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The Theory of Ferromagnetism of Metals and Alloys at Low Temperatures

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Formulas are obtained for the temperature dependence of spontaneous magnetization near absolute zero for a ferromagnetic lattice consisting of one kind of atoms in the case which in the number of electrons with uncompensated spins is greater than the number of atoms, and for lattices of binary ordered alloys of various structure. In the calculation, use is made of the method of approximate second quantization. It is shown that, in all cases considered, the theory leads to the temperature dependence of spontaneous magnetization of the form of a 3/2 power law.

1. INTRODUCTION

ONE of the problems of the theory of ferromagnetism is the deduction of a formula for the temperature dependence of spontaneous magnetization. This formula has been obtained for the ideal case, namely, for the ferromagnetic lattice of weakly interaction hydrogen–like atoms in the low temperature region. In this case,[1] the specific spontaneous magnetization is equal to

$$\sigma_S = n\mu_0 [1 - (T/\theta')^{3/2}], \qquad (1.1)$$

where n is the number of atoms and the number of electrons per unit mass, μ_0 is the Bohr magneton, $\theta' = 4.17\,(2c)^{2/3}\,J/k_0$, $c = 1/2, 1, 2$ for the simple, space-centered and face-centered cubic lattices, respectively, J = exchange integral, k_0 is Boltzmann's constant.

Real crystals of ferromagnetic elements have: 1) siginificant electrical conductivity, 2, a number of electrons with uncompensated magnetic moments that is not equal to the number of ions in the lattice. The theory of ferromagnetism with account of the state of polarization and the effect of the conductivity of the electrons on the spontaneous magnetization was developed in the researches of Vonsovskii,[2] and Turov.[3] In the most general form, the theory of the polar model of the metal was recently developed by Bogoliubov and Tiablikov.[4,5]

Möller[6] made an attempt to generalize the theory of the nonconducting ferromagnetic lattice to the case in which the number of electrons with uncompensated moments is greater than the number of atoms, and obtained a formula, similar to Eq. (1.1), but with this difference, that $\theta' = 4.17\,(2cz)^{2/3}\,zJ/k_0$, where z is the number of electrons with uncompensated spins per atom. Later, Holstein and Primakoff deduced a formula for the temperature dependence of spontaneous magnetization with account of magnetic interaction. When the interaction terms are discarded, the formula of Holstein and Primakoff reduces to that of Möller.

In the researches of Refs. 6 and 7, the exchange integrals between the electrons of neighboring atoms did not differ, but the exchange integrals between the electrons of one and the same atom did not enter into the calculation. This corresponded to an implicit assumption that the states of the electrons belonging to one atom differ only in the spin function. As a result, a series of terms fall out in the calculation of the lowest energy levels, as will be shown.

However, we can also begin from another, more consequential assumption, namely that the unperturbed wave functions of the electrons belonging to any atom differ not only in their spin functions, but also in the functions of the coordinates of the electrons. In this case it is necessary to take it into account that the exchange integrals between electrons of corresponding atoms differ in their dependence on whether electrons are exchanged which are found in identical states, or electrons which are found in different states. Moreover, we must take into account the exchange integrals between the electrons of one and the same atom.

Our problems are then the following: 1) to obtain the theoretical dependence of the spontaneous magnetization on the temperature, near absolute zero, in the case in which the number of electrons with uncompensated magnetic moments is larger than the number of atoms; 2) to derive formulas for the temperature dependence of spontaneous magnetization in the region of low temperatures for binary ferromagnetic ordered alloys of different crystalline structure and different composition.

2. GENERAL FORM OF THE HAMILTONIAN OF THE PROBLEM AND ITS DIAGONALIZATION

Let us consider the general case of a multicomponent crystal, consisting of N atoms of h different types, located at the points of the lattice; each of the atoms has z_h ferromagnetic electrons which differ in state one from another. Altogether, there are $n = \Sigma N_h z_h$ electrons in the lattice, where N_h is the number of atoms of type h and $\Sigma N_h = N$. (It must be noted that the type of atom is also determined here by what neighbors surround it. Two identical atoms can belong to different types h.)

