorporated. The configuration-averaged partial scattering matrix describing scattering by the exchange bonds is found (this matrix depends on the concentrations of the frustrated and normal exchange bonds), and the mass operator for $\langle \hat{G} \rangle$ is evaluated without allowance for fluctuation correlations.

1. INTRODUCTION

The properties of disordered systems, particularly those of disordered (amorphous) magnets, are actively being studied at the present time.¹⁻⁵ The theoretical description of disordered systems encounters fundamental difficulties stemming primarily from the absence of translational invariance and from the problem of configurational averaging.

In the theory of disordered magnets (quenched alloys), widespread use is made of "lattice" models which attribute the disorder in the distribution of the spins over sites of the crystal lattice to the presence of competing (in magnitude and sign) exchange interactions. The magnetic properties of such a system are described by the Heisenberg Hamiltonian

$$\mathcal{H} = - \sum_{fm} I_{fm} \mathbf{S}_f \cdot \mathbf{S}_m, \quad I_{fm} = I_{mf}, \quad (1.1)$$

where f and m are lattice sites, I_{fm} are exchange parameters, and \mathbf{S}_f is the spin operator at site f . Although in the general case the exchange interaction can be long-ranged and oscillatory (the RKKY mechanism), here we shall consider only cases in which I_{fm} is nonzero only for nearest neighbors. In this situation two different models can be used to describe the fluctuations in the magnitude and sign of I_{fm} : the random-site model (see, e.g., Ref. 6) and the random-bond model.

In this paper we investigate the properties of a system described by Hamiltonian (1.1) for spin $S = 1/2$ in the random-bond model, in which the exchange parameter (bond) I_{fm} is distributed randomly throughout the lattice. In the simplest case the distribution function is of the form

$$\rho(I_{fm}) = \nu \delta(I_{fm} - K) + (1 - \nu) \delta(I_{fm} - J), \quad (1.2)$$

$$K < 0, \quad J > 0, \quad \lambda = |K|/J,$$

where ν is the concentration of negative (antiferromagnetic) K bonds, $\nu = N_K/N_c$, N_K is the number of K bonds, $N_c = zN/2$ is the total number of bonds, and z is the number of nearest neighbors. For simplicity we consider only alternating lattices.

Even with these restrictions the properties of the model have a far from trivial description.

First of all, there is the problem of the ground state. A goodly number of studies have been made of the magnetic phase diagram of the system for the Ising part of Hamiltonian (1.1) with the two-spike distribution (1.2). Both analytical calculations (see, e.g., Refs. 7–10) and Monte Carlo calculations^{11,12} show that, depending on the relationship of the parameters ν , λ , and z (and also the lattice dimensionality d), the ground state of the system ($T = 0$) can be a disordered ferromagnet [for $\nu \leq \nu_{FM}(\lambda)$], a spin glass [for $\nu_{FM}(\lambda) \leq \nu \leq \nu_{AFM}(\lambda)$], or a disordered antiferromagnet [for $\nu \geq \nu_{AFM}(\lambda)$], where $\nu_{FM}(\lambda)$ and $\nu_{AFM}(\lambda)$ are the critical concentrations. It should be stressed that in any of these phases the ground state is a complex spin configuration consisting of two spin subsystems: "up" and "down". This is indicated by experimental studies of the paramagnetic susceptibility of disordered ferromagnets,¹³ where it is found that the temperature dependence is like that of a ferrimagnet.

Second, there arises the problem of describing the excitation spectrum of the system above the various ground states. The coherent-potential method, which has been used^{14,15} to describe the ferromagnetic state, ignores the existence of the two spin subsystems (the disordered ferromagnet is approximated by a translationally invariant medium with a certain average spin at every lattice site). In actuality, the spin-wave spectrum of a disordered ferromagnet should contain ferrimagnet-like optical branches in addition to the acoustic branch. Analogous conclusions can be reached for the excitation spectra of the spin glass and antiferromagnet as well. It is thus necessary to develop a technique for calculating the excitation spectra of Heisenberg magnets that reflects in an essential way the presence of the two spin subsystems.

Third, the solution of these problems can serve as a foundation on which to construct a thermodynamics of disordered magnets.

In the present paper we shall concentrate on solving the second problem, assuming that the problem of the ground state has, at least in principle, been solved.

2. GROUND STATE

The construction of an exact wave function for the ground state of a disordered Heisenberg magnet with Hamiltonian (1.1) and distribution function (1.2) is an extremely complicated problem, since there is a random distribution of "up" and "down" spins over the lattice sites. To find an approximate description of the ground state, let us separate Hamiltonian (1.1) into Ising \mathcal{H}_0 and transverse \mathcal{H}_1 parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \quad \mathcal{H}_0 = -\frac{1}{4} \sum_{jm} I_{jm} \delta_j \delta_m, \quad \delta_j = 2S_j^z. \quad (2.1)$$

We proceed from the assumption that \mathcal{H}_0 plays the principal role in the formation of the ground state, while \mathcal{H}_1 gives only a small correction due to zero-point vibrations. This is in fact the case for ideal ferrimagnets and antiferromagnets.

Let $\{\sigma_f^0\}$ be the spin configuration corresponding to the minimum of \mathcal{H}_0 , i.e.,

$$E_0 = -\frac{1}{4} \sum_{jm} I_{jm} \sigma_f^0 \sigma_m^0 = -\frac{1}{8} \sum_f \sigma_f^0 \varepsilon_f^0, \quad (2.2)$$

where ε_f^0 is the local field at site f :

$$\varepsilon_f^0 = \sum_m I_{fm} \sigma_m^0, \quad \sigma_m^0 = \pm 1. \quad (2.3)$$

It is seen from (2.2) that a necessary condition for a minimum is that $\sigma_f^0 \varepsilon_f^0 \geq 0$, which implies that the spin direction is uniquely determined by the sign of the local field¹⁾

$$\sigma_f^0 = \text{sign } \varepsilon_f^0. \quad (2.4)$$

The distribution $\{\sigma_f^0\}$ is thus uniquely related to the distribution $\{\varepsilon_f^0\}$ of the local fields. The assignment of a spin configuration $\{\sigma_f^0\}$ makes it possible to evaluate the correlation functions

$$\langle \sigma_f^0 \sigma_{f+r}^0 \rangle = \frac{1}{N} \sum_f \sigma_f^0 \sigma_{f+r}^0,$$

with the aid of which one can determine the character of the spatial distribution of the spins and, in particular, the presence of long-range or short-range order⁴ (the angle brackets $\langle \dots \rangle$ denote a configurational average).

