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N. A. POTAPKOV

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Abstract

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N. A. POTAPKOV

THE HAMILTONIAN OF A UNIAXIAL FERROMAGNET

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For the theory of ferromagnetism, it is of interest to obtain an expression for the Hamiltonian of a ferromagnet taking into account the magnetic interactions of electrons. Following paper ([1]), we choose the expression for the magnetic energy according to the correspondence principle. Then the energy operator of the system of electrons, with spin-orbit and spin-spin interaction taken into account, has the form

$$\mathcal{H} = -\mu \sum H S_{q_i} - \sum U_f(q_i) + \frac{1}{2} \sum \Phi(q_i - q_j) + \\ + \frac{Ze^2}{2m^2c^2} \sum \frac{L_{fq_i} S_{q_i}}{|f-q|^3} + \frac{e^2}{2m^2c^2} \sum \left(\frac{S_{iS}j}{r_{ij}^3} - \frac{3(S_i r_{ij})(S_j r_{ij})}{r_{ij}^5} \right). \quad (1)$$

Here H is the external magnetic field; m is the mass; e is the charge; q is the coordinate; L is the orbital angular-momentum operator; S is the spin operator of the electron; μ is the Bohr magneton; Ze is the effective charge of the ion; $\Phi(q_i - q_j)$ is the energy of electrostatic interaction; $U(q_i)$ is the sum of the kinetic energy and the potential energy of the electron in the field of the lattice atoms.

The last two terms represent the spin-orbit and spin-spin interaction of the electrons. The Hamiltonian depends on the coordinates and spin variables of the electrons. The aim of the work is to transform the Hamiltonian to a representation in the form of second quantization, since this substantially simplifies the problem of determining the energy eigenvalues of the system. The method of second quantization was developed in ([2–7]) and, in its most complete form, in ([8]).

Following ([8]), we expand the many-electron wave function in a product of one-electron functions $\psi_\alpha(x)$, where α is a set of quantum numbers, and x denotes the coordinates (including spin). Then, substituting the expansion into the wave equation and carrying out the corresponding transformations, we obtain the Hamiltonian of the system in the second-quantization representation:

$$\mathcal{H} = -\mu \sum \langle \alpha | H S_q | \alpha' \rangle a_\alpha^+ a_{\alpha'} + \sum \left\langle \alpha \left| \sum U_f(q) \right| \alpha' \right\rangle a_\alpha^+ a_{\alpha'} +$$

$$
\begin{aligned}
&+\frac{1}{2}\sum\langle\alpha_1\alpha_2|\Phi(q_1-q_2)|\alpha'_1\alpha'_2\rangle a^+_{\alpha_1}a^+_{\alpha_2}a_{\alpha'_2}a_{\alpha'_1}+\\
&+\frac{Ze^2}{2m^2c^2}\sum\left\langle\alpha\middle|\sum\frac{1}{|f-q|^3}L_{fq}S_q\middle|\alpha'\right\rangle a^+_{\alpha}a_{\alpha'}+\\
&+\frac{e^2}{2m^2c^2}\sum\left\langle\alpha_1\alpha_2\middle|\frac{S_1S_2}{r_{12}^3}-\frac{3(S_1r_{12})(S_2r_{12})}{r_{12}^5}\middle|\alpha'_1\alpha'_2\right\rangle a^+_{\alpha_1}a^+_{\alpha_2}a_{\alpha'_2}a_{\alpha'_1}. \qquad (2)
\end{aligned}
$$

Here a, a^+ are Fermi operators satisfying the permutation relations

$$a_\alpha a_\alpha = a^+_\alpha a^+_\alpha = 0, \qquad a_\alpha a^+_{\alpha'} + a^+_{\alpha'} a_\alpha = \delta_{\alpha\alpha'}. \qquad (3)$$

The matrix elements $\langle\alpha|\alpha'\rangle$ and $\langle\alpha_1\alpha_2|\alpha'_1\alpha'_2\rangle$ are calculated from one-electron wave functions. The summation over α is carried out over all quantum states of the electrons in the crystal. As a result of the influence of the crystal field, the distribution of electrons may change in comparison with that which occurs for an isolated atom. For example, in solid-state theory the outer electrons are considered to be completely collectivized. For the inner electrons, the concept of electron shells is retained, and their wave functions may be obtained from the corresponding wave functions of electrons in the isolated atom, taking account of the symmetry of the crystal.

In what follows we shall take into account the contribution to the energy operator only from electrons of unfilled inner shells (d-electrons). The wave functions of d-electrons in ferromagnets with uniaxial symmetry may be taken in the form

$$\psi_\alpha(x) = \psi_{fm\sigma}(qs) = \varphi_{fm}(q)\chi_\sigma(s), \qquad (4)$$

where f is the site number; m is the magnetic and σ the spin quantum number; q denotes the spatial coordinates, and s the spin coordinate.

Thus, in our case the quantum states of the electrons are characterized by the lattice-site number, the magnetic and spin quantum numbers, and the summation in the Hamiltonian (2) is carried out over the indices $\alpha = f, m, \sigma$.

States with different m in the isolated atom will be degenerate; in the crystal, owing to the influence of the surrounding atoms, the degeneracy is removed and the energy level is split. In the d-shell, the states corresponding to the smallest energy values will be filled. We define the ground state of the system by the relation

$$\sum_{m\sigma} n_{fm\sigma} = n_f = n_e, \qquad (5)$$

where n_e is the number of d-electrons per atom. This state satisfies the equation

$$\mathcal{H}_0 C_0 = E_0 C_0,$$

where $\mathcal{H}_0$ is the operator containing terms diagonal with respect to the numbers f, m.