The Hamiltonian of such a system, in the case in which only electrostatic interactions are taken into account, can be described in the following form:

$$\hat{H} = U_0 - \frac{\hbar^2}{2m} \sum_{(f,g)} \Delta q_{f,g} + \sum_{(f,f',g')} U_f(q_{f'g'}) + \sum_{(f,f',g,g')} \Phi(q_{fg}, q_{f'g'}). \tag{2.1}$$

Each electron of the system is characterized by two indices f and g: the index f defines the number of the lattice point at which the electron is located, and the index g defines the quantum state of the given electron in the atom. Inasmuch as only a single atom of any type can be located at a given lattice point f, we can neglect the indices h (which characterize the type of atom at the point f) in Eq. (2.1) and in subsequent expressions. The quantity U_0 is the constant potential energy of electrostatic interaction of the ions. These ions are assumed to be fixed at the points of the lattice, The quantity m is the electronic mass, Δq_{bg} is the Laplace operator in the coordinates of the electron f, g; U^f is the interaction potential of the electron with any ion; Φ is the interaction energy of the electrons.

Transforming to the representation of second quantization, the Hamiltonian (2.1) can be written in the form

$$\hat{H} = U_0 + \sum L(f, g, f', g')\, \hat{a}^+_{fg\sigma}\, \hat{a}_{f'g'\sigma} + \frac{1}{2} \sum F(f_1, g_1, f_2, g_2;\ f_1', g_1', f_2', g_2') \times \hat{a}^+_{f_1g_1\sigma_1}\, \hat{a}^+_{f_2g_2\sigma_2} \hat{a}_{f_2'g_2'\sigma_2}\, \hat{a}_{f_1'g_1'\sigma_1}, \tag{2.2}$$

where L and F are the matrix elements of the additive and binary parts of the operator (2.1) in the system of single particle functions, $\hat{a}^+$ and $\hat{a}$ are the second quantization operators in Fermi statistics; the summation is carried out over all indices.

The unexcited wave function in the second quantization representation $c_0(\ldots N_{fg\sigma})$ is defined by a system of unitary occupation numbers:

$$N_{fg\sigma} = \sum_{(\sigma)} n_{fg\sigma} = \sum_{(\sigma)} \hat{a}^+_{fg\sigma} \hat{a}_{fg\sigma} = 1. \tag{2.3}$$

Making use of the operator form of perturbation theory,[5] we can obtain the equivalent Hamiltonian of the secular equation of the third approximation in the following form:

$$\hat{\tilde{H}}\, \tilde{G}_0 = -\frac{1}{2} \sum J(f, g, f', g')\, \hat{a}^+_{fg\sigma} \hat{a}^+_{f'g'\sigma'} \hat{a}_{f'g'\sigma}\, \hat{a}_{fg\sigma'}, \tag{2.4}$$

where $J(f, g, f', g')$ is the exchange integral. The summation is carried out over all indices under the necessary conditions:

$$f \neq f', \quad \text{if} \quad g = g'; \qquad g \neq g, \quad \text{if} \quad f = f'. \tag{2.5}$$

Finding the spectrum of the energy eigenvalues of the system of electrons under consideration requires diagonalization of the Hamiltonian (2.4). For this purpose, we make use of the method of approximate second quantization in the form developed by Bogoliubov and Tiablikov.[5] Applying this method to the general case, we can change Eq. (2.4) to the following form:

$$\hat{\tilde{H}} = E_0 + \sum_{(f,g)} \Big\{ \sum_{(f'g')} J(f,g,f',g') \Big\} \hat{b}^+_{fg} \hat{b}_{fg} - \sum_{(f,g,f',g')} J(f,g,f',g')\, \hat{b}^+_{fg} \hat{b}_{f'g'}, \tag{2.6}$$

where $\hat{\xi}^+_k$ and $\hat{\xi}^+_k$ are the operators of second quantization in Bose statistics.

Diagonalization of the appropriate quadratic form is brought about with the aid of the canonical transformation:

$$\hat{b}^{+}_{fg} = \sum_{(k)} U^{*}_{k}(f,\ g)\hat{\xi}^{+}_{k}, \tag{2.7}$$

$$\hat{b}_{fg} = \sum_{(k)} U_{k}(f,\ g)\,\hat{\xi}_{k},$$

where $\hat{\xi}^{+}_{k}$ and $\hat{\xi}^{+}_{k}$ are operators which are also subject to Bose statistics, and the eigenvalues E_k and $U_k(f,g)$ are determined by a set of n equations in terms of the number of possible values f and g:

$$E_k U_k(f,g) = \Big\{ \sum_{(f',g')} J(f,\ g,\ f',\ g') \Big\} U_k(f,g) \quad (2.8)$$

$$- \sum_{(f',g')} J(f,\ g, f',g')\, U_k(f',\ g') \quad (2.8)$$

and the normalization condition

$$\sum_{(f,g)} U^{*}_{k}(f,g)\, U_{k'}(f,g) = \delta(k - k'). \tag{2.9}$$

We shall seek the solution of the set (2.8) in the following form:

$$U_k(f_h,\ g) = N^{-1/2} U_k(g,\ h) \exp\{i(\mathbf{k}\mathbf{f}_h)\}. \tag{2.10}$$

Here h is an index characterizing the type of atom in lattice site f.

