ON THE THEORY OF ANISOTROPY OF CUBIC CRYSTALS

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Abstract

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ON THE THEORY OF ANISOTROPY OF CUBIC CRYSTALS

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Magnetic anisotropy is characterized by the so-called anisotropy constants ([1]). The dependence of the anisotropy constants on temperature for cubic crystals was considered in work ([2]) by means of the method of approximate secondary quantization without taking into account the interaction of spin waves.

In the present work the spin-wave interaction is taken into account for anisotropic ferromagnets with cubic symmetry. The spin-wave interaction is treated by Dyson' s method ([3]).

The Hamiltonian of the system is

$$\mathcal{H} = \mu \sum_{j} (HS_j) - \frac{1}{2} I \sum_{j\delta} (S_j S_{j+\delta}) + \frac{1}{4!}\, \delta I \sum_{\substack{j,\ \delta_1, \delta_2, \delta_3,\ \alpha' \\ \delta_1 \neq \delta_2 \neq \delta_3}} S_j^{\alpha'} S_{j+\delta_1}^{\alpha'} S_{j+\delta_2}^{\alpha'} S_{j+\delta_3}^{\alpha'}, \quad (1)$$

where $\alpha' = (x', y', z')$; H is the external magnetic field; μ is the Bohr magneton; δI characterizes the magnetic interaction; I is the usual exchange integral; S_j is the spin operator of the electron belonging to the site j; δ is the vector connecting nearest-neighbor sites.

In the case of an arbitrary direction of the external magnetic field, the direction of the magnetization vector does not coincide with the direction of the crystallographic axes. It is convenient to write the Hamiltonian of the system in another coordinate system (x, y, z), with the direction of the z-axis along the magnetization vector. The operators $S^{x'}, S^{y'}, S^{z'}$ are expressed in terms of S^x, S^y, S^z as follows:

$$\begin{aligned} S^{x'} &= S^x \cos\theta \cos\varphi - S^y \sin\varphi + S^z \sin\theta \sin\varphi, \\ S^{y'} &= S^x \cos\theta \sin\varphi + S^y \cos\varphi + S^z \sin\theta \sin\varphi, \\ S^{z'} &= -S^x \sin\theta + S^z \cos\theta. \end{aligned} \quad (2)$$

We also define the operators

$$S_\lambda = N^{-1/2}\sum_j \exp(i\lambda j) S_j, \qquad S_\lambda^\pm = S_\lambda^x \pm i S_\lambda^y, \tag{3}$$

where λ is a reciprocal-lattice vector. The operators satisfy the relations

$$[S_\lambda^z S_\mu^+] = N^{-1/2} S_{\lambda+\mu}^+, \qquad [S_\lambda^z S_\mu^-] = -N^{-1/2} S_{\lambda+\mu}^-,$$

$$[S_\lambda^+ S_\mu^-] = +2N^{-1/2} S_{\lambda+\mu}^z. \tag{4}$$

The ground state of the system is defined by

$$S_j^-|0\rangle = 0, \qquad S_j^z|0\rangle = -S|0\rangle \tag{5}$$

for all j, or, equivalently,

$$S_\lambda^-|0\rangle = 0, \qquad S_\lambda^z|0\rangle = -N^{1/2} S\delta_{\lambda 0}|0\rangle \tag{6}$$

for all λ. Following Dyson, we define the excited states as follows:

$$|a\rangle = \prod_\lambda \left[(2S)^{-1/2\, a_\lambda}(a_\lambda!)^{-1/2}(S_\lambda^+)^{a_\lambda}\right]|0\rangle, \tag{7}$$

where a_λ is the number of spin waves with wave vector λ. States with $\sum a_\lambda > 1$ are not normalized and are not orthogonal. The nonorthogonality of the states $|a\rangle$ gives rise to an interaction between spin waves, called the kinematic interaction.

