

- ¹P. Hu, R. C. Dynes, and V. Narayanamurti, *Phys. Rev.* **B10**, 2786 (1974).
- ²A. I. Golovashkin, K. V. Mitsev, and G. P. Motulevich, *Zh. Eksp. Teor. Fiz.* **68**, 1408 (1975) [*Sov. Phys. JETP* **41**, 701 (1976)].
- ³R. C. Dynes, V. Narayanamurti, and J. P. Garno, *Phys. Rev. Lett.* **39**, 229 (1977).
- ⁴K. E. Gray and H. W. Williamson, *J. Low Temp. Phys.* **31**, 911 (1978).
- ⁵J. J. Chang and D. J. Scalapino, *Phys. Rev.* **B10**, 4047 (1974).
- ⁶V. G. Baru and A. A. Sykhanov, *Pis'ma Zh. Eksp. Teor. Fiz.* **21**, 209 (1975) [*JETP Lett.* **21**, 93 (1975)].
- ⁷L. N. Smith, *J. Low Temp. Phys.* **28**, 519 (1977); D. I. Scalapino and B. A. Huberman, *Phys. Rev. Lett.* **39**, 1365 (1977).
- ⁸V. F. Elesin, *Zh. Eksp. Teor. Fiz.* **71**, 1490 (1976) [*Sov. Phys. JETP* **44**, 780 (1976)].
- ⁹V. F. Elesin, *Zh. Eksp. Teor. Fiz.* **73**, 355 (1977) [*Sov. Phys. JETP* **46**, 185 (1977)].
- ¹⁰V. F. Elesin, V. E. Kondrashov, and Yu. M. Sklyarov, *Fiz. Tverd. Tela (Leningrad)* **18**, 3393 (1976) [*Sov. Phys. Solid State* **18**, 975 (1976)].
- ¹¹I. K. Kirichenko and V. P. Seminozhenko, *Fiz. Nizk. Temp.* **3**, 987 (1977) [*Sov. J. Low Temp. Phys.* **3**, 479 (1977)].
- ¹²A. G. Aronov and B. Z. Spivak, *Fiz. Nizk. Temp.* **4**, 1365 (1978) [*Sov. J. Low Temp. Phys.* **4**, 641 (1978)].
- ¹³V. F. Elesin and E. B. Levchenko, *Fiz. Tverd. Tela (Leningrad)* **20**, 2459 (1978) [*Sov. Phys. Solid State* **20**, 1419 (1979)].
- ¹⁴V. F. Elesin, *Zh. Eksp. Teor. Fiz.* **66**, 1755 (1974) [*Sov. Phys. JETP* **39**, 862 (1974)].
- ¹⁵G. M. Éliashberg, *Zh. Eksp. Teor. Fiz.* **61**, 1254 (1971) [*Sov. Phys. JETP* **34**, 668 (1972)]; *Pis'ma Zh. Eksp. Teor. Fiz.* **11**, 186 (1970) [*JETP Lett.* **11**, 114 (1970)].
- ¹⁶R. A. Vardanyan and B. I. Ivlev, *Zh. Eksp. Teor. Fiz.* **65**, 2315 (1973) [*Sov. Phys. JETP* **38**, 1156 (1974)].
- ¹⁷V. F. Elesin, *Fiz. Tverd. Tela (Leningrad)* **19**, 2977 (1977) [*Sov. Phys. Solid State* **19**, 1744 (1977)].
- ¹⁸A. G. Aronov and B. Z. Spivak, *Fiz. Tverd. Tela (Leningrad)* **18**, 541 (1976) [*Sov. Phys. Solid State* **18**, 312 (1976)].
- ¹⁹J. T. C. Yeh and D. N. Laugenberg, *Bull. Am. Phys. Soc.* **21**, 404 (1976).
- ²⁰A. A. Andronov, A. A. Vitt, and S. É. Khaikin, *Teoriya kolebanií (Theory of Oscillations)*, Fizmatgiz, 1959 (Eng. Transl., Pergamon, 1966).
- ²¹A. F. Volkov and Sh. M. Kogan, *Usp. Fiz. Nauk* **96**, 633 (1968) [*Sov. Phys. Usp.* **11**, 881 (1969)].
- ²²F. G. Bass, V. S. Bochkov, and Yu. G. Gurevich, *Zh. Eksp. Teor. Fiz.* **58**, 1814 (1970) [*Sov. Phys. JETP* **31**, 972 (1970)].
- ²³K. E. Gray, *Solid State Commun.* **26**, 633 (1970).

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Contribution to the theory of ferromagnets with admixture of antiferromagnetic bonds

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It is shown that replacement of one ferromagnetic bond in a ferromagnet by an antiferromagnetic bond leads to appearance of local energy levels. The spectrum of these levels and their contribution to the thermodynamic functions are investigated. For a spin $s = 1/2$, the problem is solved exactly and an expression is obtained for the only energy level existing in this case and for the wave function. At $s > 1/2$ the problem is solved approximately. In this case several local levels can exist. Their energies are calculated. Turning on an external magnetic field causes these levels to cross, and this leads in turn to strong bursts of the susceptibility and of the heat capacity in magnetic field corresponding to the level crossing.