Then, after elementary transformations, a system of equations is obtained for the determination of the eigenvalues of the energy E_k. The number of these equations is equal to Σz_h:

$$\begin{aligned} E_k U_k(g,\ h) = {} & \sum_{(g'h')} I^{(k)}_{g,g',h,h'} U_k(g',\ h') \\ & + \Big\{ \sum_{(g',h')} I_{g,g',h,h'} \Big\} U_k(g,h) - \\ & - \sum_{(g',h')} I_{g,g',h_1h'} U_k(g',h'), \end{aligned} \tag{2.11}$$

where the following notation is used:

$$\begin{aligned} & I^{(k)}_{g,g',h,h'} \\ & = \sum_{(f',h')} J(f_h, g,\ f'_{h'},\ g')\ \{1 - \exp[-ik(f'_{h'} - f_h)]\}, \end{aligned} \tag{2.12}$$

$$I_{g,g',h,h'} = \sum_{(f',h')} J(f_h,\ g,\ f'_{h'}, g'),$$

and the $U_k(f,g)$ satsifying the following normalization condition, as is easy to verify:

$$\sum_{(g,h)} U^{*}_{k}(g,\ h)\, U_{k'}(g,\ h) = \delta(k - k'). \tag{2.13}$$

We thus see that the problem of finding the energy spectrum of a system of electrons of a multi-component crystal reduces to the solution of the set $z = z_A + z_B + \ldots + z_h$ linear homogeneous equations (2.11) for the unknown functions $U_k(g, h)$.

In the general case, all the unknown functions $U_k(f,g)$ are different, and consequently, all the equations of the set are different. However, in particular cases, some equations (and sometimes, all of them) can, from the physical meaning of the problem, be shown to be identical, and therefore the order of the set is decreased, which permits us finally to develop the solution and find the spectrum E_k. For example, in the case of a pure metal, which has only a single ferromganetic electron per atom ($z_B = z_C = \ldots = z_h = 0$, $z_a = 1$), the solution of the problem reduces to the solution of a single equation.[5] If there were not one but z ferromagnetic electrons in each atom in the crystalline lattice of the pure metal, then finding the spectrum of the energy E_k would require the solution of a set of z equations.

In the lattice of a disordered alloy, the different atoms f will have a different number of nearest neighbors of dffferent types and, consequently, their equations will be located in different conditions. The number of different equations of the system (2.11) can be shown to be sufficiently large and will be determined by the number of possible combinations of neighboring atoms of different types at each of the atoms of the alloy.

It therefore follows that the degree of the equation for obtaining E_k, which is obtained by equating the determinant of the system (2.11) to zero (and consequently, the number of possible energy levels E_k), will be larger the larger the number of electrons found in the lattice of the alloy under different conditions, in particular. as the ordering of the lattice becomes less. In the ordering, the number of possible values of E_k decreases, and therefore the formula for the dependence of the spontaneous magnetization on the temperature must change. Calculation in the general case of binary alloys cannot be carried through to completion, and we limit ourselves to a consideration only of a series of completely ordered structures of binary alloys.

3. TEMPERATURE DEPENDENCE OF THE SPONTANEOUS MAGNETIZATION OF A METAL WITH TWO FERROMAGNETIC ELECTRONS PER ATOM

Let there be two ferromagnetic electrons in each of N atoms of a crystal, located in two possible low energy states (we shall conditionally give the index g the values 1 and 2). Then, setting the determinant of the set (2.11) to zero, and taking it into consideration that $I_{21}^{(k)} = I_{12}^{(k)*}$ and $I_{21} = I_{12}$, we obtain a quadratic equation for the determination of E_k which gives the following two solutions:

$$E_k = \frac{1}{2}\{2|I_{12}| + I_{11}^{(k)} + I_{22}^{(k)} \pm \sqrt{[I_{11}^{(k)} - I_{22}^{(k)}]^2 + 4[|I_{12}^{(k)} - I_{12}|]^2}\}. \tag{3.1}$$