For describing the type of ground state one can also use more coarse-grained characteristics. Let N_A be the number of sites with spin "up" (these sites are denoted $\alpha, \alpha', \dots, \sigma_\alpha^0 = +1$) and N_B be the number of sites with spin "down" (sites $\beta, \beta', \dots, \sigma_\beta^0 = -1$); $N_A + N_B = N$. The system is characterized by a relative magnetization

$$\sigma(0) = \langle \sigma_f^0 \rangle = (N_A - N_B)/N, \quad (2.5)$$

which is nonzero in the ferromagnetic state. For identification of the antiferromagnetic state it is convenient to introduce two sublattices (1 and 2), which correspond to the ideal antiferromagnet ($\nu = 1$). Denoting by f, f', \dots the sites of sublattice 1 (spins "up" in the ideal antiferromagnet) and by m, m', \dots the sites of sublattice 2, we have by definition the relative sublattice magnetizations

$$\sigma_1(0) = \frac{2}{N} \sum_{f \in 1} \sigma_f^0 = \langle \sigma_f^0 \rangle_1, \quad \sigma_2(0) = \frac{2}{N} \sum_{m \in 2} \sigma_m^0 = \langle \sigma_m^0 \rangle_2 = -\sigma_1(0), \quad (2.6)$$

which are nonzero in the antiferromagnet state and identically zero in the spin-glass phase.

Let us introduce the distribution function $P(\varepsilon)$ of the local fields in the ground state of the system; a functional of $\rho(I_{jm})$, this distribution function describes the type (ferromagnet, spin glass, antiferromagnet) and energy structure of the ground state. For the model under study, in which I_{jm} takes on only two values $J > 0$ and $K < 0$, there is a finite number of local-field types, which are characterized by different distributions of the J and K bonds and of spin states in a cluster (by cluster we mean a spin surrounded by z nearest neighbors). The local field acting on such a spin is given by formula (2.3). Let us write the function $P(\varepsilon)$ in the form

$$P(\varepsilon) = \sum_j W_j \delta(\varepsilon - \varepsilon_j^0), \quad \sum_j W_j = 1, \quad (2.7)$$

where ε_j^0 is the local field of the j th type and W_j is the probability of its occurrence in the ground state of the system. Using (2.4) and (2.7), we find

$$\frac{E_0}{N} = -\frac{1}{8} \int d\varepsilon P(\varepsilon) \varepsilon \text{sign}(\varepsilon) = -\frac{1}{8} \int d\varepsilon P(\varepsilon) |\varepsilon|, \quad (2.8)$$

$$\sigma(0) = \int d\varepsilon P(\varepsilon) \text{sign}(\varepsilon)$$

$$= \int_0^\infty P(\varepsilon) d\varepsilon - \int_{-\infty}^0 P(\varepsilon) d\varepsilon = \sigma_A(0) - \sigma_B(0),$$

where $\sigma_A(0) = N_A/N$ and $\sigma_B(0) = N_B/N$ are the fractions of sites with spin "up" (subsystem A) and "down" (subsystem B) in the ground state.

In the ferromagnetic state the envelope of the distribution function $P(\varepsilon)$ should obviously be asymmetric to provide for $\sigma(0) > 0$. In the antiferromagnetic and spin-glass states, however, the envelope should become symmetric, so that $\sigma(0) = 0$. To describe the antiferromagnetic state it is convenient to introduce the distribution function of the local fields for each sublattice:

$$P_i(\varepsilon) = \sum_j W_j^{(i)} \delta(\varepsilon - \varepsilon_j^0), \quad \int P_i(\varepsilon) d\varepsilon = 1, \quad i=1, 2, \quad (2.9)$$

where $W_j^{(i)}$ is the probability of occurrence of the local field of type j in the i th sublattice: $P(\varepsilon) = 1/2(P_1 + P_2)$. In the antiferromagnetic state sublattice 1 is occupied predominantly by "up" spins, so the shape of $P_1(\varepsilon)$ is analogous to $P(\varepsilon)$ in the ferromagnetic state. Because the sublattices are mirror images of each other, the functions $P_i(\varepsilon)$ have the properties

$$P_2(\varepsilon) = P_1(-\varepsilon), \quad \int P_i(\varepsilon) \text{sign}(\varepsilon) d\varepsilon = \sigma_i(0) \quad \text{for AFM}, \quad (2.10)$$

$$P_2(\varepsilon) = P_1(\varepsilon) = P_{\text{SG}}(\varepsilon), \quad \int P_{\text{SG}}(\varepsilon) \text{sign}(\varepsilon) d\varepsilon = 0 \quad \text{for SG}.$$

These distributions reflect the type and energy structure (local or short-range order) of the ground-state of a disordered Ising magnet. Although they can be expressed analytically in certain limiting cases, they have nevertheless been evaluated by the Monte Carlo method.¹¹

The distribution function of the local fields retains its meaning at finite temperatures, where the local field

$$\varepsilon_j = \sum_m I_{jm} \sigma_m, \quad \sigma_m = \langle 2S_m^z \rangle_T \quad (2.11)$$

depends on the thermodynamic averages σ_m . For the Ising Hamiltonian we have the formal solution $\sigma_j = \tanh(\varepsilon_j/2T)$, which implies that the spin direction is determined as before by the sign of the local field. Henceforth, for the sake of generality, we shall use functions $P(\varepsilon)$ and $P_1(\varepsilon)$ which are implicit functions of temperature, the local fields in them being defined by (2.11).