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1. INTRODUCTION

This paper deals with the properties of a Heisenberg ferromagnet with low concentration of randomly disposed antiferromagnetic bonds. Many recent papers are devoted to models of this kind in connection with the spin-glass problem (a detailed bibliography can be found in the reviews^{1,2}). In practice, however, in all the papers the problem was solved in the molecular-field approximation or for the case of an infinite interaction radius (see, e.g., Refs. 3–5 and the references therein), and for the most part, furthermore, for an Ising magnet. No attention was paid whatever to all the phenomena connected with the presence of localized spin-wave excitations in the ferromagnet. It is these phenomena to which the present paper is devoted. We confine ourselves here to the case of low concentration

of the antiferromagnetic bonds.

It must be noted first that the cited papers¹⁻⁵ dealt with a problem with a Gaussian distribution of the exchange integrals, i.e., with a purely model problem. On the other hand, there exist magnets in which the exchange integrals can be randomly both ferromagnetic and antiferromagnetic. This situation arises when the interaction is via indirect exchange and the crystal contains two sorts of atoms that effect the indirect exchange, the first leading to ferromagnetic exchange the second to the antiferromagnetic one. Examples of such substances are the alloys $\text{CrTe}_{1-x}\text{Sb}_x$ (Ref. 6) and $\text{Co}(\text{S}_x-\text{Se}_{1-x})_2$,^{7,8} where CrTe and CoS_2 are ferromagnets and CrSb and CoSe_2 are antiferromagnets. We consider therefore a ferromagnet with nearest-neighbor interaction and with a ferromagnetic exchange integral J , con-

taining a small admixture of antiferromagnetic exchange bonds I . It turns out that at $I > 2J$ the purely ferromagnetic state is unstable and the spins that surround the antiferromagnetic bond begin to deviate from the direction of spontaneous magnetization. This deviation decreases exponentially with distance. Such formations are in effect localized spin waves.

Since the projection of the total angular momentum on the z axis commutes with the exchange Hamiltonian, we shall characterize the ground state of the system by the deviation ΔM of this projection, from the maximum possible value sN , where s is the spin of the individual atom and N is the number of atoms in the crystal. If I does not exceed greatly the threshold value $2J$, when the ground state corresponds to the case $\Delta M = -1$. It is easily understood that for $s = \frac{1}{2}$ this is the ground state for all $I > 2J$. In fact, it will be shown below that what deviate mainly are the spins in contact with the antiferromagnetic coupling. The deviation for their nearest neighbors is quite small. If the latter deviation is neglected then it is clear that the case $\Delta M = -2$ for $s = \frac{1}{2}$ corresponds to total flip of the spins in contact with the antiferromagnetic coupling, a situation that is energetically unfavorable, since we gain nothing in the antiferromagnetic exchange and lose in the ferromagnetic one. Therefore the energy corresponding to $\Delta M = -2$ will be higher for $s = \frac{1}{2}$ than that of the purely ferromagnetic state, and at $s = \frac{1}{2}$ the ground state corresponds to $\Delta M = 0$ at $I < 2J$ and to $\Delta M = -1$ at $I > 2J$.

It turns out that the case $\Delta M = -1$ can be solved exactly. The problem for $s = \frac{1}{2}$ has therefore an exact solution at all I , and for other s it has a solution in some interval of I . This simplest case will be considered in Sec. 2.

Next, if $s > \frac{1}{2}$, then at sufficiently large I the ground state corresponds to $\Delta M < -1$. This means, so to speak, two and more spin waves localized in one place. It is then necessary to take into account the interaction of these spin waves with one another. Naturally, this problem can no longer be solved exactly. We solve it approximately in Sec. 3. In Sec. 4 we consider the thermodynamics in an approximation linear in the concentration of the antiferromagnetic couplings. It turns out that at low temperatures the thermodynamic quantities are oscillating functions of the external magnetic fields, and at higher temperatures the oscillations become smoothed out, but all the quantities are anomalously large compared with their ordinary values.

2. THE CASE $\Delta M = -1$

The Hamiltonian is of the form

$$H = - \sum_{ij} J_{ij} s_i s_j - h \sum_i s_i^z \quad (1)$$

where J_{ij} is the exchange integral, s_i is the spin operator, h is the external magnetic field, and i and j number of lattice sites.