We are interested in the case of small values of the wave number k, which are had at low temperatures. Taking into consideration only the exchange interval between nearest neighbor atoms, expanding (2.12) in a series in k and considering only the first terms of the expansion, we obtain for the particular case of a simple cubic lattice

$$\begin{aligned} I_{11}^{(k)} &\approx a^2 J(f,\ 1,\ f',\ 1)\,k^2 = a^2 J_{11} k^2; \\ I_{22}^{(k)} &\approx a^2 J(f,\ 2,\ f',\ 2)\,k^2 = a^2 J_{22} k^2; \\ I_{12}^{(k)} &\approx a^2 J(f,\ 1,\ f',\ 2)\,k^2 = a^2 J_{12} k^2; \\ I_{12} &= J(f,\ 1,\ f,\ 2) + 6J(f,\ 1,\ f',\ 2) = J_{12}^0 + 6J_{12}, \end{aligned} \tag{3.2}$$

where a is a parameter of the crystalline lattice, J_{11}, J_{22} are the exchange integrals between the electrons of adjacent atoms, located at identical positions, J_{12}^0 is the exchange integral between two electrons located in different states in the same atom, J_{12} is the analogous exchange integral for two nearest neighbors.

The following expressions are then obtained for the values $E_k^{(1)}$ and $E_k^{(2)}$:

$$E_k^{(1)} = \frac{a^2}{2}(J_{11} + J_{22} + 2J_{12})\,k^2, \tag{3.3}$$

$$E_k^{(2)} = 2(J_{12}^0 + 6J_{12}) + \frac{a^2}{2}(J_{11} + J_{22} - 2J_{12})\,k^2,$$

and the Hamiltonian has the following diagonal form:

$$\hat{H} = E_0 + \sum_{(k)} E_k^{(1)} \hat{N}_k^{(1)} + \sum_{(k)} E_k^{(2)} \hat{N}_k^{(2)}, \tag{3.4}$$

$$\hat{N}_k^{(1)} = \hat{\xi}_k^{(1)+} \hat{\xi}_k^{(1)}, \quad \hat{N}_k^{(2)} = \hat{\xi}_k^{(2)+} \hat{\xi}_k^{(2)}.$$

If we take into account the effect on the electron of the external magnetic field H, then the eigenvalues of the energy operator can be written in the form

$$\hat{H} = E_0 - 2\mu_0 HN + \sum_{(k)} \{E_k^{(1)} + 2\mu_0 H\} N_k^{(1)} + \sum_{(k)} \{E_k^{(2)} + 2\mu_0 H\} N_k^{(2)}, \tag{3.5}$$

where $N_k^{(1)}$ and $N_k^{(2)}$ are the occupation numbers, which take on all the integral values from zero.

Now, constructing the phase sum and carrying out standard calculations, we obtain the following relation for the mean magnetic moment M of the system of electrons under discussion:

$$\begin{aligned} M &= \left(k_0 T \frac{\partial \ln Z}{\partial H}\right)_{H=0} \\ &= 2\mu_0 H - \frac{\mu_0 G}{\pi^2} \times \int_0^\infty \frac{k^2 dk}{\exp\{a^2 k^2 (J_{11} + J_{22} + 2J_{12}) / 2k_0 T\} - 1} \\ &\quad - \frac{\mu_0 G}{\pi^2} \times \int_0^\infty \frac{k^2 dk}{\exp\{[a^2 k^2 (J_{11} + J_{22} - 2J_{12}) + 4(J_{12}^0 + 6J_{12})] / 2k_0 T\} - 1}, \end{aligned} \tag{3.6}$$

where $G = Na^3/2c$ and $c = 1/2$, 1,2 for simple, body-centered and face-centered lattices, respectively, k_0 = Boltzmann's constant.

The integrals entering into Eq. (3.6) are computed in elementary fashion, and the formula for the temperature dependence of the spontaneous magnetization of a ferromagnet possessing two electrons per atom takes the form:

$$M = M_0\left\{1 - \frac{1,306}{4c\pi^2}\left(\frac{2k_0T}{J_{11}+J_{22}+2J_{12}}\right)^{3/2}\right. \quad (3.7)$$

$$- \frac{0,4431}{4c\pi^2}\left(\frac{2k_0T}{J_{11}+J_{22}-2J_{12}}\right)^{3/2}$$

$$\left. \times \exp\left[-\frac{2(J^0_{12}+6J_{12})}{k_0T}\right]\right\}.$$

At low temperatures, and for J°_{12} and J_{12} having the order of usual exchange integrals (10^{14} erg),[12] $J^{\circ}_{12} + 6J_{12} >> k_0 T$, the third term in the curly brackets is small in comparison with the second, and Eq. (3.7) leads in practice to the same law of dependence of M on T as in the Bloch-Möller formula (1.1) for the case $z = 2$. Here

$$\theta' = 3.88\,(4c)^{2/3}\,(J_{11}+J_{22}+2J_{12})\,/\,2k_0. \quad (3.8)$$

However, it should be noted that this dependence is obtained by us as the special case of a general formula. The general formula is derived with the aid of a method which differs essentially from the method used by Möller and by Holstein and Primakoff in deriving similar expressions.