3. EQUATIONS FOR THE GREEN FUNCTIONS. ZEROth APPROXIMATION FOR THE CONFIGURATION-AVERAGED GREEN FUNCTION

The Green function formalism is widely used in the theory of disordered systems, since the experimentally observable characteristics of the system can be found in terms of such functions.¹⁻³

The equation for the Green function $\langle \langle S_j^+ | S_{j'}^- \rangle \rangle_E$ in the Tyablikov approximation¹⁶ can be written

$$(E - \varepsilon_j) \langle \langle S_j^+ | S_{j'}^- \rangle \rangle_E = \delta_{jj'} \sigma_j - \sigma_j \sum_m I_{jm} \langle \langle S_m^+ | S_{j'}^- \rangle \rangle_E. \quad (3.1)$$

In place of $\langle \langle S_j^+ | S_{j'}^- \rangle \rangle_E$ it is convenient to introduce the function

$$G_{jj'}(E) = \sigma_j^{-1} \langle \langle S_j^+ | S_{j'}^- \rangle \rangle_E,$$

the equation for which,

$$G_{jj'}(E) = \delta_{jj'} g_j(E) - g_j(E) \sum_m V_{jm} G_{mj'}(E), \quad (3.2)$$

$$g_j(E) = (E - \varepsilon_j)^{-1}, \quad V_{jm} = I_{jm} \sigma_m$$

is written in terms of the locators $g_j(E)$. In matrix form we have

$$\hat{G} = \hat{g} - \hat{g} \hat{V} \hat{G}, \quad \hat{g} = (I\hat{E} - \hat{\varepsilon})^{-1}, \quad (3.3)$$

where \hat{I} is the unit matrix and $\hat{\varepsilon}$ is the diagonal matrix $\hat{\varepsilon}_{jm} = \delta_{jm} \varepsilon_j$.

The equation for \hat{G} can be written in a different form:

$$\sum_m [E\delta_{jm} - H_{jm}] G_{mj'} = \delta_{jj'}, \quad H_{jm} = \varepsilon_j \delta_{jm} - V_{jm}, \quad (3.4)$$

or

$$(E\hat{I} - \hat{H}) \hat{G} = \hat{I}, \quad \hat{H} = \hat{\varepsilon} - \hat{V}. \quad (3.5)$$

The matrix H has the property^{3,17}

$$\sum_{(m \neq j)} H_{jm} = -H_{jj} = -\varepsilon_j, \quad (3.6)$$

which permits us to represent it in the form

$$\hat{H} = \sum_p \hat{h}(p), \quad (3.7)$$

where the summation is over all nearest-neighbor pairs $p = (fm)$. The partial matrix $\hat{h}(fm)$, like all the other matrices, has dimensionality $N \times N$, but it contains only four non-zero matrix elements

$$[\hat{h}(fm)]_{j'm'} = \delta_{j'j} (\delta_{m'f} - \delta_{m'm}) V_{jm} + \delta_{j'm} (\delta_{m'm} - \delta_{m'j}) V_{mj}. \quad (3.8)$$

This matrix can be represented symbolically as a 2×2 sub-

matrix

$$\hat{h}(fm) = \begin{vmatrix} V_{jm} & -V_{jm} \\ -V_{mj} & V_{mj} \end{vmatrix}, \quad V_{jm} = I_{jm} \sigma_m, \quad V_{mj} = I_{jm} \sigma_j.$$

The equation for \hat{G} in both its forms and relations (3.6)–(3.8) will be used extensively in what follows.

The basic problem of the theory is to evaluate the configuration-averaged Green functions. To describe the ferromagnetic state one must find $\langle G_{ff+R}(E) \rangle \equiv \langle G_R(E) \rangle$, in terms of which we can express, in particular, the density of states

$$\rho(E) = -\frac{1}{\pi} \text{Im} \langle G_{ff}(E+i0) \rangle, \quad \int \rho(E) dE = 1. \quad (3.9)$$

In a two-sublattice antiferromagnet we must introduce intrasublattice ($G_{ff'}$ and $G_{mm'}$) and intersublattice (G_{fm} and $G_{m'f}$) Green functions and carry out the configurational averaging over the sublattices. In any case the averaging “restores” the translational invariance, so that the configuration-averaged Green functions can be expanded in Fourier series. For the ferromagnetic state

$$\langle G_R(E) \rangle = \frac{1}{N} \sum_k e^{-ikR} G_k(E), \quad G_k(E) = \sum_R e^{ikR} \langle G_R(E) \rangle, \quad (3.10)$$

where the vectors k belong to the first Brillouin zone. For the antiferromagnetic state we introduce the intrasublattice [$G_{11}(q, E)$ and $G_{22}(q, E)$] and intersublattice [$G_{12}(q, E)$ and $G_{21}(q, E)$] Fourier transforms of the configuration-averaged (over the sublattices) Green functions, where the vectors q belong to the halved Brillouin zone.

The formalism set forth below (in matrix notation) is suitable for describing the properties of any state of the system.

4. ZEROth APPROXIMATION FOR THE CONFIGURATION-AVERAGED GREEN FUNCTION

Let us average equation (3.3) with the aid of the decoupling

$$\langle \hat{g} \hat{V} \hat{G} \rangle \approx \langle \hat{g} \hat{V} \rangle \langle \hat{G} \rangle. \quad (4.1)$$

The Green function found in this simplest version of configurational averaging will be denoted \hat{G}_0 :

$$\hat{G}_0 = (I + \langle \hat{g} \hat{V} \rangle)^{-1} \langle \hat{g} \rangle, \quad (4.2)$$

and will be called the zeroth approximation. Let us consider separately the structure of \hat{G}_0 in the homogeneous ferromagnetic and two-sublattice antiferromagnetic states of the system.

a) Homogeneous state

In the site representation the equation for \hat{G}_0 is of the form

$$G_R^0(E) = \delta_{R,0} \langle g_j(E) \rangle - \left\langle g_j(E) \sum_{j+h} V_{j,j+h} \right\rangle G_{j+h, j+R}^0(E), \quad (4.3)$$

where h represents the vectors joining nearest neighbors. After a Fourier transformation we obtain

$$G_k^0(E) = \langle g_f(E) \rangle - \left\langle g_f(E) \sum_h V_{f,f+h} e^{ikh} \right\rangle G_k^0(E) \\ = g(E) - M_0(k, E) G_k^0(E).$$