The purely ferromagnetic state Ψ_0 is defined as follows:

$$s_i^z \Psi_0 = s \Psi_0, \quad s_i^+ \Psi_0 = 0. \quad (2)$$

The wave function Ψ_1 of the state with $\Delta M = -1$ can be written in the form

$$\Psi_1 = \frac{1}{(2s)^{1/2}} \sum_i \varphi_i s_i^- \Psi_0. \quad (3)$$

It is easy to obtain for φ_i the equation

$$(\varepsilon_i - h) \varphi_i - 2s \sum_j J_{ij} (\varphi_i - \varphi_j) = 0. \quad (4)$$

Here $\varepsilon_i = E_1 - E_0$ and E_i is the energy of the state Ψ_i . Equation (4) was used by a number of authors to study various disordered magnets—see, e.g., the book by Izyumov and Medvedev.⁹ If $\Delta M = -p$, where $p > 1$, then an equation similar to (4) can be obtained for the wave function $\varphi_{i_1} \dots \varphi_{i_p}$ of a complex of p coupled spin waves, with account taken of their repulsion. Such an equation was obtained, e.g., in Ref. 10. We, however, will use for $p > 1$ an operator equation. From (1) we get, using the known commutation relations,

$$i \frac{\partial s_i^+}{\partial t} = h s_i^+ + 2 \sum_j J_{ij} (s_i^+ s_j^z - s_j^+ s_i^z). \quad (5)$$

We shall use Eq. (5) in the next section to study the spectrum at $p > 1$.

We proceed now to a detailed study of Eq. (4). It is easy to show, using (3), that the magnetization at the i -th site is equal to

$$s_i^{(z)} = s - |\varphi_i|^2, \quad \sum_i |\varphi_i|^2 = 1. \quad (6)$$

The normalization condition is equivalent to the condition $\Delta M = -1$. Let the antiferromagnetic coupling be between sites 0 and 1 (see Fig. 1a). Then Eq. (4) takes the form

$$\begin{aligned} (\varepsilon_i - h) \varphi_i - 2sJ \sum_j (\varphi_i - \varphi_j) &= V_i; \\ V_i &= 0 \text{ for } i \neq 0, 1, \\ V_i &= -V_0, \quad V_0 = 2s(I+J)(\varphi_1 - \varphi_0). \end{aligned} \quad (7)$$

The sum over j in (7) is over the nearest neighbors, J and I are the ferromagnetic and antiferromagnetic exchange integrals. We shall consider henceforth, for the sake of argument, a simple cubic lattice. Generalization to other lattices is elementary.

For a simple cubic lattice, the solution of (7) is

$$\begin{aligned} \varphi_i &= \sum_j G_{ij}^{(0)} (\varepsilon_i - h) V_j, \\ G_{ij}^{(0)}(\omega) &= \frac{1}{N} \sum_{\mathbf{k}} \frac{\exp[i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)]}{\omega - \varepsilon_{\mathbf{k}} + i\delta}, \end{aligned} \quad (8)$$

From (7) and (8), taking into account the normalization condition (6), we obtain the condition for the existence of a level and the explicit form of φ_i :

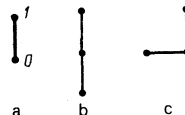


FIG. 1.

$$\varphi_i = \frac{G_{i1}^{(0)} - G_{i0}^{(0)}}{G_{01}^{(0)} - G_{00}^{(0)}} \varphi_0, \quad (9)$$

$$\varphi_0^2 = \left[\sum_i \left(\frac{G_{i1}^{(0)} - G_{i0}^{(0)}}{G_{01}^{(0)} - G_{00}^{(0)}} \right)^2 \right]^{-1},$$

$$4s(I+J)(G_{01}^{(0)} - G_{00}^{(0)}) = 1.$$

The equation for the level energy ε_1 can be rewritten in the form

$$[3 - c(\varepsilon_1 - h)]/c(\varepsilon_1 - h) = I/J, \quad (10)$$

$$c(\omega) = 12sJ(G_{01}^{(0)} - G_{00}^{(0)}) = 1 - \omega G_{00}^{(0)}(\omega).$$

The last equation can be easily obtained from the definition of $G_{ij}^{(0)}$ in (8). Using the tables of the function $G_{00}^{(0)}(\omega)$ (they are given, for example, in the book by Izyumov and Medvedev⁹), it is easily seen that at $\omega < 0$ the quantity $(3 - c)/c$ increases monotonically and its minimum value, 2, occurs at $\omega = 0$. It follows therefore that the critical value of I , at which a level first appears is equal to $2J$. At $I > 2J$ we have $\varepsilon_1 - h < 0$ and a real local level. At $I < 2J$ we have $\varepsilon_1 - h > 0$ and a quasilocal level near the threshold. Since $\text{Im}G_{00}^{(0)}(\omega) \sim \omega^{1/2}$ at $\omega > 0$, it is seen from (10) that the ratio of the damping to the level frequency is of the order of $(\varepsilon_1 - h)^{3/2}$. We note that in scattering of an ordinary spin wave by inhomogeneities we also have $\gamma(k) \sim \omega^{3/2} \varepsilon(k)$.