Equation (3.17) permits us to carry out an estimate of the various exchange integrals from the temperature dependence of the spontaneous magnetization, known from experiment. The estimate from Eq. (3.8) gives, for iron, $J_{11} + J_{22} + 2J_{12} \approx 800\,k_0$. If both electrons are found in a single shell, we can set $J_{11} = J_{22} = J$, and then our estimate gives $J_{11} + J_{12} \approx 400\,k_0$, i.e., for $J_{12} > 0$, $J < 400\,k_0$ For $J_{12} \approx J_{11} = J$; $J \approx 200\,k_0$.

4. TEMPERATURE DEPENDENCE OF THE SPONTANEOUS MAGNETIZATION OF A METAL WITH *z* FERROMAGNETIC ELECTRONS PER ATOM

For the approximate solution of the problem of the determination of the energy spectrum of a ferromagnet with z ferromagnetic electrons per atom, and for the determination of the character of the tempertture dependence of its spontaneous magnetization, we made use of a method similar to that used by Born[8] for the calculation of the frequency spectrum of the characteristic vibrations of a crystalline lattice. His method consisted of an expansion in powers of a small parameter of the k coefficients for the unknowns and the unknowns themselves in a system of linear homogeneous equations (2.11), and the consequent determination of the coefficients of these expansions.

Let us write (2.11) in the following form:

$$(A_g - E_k)\,U_k(g) + \sum_{(g'\neq g)} A_{gg'}\,U_k(g') = 0, \quad (4.1)$$

$$A_g = I^{(k)}_{gg} + \sum_{(g\neq g')} I_{gg'}, \quad (4.2)$$

$$A_{gg'} = I^{(k)}_{gg'} - I_{gg'} \quad (g, g' = 1, 2, \ldots, z).$$

The condition for the solvability of the set of equations (4.1) is the vanishing of its determination. This gives us an equation of degree z for the determine of the z eigenvalues of the energy E_k, wherein, inasmuch as the coefficients A are of Hermitian form, all the E_k will be real.

For the approximate determination of the eigenvalues of the energy just mentioned, we make use of the fact that as $T \to 0$, the wave number k is a small quantity and we expand the coefficients A_g, $A_{gg'}$, and also E_k and $U_k(g)$ in series in k. Limiting ourselves to the quadratic terms, we get

$$A_g = A^{(0)}_g + |k|^2 A^{(2)}_g, \quad (4.3)$$

$$E_k = E^{(0)}_k + |k|^2 E^{(2)}_k,$$

$$A_{gg'} = A^{(0)}_{gg'} + |k|^2 A^{(2)}_{gg'},$$

$$U_k(g) = U^{(0)}_k(g) + |k|^2 U^{(2)}_k(g).$$

Here

$$A^{(0)}_g = \sum_{(g\neq g')} I_{gg'}, \quad A^{(0)}_{gg'} = -I_{gg'} - J^0_{gg'},$$

$$A^{(2)}_g = a^2 J_{gg}, \quad A^{(2)}_{gg'} = a^2 J_{gg'},$$

and by J_{gg}, $J_{gg'}$ and $J^{\circ}_{gg'}$ we mean

$$J(f, g, f' \pm 1, g),$$

$$J(f, g, f \pm 1, g') \text{ и } J(f, g, f, g').$$

and $J(f, g, f, g')$.

