The Quantum Theory of Magnetostriction

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On the basis of the theory of the polar model of a metal in the form developed by Bogoliubov and Tiablikov, starting from the calculation of the magnetic and magnetoelastic interaction of the electrons in the lattice, a step-by-step quantum mechanical theory of magnetostriction of hexagonal monocrystals is developed. The low temperature energy spectrum of the crystal is calculated, as well as the free energy and the temperature dependent of the constants of magnetostriction.

INTRODUCTION

THE quantum theory of ferromagnetism began its development after it had been established by the researches of Frenkel'[1] and later by Heisenberg[2] that the basic property of ferromagnets—the presence of spontaneous magnetization—was explained by electrical exchange forces. The classical theory of magnetic-anisotropic properties of ferromagnets, which is fundamental to the theories of the curves of technical magnetization, is connected with the well-known researches of Akulov[3], who also pointed out that the magnetic anisotropic properties of ferromagnets are determined by the magnetic interaction of electron spins and orbits in the ferromagnetic crystal. The most important magneto-anisotropic properties of ferromagnets are the magnetic-energetic anistropy and magnetostriction. The quantum theory of these properties must be built on the basis of both exchange and magnetic interactions. If we can say that a sufficient number of researches, both Soviet and foreign[4-6], were devoted to the theory of magnetic anisotropy, we must add that the quantum theory of magnetostriction has been only very slightly investigated. Only one research, due to Vonsovskii[7], is devoted to this problem. In this work, a quantum mechanical analysis is given, with the use of the method of energetic centers of gravity, of the phenomenon of magnetostriction in cubic crystals for the region of temperatures close to the Curie point.

The aim of the present work was the step-by-step formation of a quantum mechanical theory of magnetostriction of ferromagnetic monocrystals with hexagonally symmetric lattices at low temperatures. The analysis is made on the basis of the theory of the polar model of a metal in the form developed by the researches of Bogoliubov and Tiablikov[8,9], i.e., in the many electron scheme with the use of the method of approximate second quantization.

MODEL OF THE SYSTEM AND THE INITIAL HAMILTONIAN

We shall consider the crystalline lattice of hexagonal symmetry; let a "ferromagnetic" electron in the ground state be located at each lattice site. We shall assume that the atoms in the lattice are placed sufficiently far apart that the overlap of the orbits of electrons at neighboring sites is not great. We shall assume that the integral of non-orthogonality of the atomic wave functions of the different nodes is small in comparison to unity. In the corresponding scheme of excitation, the wave function of the ground state is completely determined by the occupation number for all sites. It is also assumed that the ground level of the system is separated from the excited levels by an energy gap. We shall consider the introduction of a system of ferromagnetic electrons in this lattice only in the range of low temperatures, where

1 Ia. I. Frenkel', Z. Phys. **49**, 31 (1928)

2 W. Heisenberg, Z. Phys. **49**, 619 (1928)

3 N. S. Akulov, *Ferromagnetism*, Moscow, 1939

4 S. V. Vonsovskii, J. Exper. Theoret. Phys. USSR **8**, 1104 (1938)

5 J. Van-Vleck, Phys. Rev. 52, 1178 (1937); H. Brooks, Phys. Rev. **58**, 909 (1940)

6 S. V. Tiablikov, J. Exper. Theoret. Phys. USSR **20**, 661 (1950)

7 S. V. Vonsovskii, J. Exper. Theoret. Phys. USSR **10**, 762 (1940)

8 N. N. Bogoliubov and S. V. Tiablikov, J. Exper. Theoret. Phys. USSR **19**, 251, 256 (1950)

9 N. N. Bogoliubov, *Lectures on Quantum Statistics*, Kiev, 1949 (in Ukrainian)

the excitation of the system can be regarded as weak.

Let the system be located in an external magnetic field, sufficiently strong so that the crystal can be regarded as magnetized almost to saturation. We shall consider both exchange and magnetic interaction. In this case, as also in reference 6, the Hamiltonian of the system in "equivalent" form can be written in terms of the spin operator

$$\mathscr{H} = G_0 - \sum_{f,\alpha} \mu H^\alpha S_f^\alpha - {}^1/_2 \times \sum_{\substack{f_1, f_2 \\ \alpha, \beta}} G_{\alpha\beta}(f_1, f_2) S_{f_1}^\alpha S_{f_2}^\beta, \quad (1)$$

where $G_{\alpha\beta}(f_1, f_2)$ is the tensor of the electron interaction, which, upon ignoring the magnetic interaction, degenerates into a scalar which represents the usual exchange integral; G_0 is a constant in the sense that it is independent of the spin operators.