It is curious to note that the quantity $(3 - c)/c$ is very well approximated, in the large energy interval from 0 to $-12Js$, by the linear function

$$[3 - c(\omega)]/c(\omega) = 2 - 9\omega/32Js. \quad (11)$$

The error does not exceed 3% in this interval. Using the approximation (11), we obtain an explicit dependence of ε_1 on I/J :

$$\varepsilon_1 = h - \frac{32Js}{9} \left(\frac{I}{J} - 2 \right). \quad (12)$$

We recall that (12) is meaningful only at $\varepsilon_1 - h < 0$, since damping sets in at $\varepsilon_1 - h > 0$. We note that Eq. (12) is only a good extrapolation in a large energy interval. It does not describe correctly, however, the asymptotic behavior at $|\varepsilon - h| \ll 4Js$. In this region it is easy to obtain ε_1 from (10):

$$\varepsilon_1 = h - \frac{4Js}{3a} \left(\frac{I}{J} - 2 \right), \quad \left| \frac{I}{J} - 2 \right| \ll 1, \quad (13)$$

$$a = -4JsG_{00}^{(0)}(\omega=0) \approx 0.4926.$$

Comparison of (12) and (13) shows that the coefficients of $I/J - 2$ differ by 30%. Formula (13), however, is valid in a rather narrow range.

We consider now the asymptotic form of φ_i at $R_i \gg d$. From (8)–(10) we have

$$\varphi_i = \frac{12Js}{c} \varphi_0 (G_{i1}^{(0)} - G_{i0}^{(0)})$$

$$= -\frac{3d\varphi_0 \mathbf{R}_i \mathbf{R}_i}{2\pi c R_i^3} (1 + \kappa R_i) e^{-\kappa R_i},$$

where

$$\kappa^2 = -(e_1 - h)/2Js d^2 > 0,$$

d is the lattice constant, and $\mathbf{R}_{10} = \mathbf{R}_1 - \mathbf{R}_0$.

To conclude this section we note that if we place two

antiferromagnetic couplings in tandem, then the critical value of I decreases. For example, the configuration in Fig. 1 corresponds to $I_{cr} = 1.19J$, while the configuration in Fig. 1c corresponds to $I_{cr} = 1.13J$. By exactly the same method as used in the present section for the problem with one antiferromagnetic coupling, we can solve completely also problems with two couplings, but this will not be done here.

3. ARBITRARY ΔM

We consider now the case of arbitrary $p = -\Delta M$. We use for this purpose Eq. (5). For the case of one antiferromagnetic coupling located between sites 0 and 1, Eq. (5) can be rewritten in the form

$$i\partial s_i^+/\partial t - h s_i^+ + 2sJ \sum_j (s_j^+ - s_i^+) = W_i^+, \quad (14)$$

where

$$W_i^+ = 2sJ \sum_j \{s_j^+ (1 - s_i^+/s) - s_i^+ (1 - s_j^+/s)\}, \quad i \neq 0, 1;$$

$$W_0^+ = 2sJ \sum_{j=1} \{s_j^+ (1 - s_0^+/s) - s_0^+ (1 - s_j^+/s)\}$$

$$+ 2sJ (s_1^+ - s_0^+) + 2I (s_1^+ s_0^+ - s_0^+ s_1^+), \quad (14a)$$

$$W_1^+ = 2sJ \sum_{j=0} \{s_j^+ (1 - s_1^+/s) - s_1^+ (1 - s_j^+/s)\}$$

$$+ 2sJ (s_0^+ - s_1^+) + 2I (s_0^+ s_1^+ - s_1^+ s_0^+).$$

In contrast to Eq. (7) for φ_i , in the present case W_i differs from zero not only at $i = 0$ and 1. The formal solution of Eq. (14) is of the form

$$s_i^+(t) = \int_{-\infty}^{\infty} dt' \sum_j G_{ij}^{(0)}(t-t') W_j^+(t'), \quad (15)$$

$$G_{ij}^{(0)}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{ij}^{(0)}(\omega) e^{-i\omega t}.$$

Equations (14) and (15) can, naturally, not be solved exactly. We therefore solve them approximately, and then show that the errors of this approximate solution is of the order of several per cent. Our approximation consists of taking into account in the expression for W_i^+ in (14a) only the contribution from the antiferromagnetic coupling, i. e., from sites 0 and 1. In this case we obtain from (14) and (15)

$$s_i^+(t) = \int_{-\infty}^{\infty} dt' \{G_{i0}^{(0)}(t-t') - G_{i1}^{(0)}(t-t')\} W_0^+(t'), \quad (16)$$

$$W_0^+(t) = -2sJ (s_0^+ - s_1^+) - 2I (s_0^+ s_1^+ - s_1^+ s_0^+).$$

Equations (16) describe a diatomic antiferromagnetic molecule, and the sites 0 and 1 that enter into the molecule interact with one another and with themselves via the virtual spin waves of the ferromagnetic matrix, and the latter interaction is taken into account in the harmonic approximation. The states of such a molecule are characterized by two quantum numbers, the total angular momentum L and its projection M on the z axis. We, however, are interested only in the quantum number M . This means that we must find the state with minimal energy at a given M . It is easy to show that such a state is obtained at $L = M$. The corresponding wave function is

$$\Psi_{M,M} = \sum_m (M, M | s, s, m, M-m) \chi_{s,m}^{(1)} \chi_{s,M-m}^{(0)} \quad (17)$$