Substituting the series (4.3) in Eq. (4.1) and equating coefficients for equal powers of k to zero, we get as a consequence the system of equations of the different approximations (we restrict ourselves to the second approximation):

$$(A_g^{(0)} - E_k^{(0)})\, U_k^{(0)}(g) + \sum_{(g \neq g')} A_{gg'}^{(0)} U_k^{(0)}(g') = 0, \tag{4.4}$$

$$(A_g^{(0)} - E_k^{(0)})\, U_k^{(2)}(g) + \sum_{(g \neq g')} A_{gg'}^{(0)} U_k^{(2)}(g') \tag{4.5}$$

$$= -(A_g^{(2)} - E_k^{(2)})\, U_k^{(0)}(g) - \sum_{(g \neq g')} A_{gg'}^{(2)} U_k^{(0)}(g').$$

It is easy to show that the equation of degree z, obtained by setting the determinant of the system (4.4) equal to zero, will always have one root equal to zero, $E_{k_1}^{(0)} = 0$, namely, for the condition that the unknown $U_k^{(0)}$ are equal to each other:

$$U_k^{(0)}(1) = U_k^{(0)}(2) = \ldots = U_k^{(0)}(z) = c, \tag{4.6}$$

where c is an arbitrary constant.

Now, substituting the value $E_{k_1}^{(0)} = 0$ and solving (4.6) in a system of equations of the second approximation (4.5), we get

$$A_g^{(0)} U_k^{(2)}(g) + \sum_{(g \neq g')} A_{gg'}^{(0)} U_k^{(2)}(g') \tag{4.7}$$

$$= -\Big[(A_g^{(2)} - E_k^{(2)}) - \sum_{(g \neq g')} A_{gg'}^{(2)}\Big]\, c.$$

The system of inhomogeneous equations (4.7) is solvable only when the vector whose components are are the right sides of these equations, are orthogonal to all vectors whose components form the systems of partial solutions of the corresponding homogeneous equations. The homogeneous equations obtained from the left side of (4.7) coincide with the equations (4.4); consequently, they have a system of partial solutions (4.6). Taking this into account, and considering that $c \neq 0$, we get from the condition for the solvability of the system of equations (4.7) an equation for $E_k^{(2)}$. Solving this latter equation, and substituting the resultant expression for $E_k^{(2)}$ into (4.3), we get

$$E_{k1} = E_{k1}^{(0)} + k^2 E_{k1}^{(2)} \tag{4.8}$$

$$= \frac{1}{z}\Big\{\sum_{(g)} A_g^{(2)} + 2 \sum_{(g' < g)} A_{gg'}^{(2)}\Big\}\, a^2 k^2$$

$$= \frac{1}{z}\Big\{\sum_{(g)} J_{gg} + 2 \sum_{(g' < g)} J_{gg'}\Big\}\, a^2 k^2.$$

It is easy to note that the structure of the coefficients of the equations of the set (4.4) are such that the secular equation of this system can have only one zero root. Actually, the value $E_k^{(0)} = 0$ satisfies the system of equations (4.4) only when all the solutions of this system $U_k^{(0)}(g)$ are equal to one another. In all the remaining cases, the $E_k^{(0)}$ are different from zero and have real positive roots. In general, there are different, although multiple roots are also possible.

It should be pointed out that if there is any possibility of determining the roots $E_k^{(0)}$ of the secular equation of the system of first approximation, then the corresponding roots $E_k^{(2)}$ are also obtained, and consequently the eigenvalues E_k of the energy of the crystal. The values $E_{k_2}^{(0)}, \ldots, E_{k_z}^{(0)}$, as was shown above, are different from zero; therefore terms independent of k enter into the expressions for all the E_k except E_{kl}. Thus the character of the energy spectrum in the general case for $z > 2$ will be the same as in the particular case when $z = 2$.

The formula for the temperature dependence of the spontaneous magnetization of the ferromagnet with z uncompensated spin magnetic moments per atom will have the following form:

$$M = zN\mu_0 \Big\{1 - \frac{A_1}{z}\Big(\frac{k_0 T}{\theta_1}\Big)^{3/2} \tag{4.9}$$

$$- \frac{A_2}{z}\Big(\frac{k_0 T}{\theta_2}\Big)^{3/2} \exp\Big(-\frac{\theta_2'}{k_0 T}\Big)$$

$$\ldots - \frac{A_z}{z}\Big(\frac{k_0 T}{\theta_z}\Big)^{3/2} \exp\Big(-\frac{\theta_z'}{k_0 T}\Big)\Big\},$$

where $A_1, A_2, \ldots, A_z$ are certain constants of order 10^{-1}; but $\theta_2, \theta_3, \ldots, \theta_z, \theta_z', \ldots, \theta_2'$ are certain functions of the exchange integrals $J_{gg}, J_{gg'}$ $\times (g, g' = 1, 2, \ldots, z)$.