The magnetic interaction of the electrons in the ferromagnetic lattice brings about a displacement of the atoms from their equilibrium positions, which brings about a spontaneous deformation of the lattice. We shall consider that these displacements are not large, and that the deformations are homogeneous. Inasmuch as one can consider that $G_{\alpha\beta}(f_1, f_2) = G_{\alpha\beta}(f_1 - f_2)$ in an actual lattice, we expand each of the components of the tensor $G_{\alpha\beta}$ in a series of small displacements relative to the equilibrium position, and restrict ourselves to terms which are linear in the components of the deformation tensor u_{ij}. Then (keeping the previous designation f for the positions of the sites in equilibrium), the equivalent Hamiltonian of the spontaneously deformed lattice can be written in the form

$$\mathscr{H} = G_0 - \sum_{f,\alpha} \mu H \gamma^\alpha S_f^\alpha - {}^1/_2 \times \sum_{\substack{f_1, f_2 \\ \alpha, \beta}} G_{\alpha\beta}(f_1, f_2) S_{f_1}^\alpha S_{f_2}^\beta - {}^1/_2 \sum_{\substack{f_1, f_2 \\ \alpha, \beta}} \sum_{ij} A_{ij}^{\alpha\beta}(f_1, f_2) S_{f_1}^\alpha S_{f_2}^\beta u_{ij} \quad (2)$$

or

$$\mathscr{H} = G - {}^1/_2 \sum_{\substack{f_1, f_2 \\ \alpha, \beta}} D_{\alpha\beta}(f_1, f_2) S_{f_1}^\alpha S_{f_2}^\beta - \sum_{f,\alpha} \mu H \gamma^\alpha S_f^\alpha, \quad D_{\alpha\beta}(f_1, f_2) = G_{\alpha\beta}(f_1, f_2) + \sum_{ij} u_{ij} A_{ij}^{\alpha\beta}(f_1, f_2), \quad (3)$$

where $A_{ij}^{\alpha\beta}(f_1, f_2)$ is the tensor of magnetic interaction, γ^α is the direction cosine of the magnetic field. (Inasmuch as the tensor $G_{\alpha\beta}$ describes the magnetic interaction in generalized form, the evident form of the dependence of $A_{ij}^{\alpha\beta}$ on the components $G_{\alpha\beta}$ and their derivatives is not brought out here, and will not be made use of in what follows.) In this manner, the Hamiltonian of the system in the form (2) will appear as the initial Hamiltonian of our problem.

The calculation of the terms of magnetic and magneto-elastic interaction permits the removal of exchange degeneracy even in the zeroth approximation. The parametric character of the dependence of the Hamiltonian (2) on the components of the deformation tensor makes possible the use of the general scheme of the method of finding the ground level and the energy spectrum that is described in the book of Bogoliubov[9]. For this purpose, we express the Hamiltonian (3) by Fermi operators $a_{f\nu}$ making use of the well-known relations

$$S_f^x = a_{f,-1/2}^+ a_{f,1/2} + a_{f,1/2}^+ a_{f,-1/2}, \quad S_f^y = i(a_{f,1/2}^+ a_{f,-1/2} - a_{f,-1/2}^+ a_{f,1/2}), \quad S_f^z = a_{f,-1/2}^+ a_{f,-1/2} - a_{f,1/2}^+ a_{f,1/2}, \quad (4)$$

with the condition

$$a_{f,-1/2}^+ a_{f,-1/2} + a_{f,1/2}^+ a_{f,1/2} = 1. \quad (5)$$

The Hamiltonian takes the form

$$\mathscr{H} = - {}^1/_2 \sum B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2') a_{f_1\nu_1}^+ a_{f_2\nu_2}^+ a_{f_2\nu_2'} a_{f_1\nu_1'} + \sum' A(f, \nu_1, \nu_1') a_{f\nu_1}^+ a_{f\nu_1'} \quad (6)$$

(for the present, we omit the constant term G_0). The quantities $B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2')$ and $A(f, \nu_1, \nu_1')$ will be completely determined as known functions of the components of the tensors $G_{\alpha\beta}$, $A_{ij}^{\alpha\beta}$ u_{ij} and the field H.

DETERMINATION OF THE GROUND LEVEL AND THE ENERGY SPECTRUM

The ground level of the system is found by a quasi-classical method, replacing the operators $a_{f\nu}$ by the c-numbers $\theta_0(f, \nu)$ which are subject to the condition

$$\sum \theta_0^*(f, \nu)\,\theta_0(f, \nu) = 1 \qquad (7)$$

and which satisfy the equations

$$-\sum B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2') \times \theta_0^*(f_2, \nu_2)\,\theta_0(f_2, \nu_2')\,\theta_0(f_1, \nu_1') + \sum A(f_1, \nu_1, \nu_2)\,\theta_0(f_1, \nu_2) = \lambda_0(f_1)\,\theta_0(f_1\nu_1). \qquad (8)$$

We transform Eq. (6) to the operators $a_{f\omega}$ with the help of the function $\theta_\omega(f, \nu)$:

$$a_{f\nu} = \sum_\omega \theta_\omega(f, \nu)\,a_{f\omega} \qquad (\omega = 0.1),$$

where the $\theta_\omega(f, \nu)$ are orthogonal to $\theta_0(f, \nu)$ and satisfy the equations

$$-\sum B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2') \times \theta_0^*(f_2, \nu_2)\,\theta_0(f_2, \nu_2')\,\theta_\omega(f_1, \nu_1') + \sum A(f_1, \nu_1, \nu_2)\,\theta_\omega(f_1, \nu_2) = \lambda_\omega(f_1)\,\theta_\omega(f_1, \nu_1). \qquad (9)$$

Introducing the operators $b_{f\omega}$ which obey the Bose statistics aproximately:

$$b_{f\omega} = \overset{+}{a}_{f0} a_{f\omega},\ b_{f\omega}^{+} = \overset{+}{a}_{f\omega} a_{f0},\ n_{f\omega} = b_{f\omega}^{+} b_{f\omega} \quad (\omega = 1), \qquad (10)$$