The configurational average appearing in this equation is easily evaluated since, owing to the isotropy of the system, the averaging includes all possible orientations of the cluster with central spin at site f :

$$M_0(k, E) = \gamma_k \left\langle g_f(E) \sum_h V_{f,f+h} \right\rangle = \gamma_k \langle g_f \epsilon_f \rangle = \gamma_k M_0(E), \quad (4.4)$$

where

$$\gamma_k = \frac{1}{z} \sum_n e^{ihn}, \quad M_0(E) = \int \frac{P(\epsilon) \epsilon d\epsilon}{E - \epsilon}. \quad (4.5)$$

We finally have the following expression for the Fourier transform of the zeroth-approximation Green function:

$$G_k^0(E) = g(E) [1 + \gamma_k M_0(E)]^{-1}, \quad (4.6) \\ g(E) = \langle g_f(E) \rangle = \int \frac{P(\epsilon) d\epsilon}{E - \epsilon}.$$

Let us establish the connection between the poles of the Green function (4.6) and the excitation spectrum of the system. The function $G_k^0(E)$ has two types of poles: the poles of $g(E)$ represent the spectrum of the local fields $\{\epsilon_j\}$, while the poles corresponding to solutions of the equation

$$1 + \gamma_k M_0(E) = 0, \quad (4.7)$$

take into account the presence of collective excitations in the system.

We shall show that Eq. (4.7) implies the existence of an acoustic branch of the spectrum. Expanding $M_0(E)$ in a series about $E = 0$, we obtain

$$M_0(E) = -1 - aE - bE^2 - \dots, \\ a = \int \frac{P(\epsilon) d\epsilon}{\epsilon}, \quad b = \int \frac{P(\epsilon) d\epsilon}{\epsilon^2}. \quad (4.8)$$

In the ferromagnetic phase we have $a > 0$, i.e., $M_0'(0) < 0$, and for small E it is sufficient to keep only the linear term in expansion (4.8). Since $\gamma_k \approx 1 - ck^2$ for small k , we obtain from (4.7) and (4.8) the relation

$$E_{FM}(k) \approx (1 - \gamma_k) / a \gamma_k \approx (c/a) k^2. \quad (4.9)$$

At the transition to the spin-glass phase the local-field distribution function becomes symmetric: $P(\epsilon) \rightarrow P_{SG}(\epsilon) = P_{SG}(-\epsilon)$, the magnetization goes to zero, and $a = 0$. In this case the acoustic branch of the collective excitations has a linear dispersion law:

$$E_{SG}(k) \approx [(1 - \gamma_k) / b \gamma_k]^{1/2} \approx (c/b)^{1/2} k. \quad (4.10)$$

As we have already mentioned, distribution function (1.2) leads to a discrete spectrum of local fields, and here Eq. (4.7) is an algebraic equation of degree n , where n is the number of local fields. One can solve Eq. (4.7) graphically after rewriting this equation in the form

$$-\frac{1}{\gamma_k} = M_0(E) = \sum_j \frac{W_j \epsilon_j}{E - \epsilon_j}, \quad -1 \leq \gamma_k \leq 1. \quad (4.11)$$

We introduce dimensionless constant-energy surfaces in the

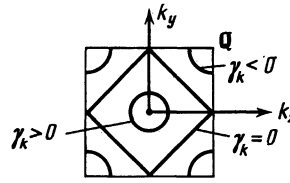


FIG. 1. The Brillouin zone for a square lattice and the constant-energy surface $\gamma_k = \text{const}$.

first Brillouin zone for the "dispersion law" $\gamma_k = \text{const}$. These surfaces include the surface $\gamma_k = 0$, which is the boundary of the halved Brillouin zone (Fig. 1). The solutions of (4.11) for $\gamma_k = 0$ represent the spectrum of the local fields $\{\epsilon_j\}$. The solutions of (4.11) over the entire range of γ_k are shown schematically in Fig. 2, from which we see that n nonoverlapping energy bands ("smeared" local fields) arise. We denote these solutions by E_{jk} , where E_{jk} , the dispersion law for spin waves in the j th band, is "genetically" related to the local field ϵ_j . The width of the j th band is equal to the difference in the energies determined from the equations $M_0(E) = 1$ and $M_0(E) = -1$ in the vicinity of ϵ_j .

The density of states in our zeroth approximation is

$$\rho_0(E) = \frac{1}{N} \sum_k \left(-\frac{1}{\pi} \right) \text{Im} G_k^0(E + i0) \\ = \frac{1}{N} \sum_k \sum_j C(E_{jk}) \delta(E - E_{jk}), \quad (4.12)$$

where the statistical weight $C(E_{jk})$ of each state depends on all the probabilities for the occurrence of the local fields, and the sum of these weights obeys

$$\sum_j C(E_{jk}) = 1$$

for any k belonging to the Brillouin zone. To obtain the excitation spectrum of the system and the density of excited states the negative solutions $E_{jk} < 0$ must be inverted ($E_{jk} \rightarrow |E_{jk}|$), since they refer to spin subsystem B . It follows from (4.9) that the density of states in the three-dimensional case will be proportional to \sqrt{E} at small values of E .

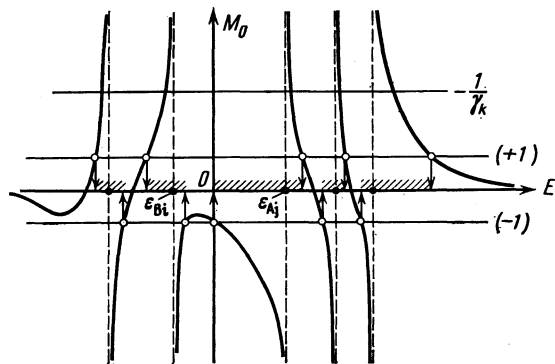


FIG. 2. Graphical solution of equation (4.11). The energy values at which $M_0(E) = -1$ correspond to the center of the Brillouin zone ($k = 0$) and the values at which $M_0(E) = 1$ correspond to the points $\mathbf{k} = \mathbf{Q} = \pi/a (\pm 1, \pm 1)$. The hatching indicates the regions in which solutions exist (the widths of the spin-wave bands).

In the spin-glass phase the spectrum becomes doubly degenerate, with a density of states in the three-dimensional case $\propto E^2$ for small E .