The nondiagonal terms of the Hamiltonian, corresponding to transitions into unfilled quantum states and to electron exchange, will be quantities of higher order of smallness in comparison with $\mathcal{H}_0$. Applying the method of projecting the Hamiltonian onto the ground state (9), we obtain an approximate expression for the Hamiltonian of the system, accurate up to terms of second order. This expression is not given here because of its cumbersome form. To write it in a more compact form, let us pass from Fermi operators to spin operators according to the formulas

$$\sum_\sigma \sigma a^+_{fm\sigma} a_{fm\sigma} = S^z_{fm}, \qquad a^+_{fm-1/2} a_{fm1/2} = S^-_{fm}, \qquad a^+_{fm1/2} a_{fm-1/2} = S^+_{fm}. \tag{6}$$

After simple transformations we obtain the following expression for the Hamiltonian of the system:

$$\begin{gathered} \mathcal{H} = -\mu \sum H S_f - \frac{1}{2} \sum I(f_1 m_1, f_2 m_2) S_{f_1 m_1} S_{f_2 m_2} - \\ -\frac{1}{2} \sum \delta I(f_1 m_1, f_2 m_2) S^z_{f_1 m_1} S^z_{f_2 m_2} - \\ -\sum B_{fm} \left\{ m - \frac{B_{fm}}{2} \left[\frac{(2-m)(3+m)}{E_{m+1} - E_m} - \frac{(2+m)(3-m)}{E_{m-1} - E_m} \right] \right\} S^z_{fm} - \\ -\frac{1}{4} \sum B^2_{fm} \left[\frac{(2-m)(3+m)}{E_{m+1} - E_m} - \frac{(2+m)(3-m)}{E_{m-1} - E_m} \right] (S^z_{fm})^2. \end{gathered} \tag{7}$$

Here

$$\delta I = \delta I_1 + \delta I_2 + \delta I_3; \tag{8}$$

$$\begin{gathered} \delta I_1(f_1 m_1, f_2 m_2) = \\ = \frac{e^2}{2m^2c^2} \left\langle f_1 m_1 f_2 m_2 \left| \frac{S_1 S_2}{r^3_{12}} - \frac{3(S_1 r_{12})(S_2 r_{12})}{r^5_{12}} \right| f_1 m_1 f_2 m_2 \right\rangle; \end{gathered} \tag{9}$$

$$\delta I_2(f_1m_1, f_2m_2) = \frac{e^2}{2m^2c^2}\left\langle f_1m_1f_2m_2\left|\frac{S_1S_2}{r_{12}^3} - \frac{3(S_1r_{12})(S_2r_{12})}{r_{12}^5}\right|f_2m_2f_1m_1\right\rangle; \tag{10}$$

$$\delta I_3(f_1m_1f_2m_2) =$$

$$= \left(\frac{Ze^2}{2m^2c^2}\right)^2 \frac{1}{\Delta(f_1m_1f_2m_2)}\left\{\left\langle f_1m_1\left|\sum\frac{L^+_{f'q}}{|f'-q|^3}\right|f_2m_2\right\rangle\left\langle f_2m_2\left|\frac{L^-_{f'q}}{|f'-q|^3}\right|f_1m_1\right\rangle - \right.$$

$$\left. - \left\langle f_1m_1\left|\sum\frac{L^z_{f'q}}{|f'-q|^3}\right|f_2m_2\right\rangle\left\langle f_2m_2\left|\frac{L^z_{f'q}}{|f'-q|^3}\right|f_1m_1\right\rangle\right\}; \tag{11}$$

$$B_{fm} = \frac{Ze^2}{2m^2c^2}\left\langle fm\left|\frac{1}{|f-q|^3}\right|fm\right\rangle. \tag{12}$$

In their form, the first three terms of the Hamiltonian are analogous to the ferromagnet Hamiltonian used in work (^{10}). The first term of the Hamiltonian represents the Zeeman energy; the second term, the exchange electrostatic interaction. The third term describes the spin-spin and exchange spin-orbit interaction. The last two terms describe the spin-orbit interaction averaged over the wave functions of individual lattice sites. Thus, the obtained expression for the Hamiltonian of a uniaxial ferromagnet makes it possible to estimate the influence of the spin-spin and spin-orbit interaction on the magnetic properties.

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Magnetic Laboratory
Academy of Sciences of the USSR

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References

1. W. Heisenberg, Zs. Phys., **70**, 395 (1931).
2. P. Jordan, Zs. Phys., **44**, 473 (1927); **45**, 766 (1927); **75**, 648 (1932); **91**, 274 (1934).
3. P. A. M. Dirac, Proc. Roy. Soc., **A 114**, 243 (1927); **A 117**, 610 (1928); **A 118**, 351 (1928).

4. P. Jordan, O. Klein, Zs. Phys., **45**, 471 (1927).
5. P. Jordan, W. Pauli, Zs. Phys., **47**, 151 (1928).
6. P. Jordan, E. Wigner, Zs. Phys., **47**, 631 (1928).
7. W. Heisenberg, W. Pauli, Zs. Phys., **56**, 1 (1929); **59**, 168 (1929).
8. N. N. Bogolyubov, *Lectures on Quantum Statistics*, Kyiv, 1949.
9. S. V. Tyablikov, Vestn. Mosk. Univ., **3**, 35 (1949).
10. S. V. Tyablikov, ZhETF, **20**, 661 (1950).

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