The Hamiltonian (6) can be reduced, for the case of weak excitations, to a quadratic form relative to the operators $b_{f\omega}$:

$$\mathscr{H} = E_0 + \sum \{\lambda_\omega(f) - \lambda_0(f)\}\, b_{f\omega}^{+} b_{f\omega} + \sum Q(f_1, f_2, \omega_1, \omega_2)\, b_{f_1\omega_1}^{+} b_{f_2\omega_2} + {}^1/_2 \sum P^*(f_1, f_2, \omega_1, \omega_2)\, b_{f_1\omega_1} b_{f_2\omega_2} + {}^1/_2 \sum P(f_1, f_2, \omega_1, \omega_2)\, b_{f_1\omega_1}^{+} b_{f_2\omega_2}^{+}, \qquad (11)$$

where

$$Q(f_1, f_2, \omega_1, \omega_2) = \sum B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2') \times \theta_{\omega_1}^*(f_1, \nu_1)\,\theta_0^*(f_2, \nu_2)\,\theta_{\omega_2}(f_2, \nu_2')\,\theta_0(f_1, \nu_1'), \qquad (12)$$

$$P(f_1, f_2, \omega_1, \omega_2) = \sum B(f_1, f_2, \nu_1, \nu_2, \nu_1', \nu_2') \times \theta_{\omega_1}^*(f_1, \nu_1)\,\theta_{\omega_2}^*(f_2, \nu_2)\,\theta_0(f_2, \nu_2')\,\theta_0(f_1, \nu_1').$$

The problem of finding the energy spectrum reduces to the reduction of the Hamiltonian (11) to diagonal form. For this, we transform Eq. (11) according to the formulas

$$b_{f1} = \sum_k \{u_{kf}\xi_k + v_{kf}^*\xi_k^{+}\}, \qquad b_{f1}^{+} = \sum \{u_{kf}^*\xi_k^{+} + v_{kf}\xi_k\}, \qquad (13)$$

where the ξ_k are Bose operators and u_{kf} and v_{kf} are the eigenfunctions of the equations

$$E_k u_{kf_1} = \sum_{f_2} P(f_1, f_2)\, v_{kf_2} + \sum_{f_2} Q(f_1, f_2)\, u_{kf_2} + \Lambda_{f_1} u_{kf_1},$$
$$-E_k v_{kf_1} = \sum_{f_2} P^*(f_1, f_2)\, u_{kf_2} + \sum_{f_2} Q^*(f_1, f_2)\, v_{kf_2} + \Lambda_{f_1} v_{kf_1} \qquad (14)$$
$$(\Lambda_f = \lambda_1(f) - \lambda_0(f)),$$

and satisfy the condition

$$\sum_f (u_{kf} u_{k'f}^* - v_{kf} v_{k'f}^*) = \delta(k, k') \qquad (15)$$

[E_k is the eigenvalue of the system (14)]. Making use of Eq. (13), setting up pair products of the operators $b_{f\omega}$ and substituting in Eq. (11), we obtain, keeping in mind the properties of ξ_k, v_{kf}, u_{kf}

$$\mathscr{H} = E_0 - \sum E_k v_{kf}^* v_{kf} + \sum E_k \xi_k^{+} \xi_k. \qquad (16)$$

The quantity $-\Sigma\, E_k v_{kf}^* v_{kf}$ can be regarded as a correction to the energy level E_0, for which reason we denote it as ΔE_0. The quantity E_k is some function of the wave number which characterizes the spectrum of elementary excitations. The eigenvalues of the operator $\xi_k^+ \xi_k = \hat{N}_k$ are known; they are the integers 0, 1, 2, ...

Thus,

$$\tilde{\mathscr{H}} = E_0 + \Delta E_0 + \sum E_k \hat{N}_k. \quad (17)$$

The energy of the system with the Hamiltonian in the form (17) can be interpreted as the energy of an ideal gas of quasi-particles (elementary excitations), which obeys the Bose statistics; the quantity E_k will characterize the energy spectrum of the quasi-particles. The energy levels of the system will be determined by the collection of occupation numbers of the quasi-particles in the states E_k. In order to establish the dependence of the quantities ΔE_0 and E_k (which are of interest to us) on the characteristics of the system, we make use of Eqs. (14), the solutions to which we shall seek in the form

$$u_{kf} = u_k e^{ifk}, \; v_{kf} = v_k e^{ifk}. \quad (18)$$

Substituting Eq. (18) in Eq. (14) and introducing the notation

$$P(k) = \sum_{f_2} P(f_1 - f_2) e^{i(f_1 - f_2)k}, \quad (19)$$

$$Q(k) = \sum_{f_2} Q(f_1 - f_2) e^{i(f_1 - f_2)k},$$

we get

$$[(E_k - \Lambda) - Q(k)] u_k - P(k) v_k = 0, \quad (20)$$
$$P^*(k) u_k - [(E_k + \Lambda) + Q^*(k)] v_k = 0.$$