(b) Two-sublattice state

We shall omit the trivial computations and simply give the expressions for the Fourier transforms of the Green functions for the two-sublattice state:

$$\begin{aligned} G_{11}^0(q, E) &= g_1(E)/D_0(q, E), & G_{22}^0(q, E) &= g_2(E)/D_0(q, E), \\ G_{12}^0(q, E) &= -\gamma_q M_1^0(E) g_2(E)/D_0(q, E), & (4.13) \\ G_{21}^0(q, E) &= -\gamma_q M_2^0(E) g_1(E)/D_0(q, E), \end{aligned}$$

where

$$\begin{aligned} D_0(q, E) &= 1 - \gamma_q^2 M_1^0(E) M_2^0(E), \quad 1 \leq \gamma_q \leq 0, & (4.14) \\ g_i(E) &= \int \frac{P_i(\epsilon) d\epsilon}{E - \epsilon}, & M_i^0(E) &= \int \frac{P_i(\epsilon) \epsilon d\epsilon}{E - \epsilon}, \\ \gamma_q &= \frac{1}{z} \sum_h e^{iqh}. & (4.15) \end{aligned}$$

Let us briefly discuss the structure of the energy spectrum determined by the poles $D_0(q, E) = 0$ of the Green functions in the case of a discrete distribution of local fields in the antiferromagnetic and spin-glass states. In both cases the spectrum is doubly degenerate, since in the antiferromagnet one has $M_2^0(-E) = M_1^0(E)$ and in the spin glass $M_1^0(E) = M_2^0(E) \equiv M_{SG}(E)$. Near $E = 0$ we have the expansion

$$\begin{aligned} M_1^0(E) M_2^0(E) &= 1 + (2b_1 - a_1^2) E^2 + \dots, & (4.16) \\ a_1 &= \int \frac{P_1(\epsilon) d\epsilon}{\epsilon}, & b_1 &= \int \frac{P_1(\epsilon) \epsilon d\epsilon}{\epsilon^2}, \end{aligned}$$

with $2b_1 - a_1^2 > 0$, and in the spin-glass phase $a_1 = 0$. From (4.14) and (4.16) we find for small E and $q(\gamma_q \approx 1 - cq^2)$

$$E^2(q) \approx \frac{1 - \gamma_q^2}{\gamma_q^2 (2b_1 - a_1^2)} \approx \frac{c}{b_1 - a_1^2/2} q^2, \quad (4.17)$$

i.e., an acoustic branch of the spectrum with a linear dispersion law. The graphical and analytical solutions of the equation $D_0(q, E) = 0$ show that the excitation spectrum of the system consists of n nonoverlapping energy bands of spin-wave excitations (one acoustic and $n - 1$ optical) with dispersion laws $E_j(q)$, where n is the number of local fields of different moduli. The density of states of the j th band appears in the total density of states of the system with a certain statistical weight C_j , where $\sum C_j = 1$.

5. EFFECTIVE TRANSLATIONALLY INVARIANT MEDIUM. DYSON'S EQUATION AND THE T MATRIX

Let us compare the Green function \hat{G}_0 which we have obtained to a matrix \hat{H}_0 which describes the properties of an effective translationally invariant medium:

$$(E\hat{I} - \hat{H}_0)\hat{G}_0 = \hat{I}. \quad (5.1)$$

From (5.1) and (4.2) we find

$$\hat{H}_0 = E\hat{I} - \hat{G}_0^{-1} = E\hat{I} - \langle \hat{g} \rangle^{-1} (\hat{I} + \langle \hat{g} \hat{V} \rangle). \quad (5.2)$$

(a) Homogeneous case

It is easily shown that

$$(\hat{G}_0^{-1})_{fm} = \frac{1}{N} \sum_k e^{ik(f-m)} (G_k^0)^{-1} = \frac{1}{g(E)} \left[\delta_{fm} + \frac{M_0(E)}{z} \tilde{\delta}_{fm} \right], \quad (5.3)$$

where $\tilde{\delta}_{fm} = 1$ if f and m are nearest neighbors and zero otherwise. Equation (5.3) implies

$$(\hat{H}_0)_{fm} = \left(E - \frac{1}{g(E)} \right) \delta_{fm} - J_0(E) \tilde{\delta}_{fm}, \quad J_0(E) = \frac{1}{z} \frac{M_0(E)}{g(E)}. \quad (5.4)$$

After straightforward manipulations, the diagonal matrix element assumes the form $(\hat{H}_0)_{ff} = zJ_0(E)$, so that the matrix elements of \hat{H}_0 have the property (3.6). The function $zJ_0(E)$ is an effective local field in the translational medium, simultaneously incorporating both fluctuations of the spin environment and fluctuations of the exchange parameters. If the fluctuations of the environment are formally neglected (after the value of each spin is replaced by its average value σ), then $J_0(E)/\sigma$ has the meaning of an effective exchange parameter and is analogous to the coherent potential.^{1-3,14,15}

(b) Two-sublattice case

It can be shown¹⁷ by an analogous method that in the antiferromagnetic state

$$(\hat{H}_0)_{ff'} = zK_1^0(E) \delta_{ff'}, \quad (\hat{H}_0)_{fm} = -K_1^0(E) \tilde{\delta}_{fm}, \quad (5.5)$$

$$(\hat{H}_0)_{mm'} = zK_2^0(E) \delta_{mm'}, \quad (\hat{H}_0)_{mf} = -K_2^0(E) \tilde{\delta}_{mf},$$

where

$$K_i^0(E) = M_i^0(E)/zg_i(E), \quad K_2^0(-E) = -K_1^0(E). \quad (5.6)$$

As before, $zK_1^0(E)$ is the effective local field in which the spins of sublattice 1 are located. Since these spins interact only with their nearest neighbors in sublattice 2, which is occupied predominantly by "down" spins and has a relative magnetization $\sigma_2 = -|R|$, one can write

$$zK_1^0(E) = z(-|R|)(-K_1^0(E)/|R|) \equiv z(-|R|)J_0(E).$$

If one neglects the spin fluctuations of the environment, the quantity $J_0(E)$ has the meaning of an effective exchange between nearest neighbors and is analogous to the coherent potential. In an antiferromagnet the average and asymptotic values of $J_0(E)$ are negative:

$$\int J_0(E) dE < 0, \quad J_0(\pm\infty) < 0;$$

at the transition to the spin-glass phase, however, these quantities vanish.