5. TEMPERATURE DEPENDENCE OF THE SPONTANEOUS MAGNETIZATION OF ORDERED BINARY ALLOYS

Let us consider a series of binary, completely ordered, ferromagnetic alloys, and for simplicity, we assume that the atoms of both components A and B possess only one ferromagnetic electron apiece ($z_A = 1$, $z_B = 1$). This permits us to omit the index g in all the expressions below.

1. *Cubic lattice of an alloy of the type NaCl.* In this case, each atom A has 6 nearest neighbors B, and conversely, each atom B has 6 neighbors A. The indices h take only two values, A and B. The system (2.11) reduces to two linear equations which are homogeneous relative to $U_k(A)$ and $U_k(B)$.

After several transformations, taking only the exchange integrals between nearest neighbors into account, and expanding the coefficients of these equations in series in small values of the wave number k, we get, with accuracy up to terms of second order:

$$(6J_{AB} - E_k)\, U_k(A) + (J_{AB}\, a^2 |k|^2 - 6J_{AB})\, U_k(B) = 0, \qquad (5.1)$$

$$(J_{BA}\, a^2 |k|^2 - 6J_{BA})\, U_k(A) + (6J_{BA} - E_k)\, U_k(B) = 0,$$

where J_{AB} and J_{BA} refer respectively to $J(f_A, f_B)$ and $J(f_B, f_A)$. Setting the determinant of this system equal to zero, and taking it into account that $J_{AB} = J^*_{BA}$, we get a quadratic equation for E_k, which has the following solution:

$$E_k^{(1)} = J_{AB}\, a^2 k^2, \quad E_k^{(2)} = 12J_{AB} - J_{AB}\, a^2 k^2. \qquad (5.2)$$

Carrying out the usual statistical-thermodynamical calculations, we finally get the following equation for the spontaneous magnetization:

$$M = N\mu_0 - 2\mu_0 \sum_{k=0}^{N-1} \frac{1}{\exp\{J_{AB}\, a^2 k^2 / k_0 T\} - 1} - 2\mu_0 \sum_{k=0}^{N-1} \frac{1}{\exp\{[12J_{AB} - J_{AB}\, a^2 k^2] / k_0 T\} - 1}. \qquad (5.3)$$

The exponent in the first sum of this expression is essentially a positive quantity for arbitary k; therefore the first sum is convergent and can be replaced by an integral in k from 0 to ∞. In the second sum, the condition of the smallness of k plays the essential role: this sum will be convergent only for $12\, J_{AB} - J_{AB}\, a^2 k^2 > 0$ i.e., for the condition $k < \sqrt{12}\, a$. This means that in the transition from a sum to an integration in the second integral, it is necessary to set the upper limit equal to a sufficiently high finite quantity which, however, must be less than $\sqrt{12}/a$.

Thus, for the temperature dependence of the spontaneous magnetization of an alloy with a lattice of the type NaCl, we get the formula

$$M = N\mu_0 \left\{1 - \frac{1{,}306}{\pi^2} \left(\frac{k_0 T}{J_{AB}}\right)^{3/2} - \frac{1}{\pi^2} \left(\frac{k_0 T}{J_{AB}}\right)^{3/2} e^{-\alpha}\right\} \int_0^B \frac{x^2\, dx}{e^{-x^2} - e^{-\alpha}}, \qquad (5.4)$$

$$\alpha = 12J_{AB} / k_0 T, \quad B < (12J_{AB} / k_0 T)^{1/2} = \alpha^{1/2}.$$

The integral in thesecond term is a finite quantity, but $e^{-\alpha}$ for $T \to 0$ approaches ∞; therefore, for low temperatures, the second term falls off rapidly and plays no practical role.

2. CUBIC LATTICE OF AN ALLOY OF THE TYPE CsCl ($z_A = z_B = 1$)

This case is very much like the preceding. Here the atoms A or B also have as nearest neighbors atoms of B or A, respectively. The difference lies in the fact that the number of nearest neighbors is equal to 8 here, and these neighbors are located not along the crystallographic edges of the cube but along its spatial diagonals. In this case the indices h also take on only two values and the system (2.11) reduces to two linear equations which are homogeneous relative to $U_k(A)$ and $U_{k(B)}$. From the secular equation solution, we get for E_k the values

$$E_k^{(1)} = J_{AB}\, a^2 k^2, \; E_k^{(2)} = 16J_{AB} - J_{AB} a^2 k^2. \qquad (5.5)$$

For M at low temperatures, we get the same formula as (5.4), but $\alpha = 16J_{AB}/k_0 T$.