From the conditions of solvability of these equations, an expression is immediately obtained for $E(k)$, if we keep in mind that $Q(k)$ is a real quantity,

$$E_k = \{(Q(k) - \Lambda)^2 - |P(k)|^2\}^{1/2}. \quad (21)$$

In order to find ΔE_0 we must calculate $v_{kf} v^*_{kf}$; by virtue of Eq. (18) it is sufficient to find v_k^2. From Eq. (20), eliminating u_k and making use of the condition (15), we get

$$\Delta E_0 = -\frac{1}{2} \sum \frac{|P(k)|^2}{E_k + Q(k) + \Lambda} \quad (22)$$

To bypass the difficulties of solution of the system of Eqs. (8) and (9), we take advantage of the procedure set forth by Tiablikov[6]. In finding the the ground level and the minimizing form of the function $\theta_0(f, \nu)$ we can replace the components of the spin operator S_f^α by components of ordinary vectors σ_f^α. We put the relations which connect the components σ_f with the c-numbers $\theta_0(f, \nu)$, by analogy with Eq. (4), in the form

$$\sigma_f^x = \theta_0^*(f, -1/2)\theta_0(f, 1/2) + \theta_0^*(f, 1/2)\theta_0(f, -1/2), \quad (23)$$
$$\sigma_f^y = i\{\theta_0^*(f, 1/2)\theta_0(f, -1/2) - \theta_0^*(f, -1/2)\theta_0(f, 1/2),$$
$$\sigma_f^z = \theta_0^*(f, -1/2)\theta_0(f, -1/2) - \theta_0^*(f, 1/2)\theta_0(f, 1/2).$$

Instead of Eq. (7) we will have the condition

$$\sum_\alpha (\sigma_f^\alpha)^2 = 1 \quad (\alpha = x, y, z). \quad (24)$$

Keeping in mind the well-defined connection between σ_f^α and $\theta_0(f, \nu)$, we consider the quadratic form

$$E = -1/2 \sum D_{\alpha\beta}(f_1, f_2, u_{ij}) \sigma_{f_1}^\alpha \sigma_{f_2}^\beta - \sum \mu H \gamma^\alpha \sigma_f^\alpha \quad (25)$$

and seek its minimumunder the added condition (24). Consequently, the minimizing form of the value of the components σ_f^α can be determined from the system of $3N$ equations

$$-\sum_{f_2, \beta} D_{\alpha\beta}(f_1, f_2, u_{ij}) \sigma_{f_2}^\beta - \lambda(f_1)\sigma_f^\alpha = \mu H \gamma^\alpha. \quad (26)$$

We now find the expression for E_0. For this purpose, we multiply each of the Eqs. (26) by the corresponding σ_f^α and add. As a result, we obtain

$$E_0 = 1/2 \sum D_{\alpha\beta}(f_1, f_2, u_{ij}) \sigma_{f_1}^\alpha \sigma_{f_2}^\beta + \sum \lambda(f_1). \quad (27)$$

The equation for the calculation of $\theta_0(f, \nu)$ in terms of σ_f^α can be written in the form

$$\lambda_0(f_1)\theta_0(f_1, \nu) = \sum_\alpha \lambda(f_1) \sigma_{f_1}^\alpha [\partial\sigma_{f_1}^\alpha / \partial\theta_0^*(f_1, \nu)]. \quad (28)$$

We note that Eq. (9) for determining $\theta_1(f, \nu)$ is obtained from Eq. (8) by the formal substitution of $\theta_1(f_1, \nu_1)$ for $\theta_0(f_1, \nu_1)$ (here it is obvious that $\lambda_0 \to \lambda_1$). In the same way we get from Eq. (28) the equation for $\theta_1(f_1, \nu_1)$.

$$\lambda_1(f_1)\theta_1(f_1, \nu_1) = \sum_\alpha \lambda(f_1) \sigma_{f_1}^\alpha [\partial\sigma_{f_1}^\alpha / \partial\theta_0^*(f_1, \nu_1)]_{\theta_0(f_1, \nu_1) \to \theta_1(f_1, \nu_1)}. \quad (29)$$

We solve Eqs. (28) and (29) by making use of the orthogonality of the functions $\theta_0(f,\nu)$, $\theta_1(f,\nu)$; we obtain

$$\theta_0(f,-1/2)=\sqrt{(1+\sigma_f^z)/2},\ \theta_0(f,1/2)=e^{i\varphi_f}\sqrt{(1-\sigma_f^z)/2}, \tag{30}$$

$$\theta_1(f,-1/2)=\sqrt{(1-\sigma_f^z)/2},\ \theta_1(f,1/2)=e^{i(\varphi_f+\pi)}\sqrt{1+\sigma_f^z)/2}, \tag{31}$$

$$\lambda_1(f_1)=-\lambda_0(f_1)=\lambda(H).$$

It was shown earlier that the external magnetic field is sufficiently strong; moreover, we assume that because of the nearness of the system to the state of magnetic saturation of the spin of all sites one can consider the spins parallel and therefore the components σ_f^α are practically independent of the site number f.