In (17), $L, M | s, s, m, M-m$ are Clebsch-Gordan coefficients, and $\chi_{s,m}^{(i)}$ are the wave functions of the sites 0 and 1. It is very important in what follows that the operators s_0^+ and s_1^+ transform $\Psi_{M,M}$ into $\Psi_{M+1,M+1}$, or more accurately

$$\begin{aligned} s_0^+ \Psi_{M,M} &= \alpha(s, M) \Psi_{M+1, M+1}, \\ s_1^+ \Psi_{M,M} &= -\alpha(s, M) \Psi_{M+1, M+1}, \\ (s_0^+ s_1^+ - s_1^+ s_0^+) \Psi_{M,M} &= \alpha(s, M) (M+1) \Psi_{M+1, M+1}. \end{aligned} \quad (18)$$

Here $\alpha(s, M)$ is a function that depends only on M and s . The last equation in (18) is a consequence of the first two. Equations (18) can be easily obtained by using the explicit forms of the Clebsch-Gordan coefficients¹¹ at $L=M$

$$\begin{aligned} (M, M | s, s, m, M-m) &= (-1)^m A(s, M) \left(\frac{(s+m)!(s+M-m)!}{(s-m)!(s-M+m)!} \right)^{1/2}, \\ \alpha(s, M) &= A(s, M) / A(s, M+1). \end{aligned} \quad (19)$$

It is seen from (18) that all the operators in (16) transform the state $|M, M\rangle$ into $|M+1, M+1\rangle$. Calculating the matrix elements of these operators between the states $|M-1, M-1\rangle$ and $|M, M\rangle$, we get

$$\begin{aligned} \exp[-i(E_{M-1}-E_M)t] &= \int_{-\infty}^{\infty} dt' \{G_{01}^{(0)}(t-t') - G_{00}^{(0)}(t-t')\} \\ &\times \exp[-i(E_{M-1}-E_M)t'] (4Js+2IM). \end{aligned} \quad (20)$$

Recognizing that $p=2s-M$, we easily obtain from (20) the following equation for $\varepsilon_p = E_p - E_0$:

$$\begin{aligned} \frac{3-c(\omega_p-h)}{c(\omega_p-h)} &= \frac{I}{J} \left(1 - \frac{p}{2s}\right), \\ \omega_p &= \varepsilon_{p+1} - \varepsilon_p, \quad \varepsilon_p = \sum_{k=0}^{p-1} \omega_k. \end{aligned} \quad (21)$$

It is seen from (21) that $\varepsilon_1 = \omega_0$, and the equation for ω_0 coincides with Eq. (10) for ε_1 . Equation (21) solves the problem of determining the energy levels ε_p .

We consider now the corrections for this formula. To avoid the use of non-commuting operators, we consider for simplicity the problem for classical angular momenta, i.e., the problem with $p \gg 1$ and $s \gg 1$. It will be shown later that s determines only the energy scale, and that p enters as part of the combination $p/2s$, so that the smallness of the corrections is not connected with the conditions $p \gg 1$ and $s \gg 1$. This is precisely why we are using this limit. In the classical limit we have from (5)

$$\begin{aligned} \frac{\partial m_i^x}{\partial t} &= 2s \sum_j J_{ij} (m_i^y [1-m_i^z]^h - m_j^y [1-m_i^z]^h) + h m_i^y, \\ \frac{\partial m_i^y}{\partial t} &= -2s \sum_j J_{ij} (m_i^x [1-m_i^z]^h - m_j^x [1-m_i^z]^h) - h m_i^x, \end{aligned} \quad (22)$$

here

$$\begin{aligned} s_i^x &= s m_i^x, \quad s_i^y = s m_i^y, \\ s_i^z &= s(1-m_i^z)^h, \quad m_i^2 = (m_i^x)^2 + (m_i^y)^2, \end{aligned}$$

where m_i is a planar vector. We shall be interested henceforth only in a solution of the precession type, for which

$$\begin{aligned} m_i^x &= m_i \cos \omega t, \quad m_i^y = -m_i \sin \omega t, \\ \partial m_i^x / \partial t &= \omega m_i^y, \quad \partial m_i^y / \partial t = -\omega m_i^x. \end{aligned} \quad (23)$$

From (22) and (23) we obtain for the case of one antiferromagnetic coupling the following equation:

$$\begin{aligned} (\omega-h)m_i + 2Js \sum_j (m_j - m_i) &= W_i; \\ W_i &= 2Js \sum_j \{m_j [1-(1-m_i^z)^h] - m_i [1-(1-m_j^z)^h]\}, \quad i \neq 0, 1; \\ W_0 &= 2Js \sum_{j \neq 0} \{m_j [1-(1-m_0^z)^h] - m_0 [1-(1-m_j^z)^h]\} \\ &\quad + 2sJ(m_1 - m_0) + 2sI[m_1(1-m_0^z)^h - m_0(1-m_1^z)^h], \\ W_1 &= 2Js \sum_{j \neq 0} \{m_j [1-(1-m_1^z)^h] - m_1 [1-(1-m_j^z)^h]\} \\ &\quad + 2sJ(m_0 - m_1) + 2sI[m_0(1-m_1^z)^h - m_1(1-m_0^z)^h]. \end{aligned} \quad (24)$$