3 *Cubic lattice of the compound* AB_3 *of the type* $FeNi_3$ ($z_A = z_{AB} = 1$). In this case atom A will have 12 nearest neighbors of B, at a distance of $a/\sqrt{2}$ from it and located in the centers of the cube faces. Each B atom will also have 12 nearest neighbors, of which 4 will be atoms of A and 8 atoms of B. Here the atoms of A will be found in a plane while the 8 of the neighbors of type B will be found in two plane parallel to the first. Thus the atoms of A are equally distributed in the sense of symmetry of their nearest neighbors, into three types (of equal number) depending on what planes they have by way of nearest neighbors of atoms of A. It then follows that we have four types of atoms in the case under consideration and the indices h will

take on the four values A, B_1, B_2 and B_3 the system (2.11) reduces to four equations.

We identify the coordinate axes with the tetragonal axes of the cube. After the corresponding transformations and expansions of the coefficients in powers of the components k_1, k_2 and k_3 of the wave number k (with accuracy up to terms of second order) we get the following system of four linear homogeneous equations:

$$\begin{aligned}&(c_0 - E_k)\, U_k(A) + c_l\, U_k(B_l) \\ &\quad + c_m\, U_k(B_m) + c_n\, U_k(B_n) = 0, \\ &\quad c_l\, U_k(A) + (c_{ll} - E_k)\, U_k(B_l) \\ &\qquad + c_{lm}\, U_k(B_m) + c_{ln}\, U_k(B_n) = 0.\end{aligned} \tag{5.6}$$

$$c_0 = 12 J_{AB}, \tag{5.7}$$

$$c_l = \frac{1}{2} J_{AB}\, a^2 (k_m^2 + k_n^2) - 4J_{AB},$$

$$c_{ll} = 4J_{AB} + 8J_{BB},$$

$$c_{ml} = c_{nl} = \frac{1}{2} J_{BB}\, a^2 (k_m^2 + k_n^2) - 4J_{BB},$$

and the indices l, m, n run through the values 1,2,3. $J_{AB} = J_{AB_1} = J_{AB_2} = J_{AB_3}$, while $J_{BB} = J_{B\,B_m}$, since the exchange integrals here depend only on the atoms between which the electron exchange takes place, and do not depend upon the type of neighbors.

Setting the determinant of (5.6) equal to zero, we obtain a fourth degree equation for the determination of the eigenvalues E_k. We limit ourselves to the approximation solution of the problem by the method given above. Expanding the coefficients and the unknowns [in Eqs. (5.6)] in series of small k_1, k_2, and k_3 and obtaining by rough calculations systems of equations of first and second approximation, we find for $E_k^{(k)}$ the value

$$E_k^{(1)} = {}^1\!/_2\, a^2 (J_{AB} + J_{BB})\, k^2. \tag{5.8}$$

The remaining roots $E_k^{(2)}$, $E_k^{(3)}$, $E_k^{(4)}$ with the exception of the term depending on k^2 will also contain terms independent of k. We get the formula for the temperature dependence of spontaneous magnetization of the alloy under consideration (for $T \to 0°$ K) in the form

$$\begin{aligned}M = N\mu_0 \Big\{ 1 &- \frac{1{,}306}{\pi^2} \left(\frac{2k_0 T}{J_{AB} + J_{BB}} \right)^{3/2} \\ &- A \left(\frac{k_0 T}{\theta_2} \right)^{3/2} \exp\left(- \frac{\theta_2'}{k_0 T} \right) \\ &- B \left(\frac{k_0 T}{\theta_3} \right)^{3/2} \exp\left(- \frac{\theta_3'}{k_0 T} \right) \\ &- C \left(\frac{k_0 T}{\theta_4} \right)^{3/2} \exp\left(- \frac{\theta_4'}{k_0 T} \right) \Big\},\end{aligned} \tag{5.9}$$

where A, B, C are constants of the order $10,^{-1}$ and θ_2, θ_2', . . . are functions of the exchange integrals J_{AB} and J_{BB}. Here, also for low temperatures (close to $T = 0$ ° K), the terms containing exponential factors virtually vanish and the "three-halves law" must hold.

Applying the methods outlined above, we can complicate the problem and consider the case of a binary ferromagnetic alloy, the atoms of whose components have different (and not equal to unity) numbers of ferromagnetic electrons. However, as rough calculations have always shown, such a complication is not of essential interest, inasmuch as the character of the temperature dependence of spontaneous magnetization in this case is not materially changed.

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