We introduce sums over the lattice

$$\overline{G}_{\alpha\beta}=\sum_{f_2}G_{\alpha\beta}(f_1,f_2),\ \overline{A}_{ij}^{\alpha\beta}=\sum_{f_2}\overline{A}_{ij}^{\alpha\beta}(f_1,f_2). \tag{32}$$

For a hexagonal lattice (when the principal axis coincides with the axis $0Z$) the following assumptions can be made relative to the components of the tensors $G^{\alpha\beta}$ and $A_{ij}^{\alpha\beta}$:

$$\overline{G}_{\alpha\beta}=0 \quad \text{for} \quad \alpha\neq\beta; \tag{33}$$

$$\overline{G}_{11}=\overline{G}_{22}=G_0;\quad \overline{G}_{33}=G_0^a>G_0;$$

$$\overline{A}_{ij}^{\alpha\beta}=\overline{A}_{ji}^{\alpha\beta}=\overline{A}_{ij}^{\beta\alpha};\quad \overline{A}_{ij}^{\alpha\beta}=\overline{A}_{\alpha\beta}^{ij}, \tag{34}$$

$$A_{ij}^{\alpha\beta}\neq 0\begin{cases}\text{when } (\alpha\beta)\neq(ij) \text{ for } i=j \text{ and simultaneously } \alpha=\beta;\\ \text{when } (\alpha\beta)=(ij) \text{ for } i\neq j,\ \alpha\neq\beta;\end{cases}$$

the other components vanish.

Introducing the abbreviating notation:

$$-\frac{G_0+\lambda}{\mu H}=x;\quad G_0^a-G_0=\Delta;\quad \frac{\Delta}{\mu H}=\eta; \tag{35a}$$

$$A_1^1/\mu H=\varepsilon_1,\ A_2^2/\mu H=\varepsilon_2,\ A_3^3/\mu H=\varepsilon_3;\ A_2^1/\mu H=\varepsilon_1^0,\ A_2^3/\mu H=\varepsilon_2^0;$$

$$A_1^3/\mu H=\varepsilon_3^0, \tag{35b}$$

where

$$A_\alpha^\beta=A_\beta^\alpha=\sum_{ij}u_{ij}A_{ij}^{\alpha\beta}, \tag{35c}$$

we rewrite Eq. (26), taking into account the assumptions on the independence of σ_f^α on f:

$$\begin{aligned}(\varepsilon_1-x)\sigma_1+\varepsilon_1^0\sigma_2+\varepsilon_3^0\sigma_3&=-\gamma_1,\\ \varepsilon_1^0\sigma_1+(\varepsilon_2-x)\sigma_2+\varepsilon_2^0\sigma_3&=-\gamma_2,\\ \varepsilon_3^0\sigma_1+\varepsilon_2^0\sigma_2+(\varepsilon_3+\eta-x)\sigma_3&=-\gamma_3.\end{aligned} \tag{36}$$

According to Eq. (24), the σ_i are connected by the condition

$$\sum_i\sigma_i^2=1. \tag{37}$$

Because of the assumption on the strong fields, the magnitudes of η, ϵ_i, ϵ_i^0 can be considered small, and Eqs. (36) can be solved approximately under the condition (37). As a result, we obtain relatively simple expressions for σ_i and λ:

$$\sigma_1=\frac{1}{x}\left\{\gamma_1+\frac{1}{x}\left[\gamma_1\varepsilon_1+\gamma_2\varepsilon_1^0+\gamma_3\varepsilon_3^0\right]\right\}, \tag{38}$$

$$\sigma_2=\frac{1}{x}\left\{\gamma_2+\frac{1}{x}\left[\gamma_1\varepsilon_1^0+\gamma_2\varepsilon_2+\gamma_3\varepsilon_2^0\right]\right\},$$

$$\sigma_3=\frac{1}{x-\eta}\left\{\gamma_3+\frac{1}{x-\eta}\left[\gamma_1\varepsilon_3^0+\gamma_2\varepsilon_2^0+\gamma_3\varepsilon_3\right]\right\};$$

$$\lambda=-G_0-\mu H-\Delta\gamma_3^2-\xi(\gamma_i,\gamma_j,u_j), \tag{39}$$

where

$$\begin{aligned}\xi(\gamma_i,\gamma_j,u_{ij})=&(u_{11}\overline{A}_{11}^{11}+u_{22}\overline{A}_{22}^{11}+u_{33}\overline{A}_{33}^{11})\gamma_1^2\\&+(u_{11}\overline{A}_{11}^{22}+u_{22}\overline{A}_{22}^{22}+u_{33}\overline{A}_{33}^{22})\gamma_2^2\\&+(u_{11}\overline{A}_{11}^{33}+u_{22}\overline{A}_{22}^{33}+u_{33}\overline{A}_{33}^{33})\gamma_3^2+2u_{12}\overline{A}_{12}^{12}\gamma_1\gamma_2\\&+2u_{13}\overline{A}_{13}^{13}\gamma_1\gamma_3+2u_{23}\overline{A}_{23}^{23}\gamma_2\gamma_3.\end{aligned} \tag{40}$$

Substituting in the formulas for $P(f_1,f_2)$ and $Q(f_1,f_2)$ expressions for $B(f_1,f_2,\nu_1,\nu_2,\nu_1',\nu_2')$,