Let us introduce the fluctuation matrix $\hat{U} = \hat{H} - \hat{H}_0$. Then, with allowance for (5.1), Eq. (3.5) assumes the form of Dyson's equation:

$$(\hat{G}_0^{-1} - \hat{U})\hat{G} = \hat{I}, \quad (5.7)$$

whose solution can be expressed in terms of the T matrix:

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{T} \hat{G}_0.$$

The \hat{T} matrix, in turn, obeys the equation

$$\hat{T} = \hat{U} + \hat{U} \hat{G}_0 \hat{T}, \quad (5.8)$$

and the problem of finding the complete configuration-averaged Green function $\langle \hat{G} \rangle$ reduces to finding $\langle \hat{T} \rangle$.

Let us first consider the structure of \hat{U} in general form. It follows from (3.4) and (4.2) that

$$\hat{U} = (\langle \hat{g} \rangle^{-1} - \hat{g}^{-1}) - (\hat{V} - \langle \hat{g} \rangle^{-1} \langle \hat{g} \hat{V} \rangle), \quad (5.9)$$

where the first bracket corresponds to diagonal fluctuations and the second to off-diagonal fluctuations. Since the matrix elements of \hat{H}_0 in the cases under consideration satisfy condition (3.6), one can use the representation

$$\hat{U} = \hat{H} - \hat{H}_0 = \sum_p [\hat{h}(p) - \hat{h}_0(p)] = \sum_p \hat{u}(p), \quad (5.10)$$

where the summation is over all nearest-neighbor pairs $p = (fm)$. The concrete form of the partial fluctuation matrices \hat{u} for the ferromagnetic and antiferromagnetic states will be given below.

Following Velicky *et al.*¹⁸ (see also Refs. 3 and 11), we write (5.8) in the form

$$\hat{T} = \sum_p \hat{u}(p) (\hat{I} + \hat{G}_0 \hat{T}) = \sum_p \hat{Q}(p).$$

For $\hat{Q}(p)$ one easily obtains the representation

$$\hat{Q}(p) = \hat{\varepsilon}(p) \left[\hat{I} + \hat{G}_0 \sum_{p'} \hat{Q}(p') \right], \quad (5.11)$$

where $\hat{\varepsilon}(p)$ is the partial scattering matrix for scattering by the nearest-neighbor pair p :

$$\hat{\varepsilon}(p) = (\hat{I} + \hat{u}(p) \hat{G}_0)^{-1} \hat{u}(p). \quad (5.12)$$

The basic simplification of the problem of evaluating $\langle \hat{T} \rangle$ consists of neglecting fluctuation correlations and multiple-scattering effects. In this approximation (the single-bond approximation)¹⁸ we obtain

$$\langle \hat{T} \rangle = (\hat{I} - \hat{M} \hat{G}_0)^{-1} \hat{M}, \quad \hat{M} \approx \sum_p [\hat{I} + \langle \hat{\varepsilon}(p) \rangle \hat{G}_0]^{-1} \langle \hat{\varepsilon}(p) \rangle, \quad (5.13)$$

where \hat{M} , as is readily shown, is the mass operator of the pseudo-Dyson's equation

$$\langle \hat{G} \rangle = \hat{G}_0 + \hat{G}_0 \hat{M} \langle \hat{G} \rangle. \quad (5.14)$$

As can be seen from (5.13), evaluation of the translationally invariant matrix \hat{M} reduces to finding $\langle \hat{\varepsilon}(p) \rangle$ and then performing a summation.

The configurational average $\langle \hat{\varepsilon}(fm) \rangle$ for a fixed nearest-neighbor pair (fm) will be found from the following considerations.

First, a given pair has a probability ν_{AA} of being an $(\alpha\alpha')$ pair, a probability ν_{BB} of being a $(\beta\beta')$ pair, and a probability ν_{AB} of being a pair with antiparallel spins. The probabilities ν_{AA} , ν_{BB} , and ν_{AB} are essentially the concentrations of the corresponding pairs and are thus (in the general case) temperature dependent.

Second, it is necessary to introduce the concept of frustrated exchange bonds. A bond $J > 0$ is frustrated if it links a pair of antiparallel spins $(\alpha\beta)$, and, similarly, a bond $K < 0$ is frustrated if it links parallel spins $(\alpha\alpha')$ or $(\beta\beta')$. Thus, each type of pair consists of both normal (0) and frustrated (F) bonds:

$$\nu_{AA} = \nu_{AA}^0(J) + \nu_{AA}^F(K), \quad \nu_{BB} = \nu_{BB}^0(J) + \nu_{BB}^F(K), \quad (5.15)$$

$$\nu_{AB} = \nu_{AB}^0(K) + \nu_{AB}^F(J), \quad \nu_{AA} + \nu_{BB} + \nu_{AB} = 1.$$

Third, the \hat{t} matrix depends in the general case on the thermodynamic averages $\sigma_f(T)$ and $\sigma_m(T)$ on neighboring sites. For dealing with the finite-temperature case, one can introduce the relative magnetizations of subsystems A and B :

$$R_A(T) = N_A^{-1} \sum_\alpha \sigma_\alpha(T), \quad -R_B(T) = N_B^{-1} \sum_\beta \sigma_\beta(T), \quad (5.16)$$

so that $\sigma_\alpha \approx R_A(T)$, $\sigma_\beta \approx -R_B(T)$, with $R_A(0) = R_B(0) = 1$.