The action of the Hamiltonian $\mathcal{H}$ on the state $|a\rangle$ gives the expression

$$\mathcal{H}|a\rangle = \left[E_0 + \sum_\lambda a_\lambda (L + \varepsilon_\lambda)\right]|a\rangle + \sum_b Q_{ba}|b\rangle. \tag{8}$$

Here

$$E_0 = -\mu N H^z - \frac{1}{2} I\gamma_0 N S^2 + \frac{1}{4!}\delta I \gamma_{000}\omega N S^4; \tag{9}$$

$$\varepsilon_\lambda = \left[IS - \frac{6}{4!}\delta I S^3 \frac{\gamma_{000}}{\gamma_0}(1-\omega)\right](\gamma_0 - \gamma_\lambda); \tag{10}$$

$$L = \mu H^z + \frac{1}{4!}\delta I S^3 \gamma_{000}(6 - 10\omega); \tag{11}$$

$$\gamma_\lambda = \sum_\delta e^{i\lambda\delta}, \qquad \gamma_{\lambda_1\lambda_2\lambda_3} = \sum_{\delta_1,\delta_2,\delta_3} e^{i(\delta_1\lambda_1+\delta_2\lambda_2+\delta_3\lambda_3)}; \tag{12}$$

$$\omega = \cos^4\alpha_1 + \cos^4\alpha_2 + \cos^4\alpha_3, \tag{13}$$

where $\cos\alpha_i$ are the direction cosines of the magnetization vector with respect to the crystallographic axes; Q_{ba} are determined from expressions for the commutators of $\mathcal{H}$ with S_λ^+.

Let us write the energy operator $\mathcal{H}$ in another model, called the ideal spin-wave model[3]:

$$\mathcal{H} = E_0 + \sum_\lambda (L+\varepsilon_\lambda)\alpha_\lambda^*\alpha_\lambda + \sum_{\lambda\rho\sigma} \Gamma_{\rho\sigma}^\lambda \alpha_{\sigma+\lambda}^*\alpha_{\rho-\lambda}^*\alpha_\rho\alpha_\sigma + \cdots, \tag{14}$$

$\Gamma_{\rho\sigma}^\lambda$ are determined from expressions for the double commutators $[[\mathcal{H}, S_\rho^+], S_\sigma^+]$. The third term represents the scattering of two spin waves. The energy operator also contains terms describing the scattering of three and four spin waves; however, they will be omitted in calculating the free energy.

For the free energy per atom we obtain the expression

$$F = F_0 + F_A, \tag{15}$$

where F_A is the anisotropy free energy;

$$F_A = K_1^0\omega\left\{1 - \frac{1}{S}10Z_{3/2}(\beta L')\theta^{3/2} - \frac{3}{2S}\pi\nu Z_{1/2}(\beta L')\theta^{5/2} + \right.$$
$$\left. + \frac{1}{S^2}45[Z_{3/2}(\beta L')]^2\theta^3\right\}, \tag{16}$$

$$K_1^0 = \frac{1}{4!}\delta I\gamma_{000}S^4, \qquad L' = \mu H^z, \qquad \theta = \frac{T}{2\pi T_c}, \qquad Z_n(x) = \sum_{j=1}^\infty j^{-n}e^{-jx}, \qquad \nu = \frac{a^2}{v^{2/3}}.$$

The term with θ^3 in the expression for F_A represents the spin-wave interaction (scattering of two spin waves). The terms in expression (14) of the operator $\mathcal{H}$ describing the scattering of three and four spin waves give, in the free energy, contributions proportional to $\theta^{9/2}$ and θ^6, respectively. In the temperature range up to $T = \frac{1}{4}T_c$, the term describing the spin-wave interaction does not exceed 10% (for $s = 1$) and 20% (for $s = \frac{1}{2}$) of the term corresponding to the Bloch approximation.

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CITED LITERATURE

[1] S. V. Vonsovskii, Ya. S. Shur, *Ferromagnetism*, Moscow, 1948. [2] S. V. Tyablikov, A. A. Gusev, *Fiz. met. i metalloved.*, **2**, no. 3, 385 (1956). [3] F. J. Dyson, *Phys. Rev.*, **102**, 1217 (1956).

Note: Figure translations are in progress. See original paper for figures.