In analogy with (8) and (15) we can express the formal solution of (24) in the form

$$m_i = \sum_j G_{ij}^{(0)} (\omega-h) W_j. \quad (25)$$

Equations (25), however, are still too complicated to solve. To simplify them, we note that $m_i \ll 1$ if $i \neq 0$ or $i \neq 1$. Therefore the terms $\sim m_i^2$ in (24) will be neglected. We are left then in (24) only with W_i with $i=0, 1, 2, \dots, 11$, where the numbering of the sites is illustrated in Fig. 2. If we write out (25) fully after this simplification and set m_i in the left-hand side of (25) equal in succession to m_0, \dots, m_{11} , then we obtain a 12-th order system of equations. From the structure of this system it is seen that

$$\begin{aligned} m_1 &= -m_0, \\ m_2 = m_3 = m_4 = m_5 &= -m_6 = -m_7 = -m_8 = -m_9, \\ m_{10} &= -m_{11}, \end{aligned} \quad (26)$$

and thus, there are only three independent quantities, which we choose to be m_0 , m_6 , and m_{11} . We obtain for these quantities the equation

$$\begin{aligned} m_0 &= A[G(0, 0, 0) - G(1, 0, 0)] - 2Bm_6[G(1, 0, 0) - G(1, 1, 0)] - 1/2 Bm_{11}[G(1, 0, 0) - G(2, 0, 0)], \\ m_6 &= A[G(1, 0, 0) - G(1, 1, 0)] - 1/2 Bm_6[G(0, 0, 0) + G(2, 0, 0) + 2G(1, 1, 0) - G(1, 0, 0) - G(1, 2, 0) - 2G(1, 1, 1)] - 1/2 Bm_{11}[G(1, 1, 0) - G(1, 2, 0)], \\ m_{11} &= A[G(1, 0, 0) - G(2, 0, 0)] - 2Bm_6[G(1, 1, 0) - G(2, 1, 0)] - 1/2 Bm_{11}[G(0, 0, 0) - G(3, 0, 0)], \end{aligned} \quad (27)$$

where

$$\begin{aligned} A &= -\frac{I}{J} m_0(1-m_0^z)^h - m_0 + 2m_6[1-(1-m_0^z)^h] + 1/2 m_{11}[1-(1-m_0^z)^h], \\ B &= 1 - (1-m_0^z)^h, \\ G(i, j, l, \omega) &= 4Js G_{ijl}^{(0)}(\omega). \end{aligned} \quad (27a)$$

Here $G_{ijl}^{(0)}$ are the matrix elements of $G^{(0)}$ with coordinates $R = ie_x + je_y + le_z$. If we neglect in the right-hand

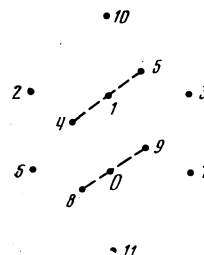


FIG. 2.

side of (27) the small terms of order m_6 and m_{11} , we get

$$\begin{aligned} m_6 &= a(\omega - h)m_0, & m_{11} &= b(\omega - h)m_0; \\ a(\omega) &= \frac{G(1, 0, 0) - G(1, 1, 0)}{G(0, 0, 0) - G(1, 0, 0)}, \\ b(\omega) &= \frac{G(1, 0, 0) - G(2, 0, 0)}{G(0, 0, 0) - G(1, 0, 0)}, \\ a(0) &= 0.1848, & b(0) &= 0.2598. \end{aligned} \quad (28)$$

It is quite clear that with increasing $|\omega|$ at $\omega < 0$ the quantities $a(\omega)$ and $b(\omega)$ will decrease, so that the contribution from m_6 and m_{11} is maximal at $\omega = h = 0$. We consider first this case.

Using the explicit form of some matrix elements⁹ and estimating the remaining ones from the asymptotic forms at large R , we obtain at $\omega = h = 0$

$$\begin{aligned} m_0 &= -1/3A + 0.1232m_6B + 0.1732m_{11}B, \\ m_6 &= -0.0616A + 0.1905m_6B + 0.013m_{11}B, \\ m_{11} &= -0.0866A + 0.053m_6B + 0.220m_{11}B. \end{aligned} \quad (29)$$