$\theta_0(f, \nu)$ and $\theta_1(f, \nu)$, we obtain

$$-Q(f_1, f_2) = \frac{1}{2}[D_{11}(f_1, f_2) + D_{22}(f_1, f_2)](1 + \sigma_3^2) \tag{41}$$

$$+ D_{33}(f_1, f_2)(1 - \sigma_3^2) - D_{12}(f_1, f_2)(1 - \sigma_3^2)\sin 2\varphi$$

$$-\frac{1}{2}[D_{11}(f_1, f_2) - D_{22}(f_1, f_2)](1 - \sigma_3^2)\cos 2\varphi$$

$$-2D_{13}(f_1, f_2)\sigma_3\sqrt{1-\sigma_3^2}\sin\varphi - 2D_{23}(f_1, f_2)\sigma_3\sqrt{1-\sigma_3^2}\cos\varphi;$$

$$-P(f_1, f_2) = [D_{11}(f_1, f_2) - D_{22}(f_1, f_2)]\left\{\frac{1}{2}(1-\sigma_3^2)\cos 2\varphi - \sigma_3 \sin 2\varphi\right\}$$

$$-2iD_{12}(f_1, f_2)\left\{\frac{1}{2}(1+\sigma_3^2)\sin 2\varphi - \sigma_3\cos 2\varphi\right\}$$

$$+\frac{1}{2}[2D_{33}(f_1, f_2) - D_{22}(f_1, f_2) - D_{11}(f_1, f_2)](1 - \sigma_3^2)$$

$$+[D_{13}(f_1, f_2) - iD_{23}(f_1, f_2)]e^{i\varphi}(1 - \sigma_3)\sqrt{1-\sigma_3^2}$$

$$-[D_{13}(f_1, f_2) + iD_{23}(f_1, f_2)]e^{-i\varphi}(1 + \sigma_3)\sqrt{1-\sigma_3^2},$$

where

$$\cos\varphi = \frac{\sigma_1}{\sqrt{1-\sigma_3^2}}, \quad \sin\varphi = \frac{\sigma_2}{\sqrt{1-\sigma_3^2}}, \quad \varphi = \operatorname{arctg}\frac{\sigma_2}{\sigma_1}. \tag{42}$$

We now have arranged all the necessary data for finding the quantities E_0, ΔE_0 and E_k of interest to us.

Making use of Eqs. (27) and (33) we get for E_0

$$E_0 = -\frac{N}{2}\left[G_0 + \frac{1}{2}\Delta\gamma_3^2 + \frac{1}{2}\xi(\gamma_i, \gamma_j, u_{ij}) + 2\mu H\right] \tag{44}$$

We introduce the Fourier decomposition

$$D_{\alpha\beta}(k) = \sum_{(f_2-f_1)\neq 0} D(f_2 - f_1)e^{-i(f_2-f_1)k} \tag{45}$$

$$= G_{\alpha\beta}(k) + \sum_{ij} u_{ij}A_{ij}^{\alpha\beta}(k).$$

Inasmuch as we have made assumptions about low temperatures, we must limit ourselves to the approximation of small wave numbers

$$G_{\alpha\beta}(k) = \overline{G_{\alpha\beta}} - \frac{1}{2}\overline{G_{\alpha\beta}f^2}k^2 + O_G(k^4), \tag{46}$$

$$A_{ij}^{\alpha\beta}(k) = \overline{A_{ij}^{\alpha\beta}} - \frac{1}{2}\overline{A_{ij}^{\alpha\beta}f^2}k^2 + O_A(k^4).$$

In such an assumption, it is of course understood that we limit ourselves to the approximation of nearest neighbors and make a definite averaging over the angles in the space of the wave numbers.

For maximum simplification of the tedious calculations, we shall use approximate forms in place of Eqs. (21) and (22):

$$E_k = Q(k) - 2\lambda, \tag{47}$$

$$\Delta E_0 = -\frac{1}{4}\sum\frac{|P(k)|^2}{E_k}. \tag{48}$$

Multiplying on the right and the left of the expression for $Q(f_1, f_2)$ in Eq. (41) by $e^{-i(fk)}$ and summing over f, we get $Q(k)$. Expanding the components

$$D_{\alpha\beta}(k) = G_{\alpha\beta}(k) + \sum u_{ij}A_{ij}^{\alpha\beta}(k)$$

in a series, in accord with Eq. (46), and substituting in $Q(k)$, and also substituting for the σ_i their values from Eq. (38) [taking into account Eq. (35)], we get

$$E_k = 2\mu H - \Delta(1 - 3\gamma_3^2) + \xi(\gamma_i, \gamma_j, u_{ij}) + \beta k^2. \tag{49}$$

The expression for β has a rather formidable appearance, but the first term is the greatest:

$$\beta = \frac{1}{2}[\overline{G_0^a f^2} + \overline{G_0 f^2}] + \ldots \quad (50)$$

It is not difficult to note that this quantity is proportional to the exchange integral. To find ΔE_0, in accordance with Eq. (48), we must find $|P(k)|^2$. The quantity $P(k)$ can be found in the same way as $Q(k)$, from Eq. (42) for $P(f_1, f_2)$. Inasmuch as $P(k)$ is a complex quantity, we can write it in the form

$$P(k) = P_r(k) + iP_i(k). \quad (51)$$

In this same approximation of Eq. (46) we get

$$|P(k)|^2 = a_0 - a_2 k^2 + a_4 k^4, \quad (52)$$

where the largest term, which we need, is

$$a_0 = \overline{P}_{r0}^2 + \overline{P}_{i0}^2. \quad (53)$$

Denoting a certain limiting value of k by n (n = a number of the order of unity), we get, approximately, for the case of moderately strong fields (omitting terms which do not depend on the field):

$$\Delta E_0 = \quad (54)$$

$$\frac{a_0 V}{16\pi\beta^{3/2}} \sqrt{2\mu H - \Delta(1 - 3\gamma_3^2) + \xi(\gamma_i, \gamma_j, u_{ij})}.$$