Let us now give explicit expressions for \hat{u} , $\hat{\varepsilon}$, and $\langle \hat{t} \rangle$ and present the results of our evaluation of the translationally invariant mass operator \hat{M} for the ferromagnetic and antiferromagnetic states.

a) Homogeneous case (FM)

In symbolic form the partial fluctuation matrix is

$$\begin{aligned} \hat{u}(fm) &= \hat{h}(fm) - \hat{h}_0(fm) \\ &= \begin{pmatrix} \xi_{fm} & -\xi_{fm} \\ -\xi_{mf} & \xi_{mf} \end{pmatrix}, \quad \begin{aligned} \xi_{fm} &= I_{fm} \sigma_m - J_0(E), \\ \xi_{mf} &= I_{fm} \sigma_f - J_0(E), \end{aligned} \end{aligned} \quad (5.17)$$

where the matrix elements are nonzero only for nearest neighbors (fm) . A direct calculation by formula (5.12) yields

$$\begin{aligned} \hat{\varepsilon}(fm) &= \frac{1}{d(fm)} \hat{u}(fm), \\ d(fm) &= 1 - (\xi_{fm} + \xi_{mf}) (G_0^0 - G_{m-f}^0). \end{aligned} \quad (5.18)$$

Because the system is (on the average) isotropic, the difference between the Green functions can be represented in the form

$$G_0^0 - G_{m-f}^0 = \frac{1}{z} \sum_{(m-f)} (G_0^0 - G_{m-f}^0) = \frac{1}{N} \sum_k (1 - \gamma_k) G_k^0 = \Delta(E). \quad (5.19)$$

Guided by the aforementioned principles for evaluating $\langle \hat{t} \rangle$, we find

$$\begin{aligned} \langle \hat{\varepsilon}(fm) \rangle &= [\nu_{AA}^0(J) \hat{\varepsilon}(fm) |_{I_{fm}=J} + \nu_{AA}^F(K) \hat{\varepsilon}(fm) |_{I_{fm}=K}] \sigma_m = \sigma_f = -R_A \\ &+ [\nu_{BB}^0(J) \hat{\varepsilon}(fm) |_{I_{fm}=J} + \nu_{BB}^F(K) \hat{\varepsilon}(fm) |_{I_{fm}=K}] \sigma_m = \sigma_j = -R_B \\ &+ [\nu_{AB}^0(K) \hat{\varepsilon}(fm) |_{I_{fm}=K} + \nu_{AB}^F(J) \hat{\varepsilon}(fm) |_{I_{fm}=J}] \sigma_j = R_A \sigma_m = -R_B \\ &= \begin{pmatrix} t_1(E) & -t_1(E) \\ -t_2(E) & t_2(E) \end{pmatrix}, \end{aligned} \quad (5.20)$$

$$t_1 = \left\langle \frac{\xi_{fm}}{d(fm)} \right\rangle, \quad t_2 = \left\langle \frac{\xi_{mf}}{d(fm)} \right\rangle.$$

The mass operator (5.13) is

$$\hat{M} = \frac{1}{1 + 2\bar{t}(E) \Delta(E)} \sum_{(fm)} \langle \hat{\varepsilon}(fm) \rangle, \quad \bar{t} = \frac{1}{2} (t_1 + t_2), \quad (5.21)$$

and its Fourier transform is

$$M_k(E) = \sum_{(l-n)} e^{ik(l-n)} (\hat{M})_{nl} = \frac{z(1-\gamma_k) \bar{t}(E)}{1 + 2\bar{t}(E) \Delta(E)}. \quad (5.22)$$

Finally, the expression for the Fourier transform of the con-

figuration-averaged Green function in the approximation of independent scattering by each exchange bond is of the form

$$G_k^{-1}(E) = [G_k^0(E)]^{-1} - M_k(E) \\ = g^{-1}(E) + z\gamma_k J_0(E) - z(1-\gamma_k) \frac{\bar{t}(E)}{1+2\bar{t}(E)\Delta(E)} \quad (5.23)$$

where $g(E)$, $J_0(E)$, $\Delta(E)$, and $\bar{t}(E)$ are given by (4.5), (4.6), (5.4), (5.19), and (5.21), while $\bar{t}(E)$ at $T=0$ is given by

$$\bar{t}(E) = v_{AA}^0 \frac{J-J_0}{1-2(J-J_0)\Delta} + v_{AA}^F \frac{K-J_0}{1-2(K-J_0)\Delta} \\ - v_{BB}^0 \frac{J+J_0}{1+2(J+J_0)\Delta} - v_{BB}^F \frac{K+J_0}{1+2(K+J_0)\Delta} \\ - (v_{AB}^0 + v_{AB}^F) \frac{J_0}{1+2J_0\Delta}. \quad (5.24)$$

(b) Two-sublattice case (AFM)

Using the Green functions \hat{G}_0 and \hat{H}_0 for the two-sublattice state of the system, we find

$$\hat{t}(fm) = \frac{1}{d(fm)} \hat{u}(fm), \quad \hat{u}(fm) = \begin{pmatrix} \xi_{fm}^{(1)} - \xi_{fm}^{(4)} \\ -\xi_{mf}^{(2)} & \xi_{mf}^{(2)} \end{pmatrix}, \quad (5.25) \\ d(fm) = 1 - [\xi_{fm}^{(1)} (G_{jf}^0 - G_{mf}^0) + \xi_{mf}^{(2)} (G_{mn}^0 - G_{jm}^0)], \\ \xi_{fm}^{(1)} = I_{fm} \sigma_m - K_1^0(E), \quad \xi_{mf}^{(2)} = I_{fm} \sigma_j - K_2^0(E).$$

We recall that the fluctuation parameters ξ are nonzero only for nearest neighbors, $f \in 1, m \in 2$. In analogy with the previous case

$$d(fm) = 1 - \xi_{fm}^{(1)} \Delta_1(E) - \xi_{mf}^{(2)} \Delta_2(E), \quad (5.26) \\ \Delta_{1,2}(E) = \frac{2}{N} \sum_q g_{1,2}(E) [1 + \gamma_q^2 M_{2,1}^0(E)] [D_0(q, E)]^{-1}$$

(the difference of the Green functions was evaluated using their explicit form (4.13) and performing a Fourier transform).