If we compare in the first equation of (29) the contribution from m_6 and m_{11} with the corresponding contribution from these quantities to A , we see that it is of the order of $a(0)$ and $b(0)$, and consequently this contribution is of the order of m_6^2/m_0^2 and m_{11}^2/m_0^2 , and such contributions were already neglected in the derivation of (27). Next, the term with m_{11} can be neglected in the equation for m_6 , and the term with Bm_6 necessitates a small correction, ≤ 0.2 , for m_6 . This correction is also of the order of m_6^2/m_0^2 , and its inclusion is an exaggeration of the accuracy. The situation is analogous in the last equation. We see thus that all the terms containing B in (29) can be neglected. Turning now to Eqs. (24), (25), and (27), this means that we need take into account in (25) only W_0 and W_1 . In this case we have from (25)

$$m_i = m_0 (G_{i0}^{(0)} - G_{i1}^{(0)}) / (G_{00}^{(0)} - G_{01}^{(0)}), \quad (30)$$

which is the analog of (9). For m_6 and m_{11} we get, naturally, Eqs. (28). For m_0 we have from (24), (25), and (28)

$$\frac{3-c}{c} = \frac{I}{J} (1 - m_0^2)^{1/2} - 1/2(4a+b) [1 - (1 - m_0^2)^{1/2}], \quad (31)$$

where $c(\omega - h)$ is defined in (10).

We now determine p . Since we are considering a cluster of 12 atoms, we have $M = 12s - p$. On the other hand $m_6 \ll 1$ and $m_{11} \ll 1$, therefore

$$p = 2s \{1 - (1 - m_0^2)^{1/2} + 2m_0^2 + 1/2 m_{11}^2\}. \quad (32)$$

Formulas (31) and (32) define ω as a function of p . From these formulas we get

$$\begin{aligned} \frac{p}{2s} &= \left(1 - \frac{3-c}{c} \frac{J}{I}\right) D, \\ D &= \left[1 + \frac{J}{2I} (4a+b)\right]^{-1} \left\{1 + \frac{4a^2+b^2}{2} \left(\frac{I}{J} + \frac{3-c}{c} + 4a+b\right)\right. \\ &\quad \left. \times \left[\frac{I}{J} + \frac{1}{2} (4a+b)\right]^{-1}\right\}. \end{aligned} \quad (33)$$

If $D = 1$, we obtain Eq. (21). The expression for D contains no parameter capable of making $|D - 1| \ll 1$. It turns out, however that there is a numerical smallness

that leads to $|D - 1| \ll 1$. For example, near the threshold $I \approx 2J$ and $|\omega - 4Js| \ll 4Js$, and there $D \approx 0.96$. We have next compiled a table of values of D at $I \approx 4J$. It turns out that when ω varies from zero to $-8Js$ the value of D differs from unity by not more than 3%. Since our entire theory cannot claim a higher accuracy, we shall not take these corrections into account.

Thus, there exists a numerical small parameter that makes Eq. (21) valid. We note that in the derivation of Eq. (33) the classical character of the problem played no role, for otherwise the answer would contain the small parameter $1/s$. In the classical limit we get from (21)

$$\begin{aligned} \frac{3-c(\omega_p-h)}{c(\omega_p-h)} &= \frac{I}{J} \left(1 - \frac{p}{2s}\right), \\ \varepsilon_p &= \int_0^p dk \omega_k. \end{aligned} \quad (34)$$

The first equation in (34) coincides with (33) at $D = 1$, and the second can be obtained directly from the classical equations of motion (22).

If we use the extrapolation (11), we obtain for ε_p from (21)

$$\varepsilon_p = ph - \frac{32Js}{9} \left(\frac{I}{J} - 2\right) p + \frac{8I}{9} p(p-1). \quad (35)$$

Formula (35) is valid so long as $\omega_{p-1} < 0$, for at $\omega_{p-1} > 0$ the quantity $c(\omega_{p-1})$ becomes complex. It is seen furthermore from (21) that the lowest level at $h = 0$ is determined by the value of the angular momentum

$$p_0 = E\{1 + 2s(1 - 2J/I)\}, \quad (36)$$

where $E(x)$ is the integer part of x . It follows from (36) that $p_0 \rightarrow 2s$ at $I \gg 2J$, a physically obvious fact.

We note that at $h \neq 0$ the relative positions of the levels change, but the decay properties of the levels do not change. This is physically obvious, since the decay is due to spin waves, and at $h \neq 0$ the spin wave spectrum has a gap equal to h .

4. THERMODYNAMICS

We consider now the contribution made by the discrete levels to the thermodynamics. The corresponding part of the free energy is

$$F(T) = -N_0 T \ln \sum_{p=0}^{p_0} \exp(-\varepsilon_p/T), \quad (37)$$

where N_0 is the total number of the antiferromagnetic bonds in the crystal. Let initially $p_0 = 1$. We then obtain from (37) for the heat capacity C and for the susceptibility χ :

$$C = N_0 \frac{\varepsilon_1^2}{4T^2} \left(\text{ch} \frac{\varepsilon_1}{2T}\right)^{-2}, \quad \chi = \frac{N_0}{4T} \left(\text{ch} \frac{\varepsilon_1}{2T}\right)^{-2}, \quad (38)$$