We note that term which corresponds to ΔE_0 in the expression for the magnetization (M_H), and which is obtained after differentiation according to H, not being dependent on temperature, keeps a finite value even at absolute zero and disappears only in infinitely large fields. This conclusion is still further confirmed by the results obtained in the researches of references 6 and 10. However, the expression for M_H is obtained much more precisely by virtue of the calculation of the magneto-elastic interaction (within the framework of the assumption on a single ferromagnetic electron per atom)*.

An estimate of the quantity a_0 shows that $a_0 \approx \Delta^2$ and, inasmuch as Δ is of the order of the first constant of magnetic anisotropy (relative to one atom), i.e., of the order of 10^{-16} - 10^{-17} erg or less, in the computation of the free energy and magnetostriction, we will not consider the correction to the ground level, since its effect on the final results will be very slight in the accepted approximation.

THE FREE ENERGY AND THE TEMPERATURE DEPENDENCE OF THE CONSTANTS OF MAGNETOSTRICTION

All quantities which characterize the energy of a spontaneously deformed crystal have now been obtained. In order to go over to macroscopic quantities, we find the sum-over-states

$$Z = \text{Spur}\{e^{-\mathcal{H}/\vartheta}\} \qquad (\vartheta = kT). \quad (55)$$

In our case the Hamiltonian $\mathcal{H}$ has the form of Eq. (17); therefore, we obtain the following expression for the free energy in the usual way:

$$\Psi = E_0 + \Delta E_0 + \vartheta\Sigma \ln(1 - e^{-E_k/\vartheta}). \quad (56)$$

Making use of Eqs. (44) and (49) for E_0 and E_k, we obtain, approximately,

$$\Psi = -\frac{1}{2}\frac{N}{V}[G_0 + \Delta\gamma_3^2 + \xi(\gamma_i, \gamma_j, u_{ij}) + 2\mu H] - \frac{\vartheta}{2\pi^2}\frac{\sqrt{\pi}}{4}\left(\frac{\vartheta}{\beta}\right)^{3/2}\exp\left\{-\frac{2\mu H - \Delta}{\vartheta}\right\} \times \exp\left\{-\frac{3\Delta\gamma_3^2 + \xi(\gamma_i, \gamma_j, u_{ij})}{\vartheta}\right\} \quad (57)$$

We are primarily interested in the character of the temperature dependence of the anisotropic and magneto-elastic terms of the free energy; therefore, we have specifically isolated in the second term of Eq. (57) the factor which contains the direction cosines of the vector of the magnetic field (at saturation, the direction of the field coincides with the direction of the magnetization).

At temperatures differing only slightly from absolute zero, the first term in Eq. (57) is the better approximation for the free energy. At high temperatures, the second term of Eq. (57) also begins to play a role. The exponential factor

$$\exp\{-[3\Delta\gamma_3^2 + \xi(\gamma_i, \gamma_j, u_{ij})]/\vartheta\} \quad (58)$$

at small values of the exponent can be expanded in a series. Inasmuch as the quantity $\xi(\gamma_i, \gamma_j, u_{ij})$

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* The problem of the magnetization of ferromagnetics in connection with a calculation of the magnetic interaction, touched upon here very superficially, requires special consideration and will be treated in another article.

[10] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940)

is of the order of the magneto-elastic energy per atom, it is 3-4 orders of magnitude smaller than Δ. Therefore, the possibility of decomposition is determined by the condition

$$\vartheta > \Delta. \tag{59}$$

This condition determines the lower temperature limit of applicability of such a decomposition; carrying out the latter, we get for the free energy of anisotropy

$$\Psi_a = -\left\{\frac{N\Delta}{2V} - \frac{3\sqrt{\pi}\Delta}{8\pi^2}\left(\frac{\vartheta}{\beta}\right)^{3/2}\exp\left[-\frac{2\mu H-\Delta}{\vartheta}\right]\right\}\gamma_3^2 \tag{60}$$

and for the free magneto-elastic energy

$$\Psi_{м.у} = -\left\{\frac{N}{2V} - \frac{\sqrt{\pi}}{8\pi^2}\left(\frac{\vartheta}{\beta}\right)^{3/2} \times \exp\left[-\frac{2\mu H-\Delta}{\vartheta}\right]\right\}\xi(\gamma_i, \gamma_j, u_{ij}) = f(\vartheta, H)\,\xi(\gamma_i, \gamma_j, u_{ij}). \tag{61}$$

It is evident by direct comparison that Eq. (60) for the free energy of anisotropy virtually coincides with the expression obtained earlier by Tiablikov[6].