Let us now give an expression for $\langle \hat{t}(fm) \rangle$. A nearest-neighbor pair has a probability $v_{ij}(I)$ of being found in state (ij, I) , which is characterized by the spin direction $i = A, B$ at site i in sublattice 1, the spin direction $j = A, B$ at site j in sublattice 2, and the exchange interaction $I = J, K$ (state A corresponds to spin "up" and B to spin "down"). The probabilities $v_{ij}(I)$ are the concentrations of the corresponding pairs. By summing over all possible states of a pair, we obtain an expression for $\langle \hat{t} \rangle$ in the form (5.20), where

$$t_1(E) = \left\langle \frac{\xi_{fm}^{(1)}}{d(fm)} \right\rangle = \frac{1}{2} \sum_I \sum_{ij} \frac{v_{ij}(I) \xi_i^{(1)}}{d(ij, I)}, \\ \xi_j^{(1)} = I \sigma_j - K_1^0(E), \\ t_2(E) = \left\langle \frac{\xi_{mf}^{(2)}}{d(fm)} \right\rangle = \frac{1}{2} \sum_I \sum_{ij} \frac{v_{ij}(I) \xi_i^{(2)}}{d(ij, I)}, \\ \xi_i^{(2)} = I \sigma_i - K_2^0(E), \\ d(ij, I) = 1 - \xi_j^{(1)} \Delta_1 - \xi_i^{(2)} \Delta_2, \quad i, j = A, B, \quad I = J, K, \quad (5.27)$$

with $\sigma_A = +1$, $\sigma_B = -1$ at $T=0$.

The mass operator (5.13) in the present case is of the form

$$\hat{M}(E) = \frac{1}{d(E)} \sum_{(jm)} \langle \hat{t}(jm) \rangle, \\ d(E) = 1 + t_1(E) \Delta_1(E) + t_2(E) \Delta_2(E). \quad (5.28)$$

We introduce the intrasublattice and intersublattice Fourier transforms of the mass operator:

$$M_{11}(q, E) = \sum_{(j-j')} e^{iq(t-j')} M_{jj'}(E), \\ M_{jj'}(E) = \frac{2}{N} \sum_q e^{-iq(t-j')} M_{11}(q, E)$$

and analogous expressions for the remaining components. A direct calculation making use of the matrix structure of $\langle \hat{t} \rangle$ yields

$$M_{11}(q, E) = \frac{zt_1(E)}{d(E)} \equiv \tilde{t}_1(E), \quad M_{12}(q, E) = -\gamma_q \tilde{t}_1(E), \\ M_{22}(q, E) = \frac{zt_2(E)}{d(E)} \equiv \tilde{t}_2(E), \quad M_{21}(q, E) = -\gamma_q \tilde{t}_2(E). \quad (5.29)$$

Solution of the pseudo-Dyson's equation (5.14) yields the result¹⁷

$$G_{11}(q, E) = \frac{g_1(E) [1 - \alpha_2(E)]}{D(q, E)}, \\ G_{12}(q, E) = -\gamma_q \frac{g_2(E) [M_1^0(E) + \alpha_1(E)]}{D(q, E)}, \\ G_{22}(q, E) = \frac{g_2(E) [1 - \alpha_1(E)]}{D(q, E)}, \\ G_{21}(q, E) = -\gamma_q \frac{g_1(E) [M_2^0(E) + \alpha_2(E)]}{D(q, E)}, \quad (5.30)$$

where

$$D(q, E) = [1 - \alpha_1(E)] [1 - \alpha_2(E)] \\ - \gamma_q^2 [M_1^0(E) + \alpha_1(E)] [M_2^0(E) + \alpha_2(E)]. \quad (5.31)$$

Thus the renormalization of the zeroth-approximation spectrum of the system on account of independent scattering processes at each exchange bond is described by the functions

$$\alpha_i(E) = g_i(E) \tilde{t}_i(E) = g_i(E) z t_i(E) / d(E), \quad (5.32)$$

each of which has a real and imaginary part, which lead to a modification of the bare spectrum and to attenuation. The results can be interpreted as follows. The sum $M_i^0 + \alpha_i$ can be written in the form

$$M_i^0 + \alpha_i = z g_i \left(\frac{M_i^0}{z g_i} + \frac{t_i}{d} \right) = z g_i (K_i^0 + t_i^*), \quad t_i^* = \frac{t_i}{d}.$$

This means that in the approximation of independent scatterers the effective exchange interaction is modified by the addition of a function proportional to the averaged partial scattering matrix.

In finding $\langle \hat{t} \rangle$ we made use of the concentrations of the normal and frustrated bonds; these concentrations can be found by analyzing all the possible types of local fields and comparing the exchange bonds which arise in each case with

the corresponding probabilities from the distribution function $P(\varepsilon)$.¹⁷

6. CONCLUSION

In the present paper we have proposed a systematic means of describing the spectral characteristics of homogeneously disordered Heisenberg lattice magnets with spin $S = 1/2$. The distribution of positive and negative exchange bonds between nearest neighbors can be made random in various ways (including the random site model) and is specified by some distribution function $\rho(I_{fm})$. Depending on the characteristics of this function the ground state of the system in the general case can be a ferromagnet, spin glass, or antiferromagnet.

The proposed theory is based primarily on the introduction of the local-field distribution function $P(\varepsilon)$, which, being a functional of $\rho(I_{fm})$, describes the type and energy structure of the ground state (i.e., the short-range order). We have given a prescription for constructing the zeroth approximation \hat{G}_0 for the configuration-averaged Green function $\langle G \rangle$; this prescription calls for the use of the distribution $P(\varepsilon)$ for evaluating the averages. From the function \hat{G}_0 one can find a unique matrix \hat{H}_0 describing an effective translationally invariant medium. The matrix elements of \hat{H}_0 are expressed in terms of an effective exchange parameter which depends on the spectral variable and is analogous to the coherent potential.

Then, with the nontrivial zeroth approximation at our disposal, we introduce fluctuations, Dyson's equation, and the scattering matrix \hat{T} . The problem of evaluating $\langle \hat{G} \rangle$ reduces to finding $\langle \hat{T} \rangle$, which in the general case is a complicated function of the partial scattering matrices $\langle \hat{t}(fm) \rangle$ which describe scattering by single exchange bonds. This theory is thus a version of the average-scattering-matrix method. For calculating $\langle \hat{t}(fm) \rangle$ we outline a method which is essentially based on the concept of frustrated and normal exchange bonds between nearest neighbors. The method developed in this paper for describing the energy spectrum of disordered magnets can apparently be used to describe the properties of other disordered systems as well.

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¹¹If $\varepsilon_f^0 = 0$ the spin at site f is "paramagnetic" and can have any orientation. The imposition of a small magnetic field along the quantization axis lifts this degeneracy, and the spin will take on the value $\sigma_f^0 = +1$.

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