$\varepsilon_1 = h + \alpha_0,$

where α_0 no longer depends on h . At typical values of the parameters, the spacing between the levels at $h = 0$ is of the order of $4Js$, i. e., of the order of T_c . Since we are interested in the case $T \ll T_c$, at the characteristic values of the parameters the heat capacity and the susceptibility are exponentially small. At finite h , how-

ever, the magnetic field can cancel α_0 (in our case $\alpha_0 < 0$). It is seen from (38) that at $h \sim -\alpha_0$ the susceptibility has a δ -like burst, and the heat capacity has two bursts at $|\varepsilon_1| \sim T$ and a dip at $|\varepsilon_1| \ll T$. Let now $p_0 > 1$ in our case. It is seen from (37) that altogether, including the pure ferromagnetic state, we have $p_0 + 1$ levels. It is easily seen that susceptibility bursts of the type (38) appear only upon intersection of only the two lower levels, and the two bursts and the dip of the heat capacity will occur when any two levels intersect. Therefore when the magnetic field is increased the susceptibility will have p_0 δ -like bursts, and the heat capacity will have $p_0(p_0 + 1)/2$ minima each bracketed by two bursts, i. e., in all $p_0(p_0 + 1)/2$ minima and $p_0(p_0 + 1)$ maxima. Since the described picture is connected only with the presence of p_0 magnetic levels, it should be observed also for other magnetic systems. In particular, the same picture is observed in the antiferromagnetic-impurity problem¹⁰ (not to be confused with the antiferromagnetic coupling).

We note that if the antiferromagnetic exchange integrals are random quantities, then we obtain near $|h + \alpha_0| \sim T$, averaging over the distribution of this random quantity:

$$C \sim N_0 T, \quad \chi \sim N_0. \quad (39)$$

We consider in conclusion the case $s \gg 1$. Here we have a region $\omega \ll T \ll T_c$ in which the described oscillations are smeared out. The sum in (37) must then be replaced by an integral. Calculating the heat capacity

and the susceptibility by the saddle-point method, we get at $h \gg T$

$$C = N_0/2, \quad \chi = -N_0 \partial p_1 / \partial h, \quad (40)$$

where p_1 is the minimum of ε_p at $h \neq 0$. Since $\partial p_1 / \partial h < 0$, it follows that χ in (40) is positive. Thus, C and χ do not depend on temperature in this region.

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¹K. H. Fisher, *Physica (Utr.)* **86-88**, 813 (1976).

²D. Sherrington, *AIP Conf. Proc.* **29**, 224 (1975).

³S. F. Edwards and P. W. Anderson, *J. Phys. F* **5**, 965 (1975).

⁴D. J. Thouless, P. W. Anderson, and P. G. Palmer, *Phil. Mag.* **35**, 593 (1977).

⁵S. Kirkpatrick and D. Sherrington, *Phys. Rev. B* **17**, 4384 (1978).

⁶F. K. Lotgering and E. W. Gorter, *J. Phys. Chem. Sol.* **3**, 238 (1957).

⁷K. Adachi, K. Sata, and M. Takeda, *J. Phys. Soc. Jpn.* **26**, 631 (1969).

⁸K. Adachi, K. Sato, and M. Matsuura, and M. Ohashi, *ibid.* **29**, 323 (1970).

⁹Yu. A. Izyumov and M. V. Medvedev, *Teoriya magnitouporyadochennykh kristallov s primesyami* (Theory of Magnetically Ordered Crystals with Impurities) Nauka, 1970 [Plenum, 1971].

¹⁰B. Ya. Balagurov and V. G. Vaks, *Zh. Eksp. Teor. Fiz.* **66**, 1135 (1974) [*Sov. Phys. JETP* **39**, 554 (1974)].

¹¹E. Wigner, *Group Theory*, Academic, 1959.

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Cross section for electron capture by a charged dislocation in a semiconductor

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The cross section for multiphoton capture of an electron by an edge dislocation in an n -type semiconductor is calculated in the quasiclassical approximation. Analytic dependence of the cross section on the electron-phonon interaction constant, on the temperature, and on the charge per dislocation unit are obtained.

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1. INTRODUCTION

According to the experimental data, an edge dislocation in a semiconductor leads to the onset of a one-dimensional band with a bottom E_D located in the forbidden band. The investigations performed to date are still insufficient for final conclusions concerning the carrier dispersion in this band, but it can be regarded as established that the width of the dislocation band E_0 is much less than its depth E_D , which is comparable with the width of the forbidden band E_g . In accordance with the general concepts, such a "deep one-dimensional band"

should contribute to the effective recombination of the excess carriers. The statistics of the electron and hole recombination in semiconductors were considered by Gulyaev,² who obtained the dependence of the lifetime of an electron-hole pair on the concentration of the excess carriers and capture cross sections. It was noted that the quantity corresponding to the capture cross section should be referred to the length of the dislocation, in view of the extended structure of the latter, and the concept of capture radius was introduced by the same token. The purpose of the present study was to find the radius for the capture of an electron by a