From the properties of the tensor $A_{ij}^{\alpha\beta}(f_1, f_2)$ for the hexagonal lattice, it follows that

$$\overline{A_{11}^{11}} = \overline{A_{22}^{22}},\ \overline{A_{11}^{22}} = \overline{A_{22}^{11}},\ \overline{A_{33}^{11}} = \overline{A_{11}^{33}} = \overline{A_{22}^{33}} = \overline{A_{33}^{22}},\ \overline{A_{23}^{23}} = \overline{A_{13}^{13}},\ \overline{A_{12}^{12}} = 2\,(\overline{A_{11}^{11}} - \overline{A_{22}^{22}}). \tag{62}$$

Inserting these relations in Eq. (61), we obtain an expression, from whose consideration it is evident that it is analogous, in the character of its dependence on γ_i and u_{ij}, to the classical expression for the magneto-elastic energy; hence, the quantities

$$\frac{\overline{A_{ij}^{\alpha\beta}}N}{2V}f(\vartheta, H) \tag{63}$$

will play the role of magneto-elastic coefficients.

Up to the present time the dependence of the energetic quantities with which we have to deal on the u_{ij} has been considered parametrically. In order to obtain clear expressions for the magnetostrictive constants, it is necessary to bring into consideration the elastic energy and to determine the equilibrium value of the components of the deformation tensor from the condition of minimum free energy. This is done in precisely the same way as in classical theory. As a result we obtain for the magnetostrictive constants the expression

$$\varkappa_i = \varkappa_i^0\left\{1 - \frac{V}{4N}\left(\frac{\vartheta}{\pi\beta}\right)^{3/2} \times \exp\left[-\frac{2\mu H-\Delta}{\vartheta}\right]\right\},\quad i = 1, 2, \ldots, 5, \tag{64}$$

where, for example,

$$\varkappa_1^0 = \frac{N}{V}\,[c_1(2\overline{A_{11}^{33}} - \overline{A_{11}^{11}} - \overline{A_{11}^{22}}) - c_2\overline{A_{33}^{33}}], \tag{65}$$

$$\varkappa_2^0 = \frac{N}{V}\,[c_3\overline{A_{11}^{22}} - c_4\overline{A_{11}^{11}} - c_5\overline{A_{33}^{33}}].$$

The coefficients c_i depend on the elastic constants of the crystalline lattice.

The quantities $A_{ij}^{\alpha\beta}$ in the complete theory depend on the matrix elements of the operators of magneto-elastic interaction, and are computed with the help of the corresponding wave functions. It is therefore natural that the resultant constants of magnetostriction can be either positive or negative. This circumstance is significant, since the classical theory accounts only for constants of positive sign. This special feature of the quantum theory of magnetostriction was pointed out earlier by Vonsovskii[7]. The dependence of the constants of magnetostriction on the magnitude of the magnetic field (which stems from the theory) is a new and significant result. We note that the necessity of such a dependence was shown by Akulov[3].

The low temperature limit of applicabliity of the resultant formulas for the free energy and the constants of magnetostriction was defined by the inequality (59) above. The upper limit is evidently determined by the basic physical assumption of the theory---consideration of only weakly interacting systems. Referring to this assumption, we throw away terms of third and fourth order relative to the operators $a_{f\omega}$ in the Hamiltonian in the operators $a_{f\omega}$. Therefore, the upper temperature limit can be fixed from an estimate of the energy contribution of the discarded terms and comparison of them with the energy contribution of those that remain. The corresponding calculation gives

$$(\vartheta / J)^{3/2} \ll 1, \tag{66}$$

where J is the exchange integral. If, for example, accuracy within 20% is desired from (66), it follows that the expression for the free energy of a ferromagnetic monocrystal (57) and the formulas obtained from it for the temperature dependence of the constants of magnetostriction are correct to the temperature of liquid hydrogen.

CONCLUSIONS

1. A systematic quantum-mechanical consideration of a system of electrons in a ferromagnetic monocrystal gives the possibility of explaining the phenomenon of magnetostriction and once more confirms that the phenomenon of magnetostriction is essentially connected to the magnetic interaction of the electrons.

2. The theory gives the temperature dependence of the constants of magnetostriction for the hexagonal crystals.

3. The constants of magnetostriction must display a dependence on the magnetic field. In connection with this fact, representations used in quantum theory involving the independence of the magnetic constants on the field require more accurate definition.

4. A definite analogy exists between the temperature dependence of the constants of magnetostriction and magnetic anisotropy, as is evident from the comparison of Eq. (60) with Eq. (61). This analogy is connected with the character of the energetic spectrum of ferromagnetics at low temperatures.

The proposed theory is clearly still incomplete. and needs, in the future, refinement and development. Its deficiencies are connected, in the first place, with the assumed model of the ferromagnetic and, in the second place, with the approximations and assumptions made in the course of the calculations. In particular, it ought to be relieved of the assumption that there must be only one ferromagnetic electron at a site; the representation of the magnetic interaction in generalized tensor form, for all its advantages of generality, still bears a phenomenological character; other types of interaction of electrons in the lattice were not studied; the case of weak fields, which evidently presents definite interest, was not considered. However, the initial aspects of the theory permit us, without any difficulties in principle, to take into account many of these factors.

In conclusion, we note that the method used in the present work for consideration of the magnetostriction of hexagonal crystals is also applicable to other problems of the quantum theory of ferromagnetism and, in particular, it can be extended to cubical crystals and to much more complicated systems (alloys, antiferromagnets). These problems, which have an independent interest, will be considered in subsequent researches.

Translated by R. T. Beyer
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