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Abstract

Full Text

PHYSICS

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ON THE THEORY OF ANISOTROPY OF FERROMAGNETIC SINGLE CRYSTALS

(Presented by Academician N. N. Bogolyubov on 8 VIII 1957)

Magnetic anisotropy is characterized by the so-called anisotropy constants, which are defined as the coefficients in the expansion of the free energy in a series in powers of the direction cosines (with respect to the crystallographic axes). From the theoretical point of view, the temperature dependence of the anisotropy constants was investigated qualitatively in ^(1,2). The dependence of the anisotropy constants on temperature and field was considered in ^(3,4), by means of the method of approximate secondary quantization.

The results ^(3,4) were obtained in the linear approximation of spin-wave theory without taking into account the interaction of spin waves. The theory of spin-wave interaction for an isotropic ferromagnet was considered by Dyson ⁽⁵⁾. He determined spin-wave states in which the Heisenberg Hamiltonian is approximately diagonal, while the corrections due to the dynamical interaction do not exceed several percent even for $T = \frac{1}{2}T_c$.

In the present work Dyson's method is applied to an anisotropic ferromagnet with hexagonal symmetry. The Hamiltonian of the system is

$$\mathcal{H} = \mu \sum_j (\mathbf{H}\mathbf{S}_j) - \frac{1}{2}I \sum_{j\delta} \mathbf{S}_j \mathbf{S}_{j+\delta} - \frac{1}{2}\delta I \sum_{j\delta} S_j^{z'} S_{j+\delta}^{z'}, \quad (1)$$

where H is the external magnetic field; μ is the Bohr magneton; δI characterizes the magnetic interaction; I is the ordinary exchange integral; S_j is the electron spin operator belonging to site j ; z' coincides with the direction of the crystallographic axis; $\vec{\delta}$ is the vector connecting nearest-neighbor sites.

Let us pass to another coordinate system, with the direction of the z -axis along the magnetization vector, and define the operators

$$S_\lambda = N^{-1/2} \sum_{\mathbf{j}} \exp(i\vec{\lambda}\mathbf{j}) S_j, \quad (2)$$

$$S_\lambda^\pm = S_\lambda^x \pm iS_\lambda^y.$$

Here $\vec{\lambda}$ is a reciprocal-lattice vector. The operators S_λ satisfy the relations

$$[S_\lambda^z S_\mu^+] = N^{-1/2} S_{\lambda+\mu}^+, \quad [S_\lambda^z S_\mu^-] = -N^{-1/2} S_{\lambda+\mu}^-, \quad [S_\lambda^+ S_\mu^-] = 2N^{-1/2} S_{\lambda-\mu}^z. \quad (3)$$

The Hamiltonian of the system is reduced to the form

$$\begin{aligned} \mathcal{H} = & \mu N^{-1/2} (\mathbf{H}\mathbf{S}_0) - \frac{1}{2} I \sum_\lambda \gamma_\lambda \mathbf{S}_\lambda \mathbf{S}_{-\lambda} - \frac{1}{2} \delta I \cos^2 \theta \sum_\lambda S_\lambda^z S_{-\lambda}^z \gamma_\lambda \\ & - \frac{1}{8} \delta I \sin^2 \theta \sum_\lambda \gamma_\lambda (S_\lambda^+ S_{-\lambda}^+ + S_\lambda^- S_{-\lambda}^- + S_\lambda^+ S_{-\lambda}^- + S_\lambda^- S_{-\lambda}^+) \\ & + \frac{1}{2} \delta I \sin \theta \cos \theta \sum_\lambda \gamma_\lambda (S_\lambda^+ S_{-\lambda}^z + S_\lambda^- S_{-\lambda}^z), \end{aligned} \quad (4)$$

where

$$\gamma_\lambda = \sum_\delta e^{i(\vec{\lambda}\delta)}.$$

The ground state of the system is determined by the formulas:

$$S_j^- |0\rangle = 0, \quad S_j^z |0\rangle = -S |0\rangle \quad (5)$$

for all j , or, equivalently,

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

for all $\vec{\lambda}$.

Following Dyson, let us define the spin-wave states

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

where a_λ is the number of spin waves with wave vector $\vec{\lambda}$.

States with $\sum a_\lambda > 1$ are neither normalized nor orthogonal. The nonorthogonality of the states (7) gives rise to an interaction between spin waves, called the **kinematic interaction**. Its physical cause is that the spin of an individual atom can assume only $2S + 1$ values. Another interaction, called **dynamic**, arises from the fact that the Hamiltonian (4) is not diagonal in the states (7).

Let us find the action of the Hamiltonian \mathcal{H} on the states $|a\rangle$:

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

where

$$E_0 = -\mu H^z N S - \frac{1}{2}(I + \delta I \cos^2 \theta) \gamma_0 N S^2, \quad (9)$$

$$L_0 = \mu H^z + \delta I S \gamma_0 \left(\cos^2 \theta - \frac{1}{2} \sin^2 \theta \right), \quad (10)$$

$$\varepsilon_{\lambda} = \left(I + \frac{1}{2} \delta I \sin^2 \theta \right) S(\gamma_0 - \gamma_{\lambda}) = I' S(\gamma_0 - \gamma_{\lambda}), \quad (11)$$

and Q_{ba} is determined from the expressions for the commutators of \mathcal{H} with S_{λ}^{\pm} . The sum of states of the system, according to (5), is expressed in the form

$$Z = \sum_u F_u^{-2} \sum_a \langle a|u\rangle \langle u| \exp(-\beta \mathcal{H}) |a\rangle, \quad \beta = \frac{1}{kT}. \quad (12)$$

The states $|u\rangle$ are defined as follows:

$$|u\rangle = \prod_j \left[(2S)^{-1/2 u_j} (u_j!)^{-1/2} (S_j^+)^{u_j} \right] |0\rangle, \quad (13)$$

where (u) is a system of numbers u_j taking the values $0, 1, \dots, 2S$,

$$F_u = \langle v|u\rangle. \quad (14)$$

Following Dyson, we express Z in the ideal spin-wave model, in which a harmonic oscillator is associated with each lattice site j .

The oscillators are described by means of creation operators η_j^* and annihilation operators η_j , satisfying the relations

$$[\eta_j, \eta_k^*] = \delta_{jk}, \quad \eta_j^* \eta_j = u_j. \quad (15)$$

The complete set of orthogonal and normalized states of the ideal system is

$$|u\rangle = \prod_j \left[(u_j!)^{-1/2} (\eta_j^*)^{u_j} \right] |0\rangle. \quad (16)$$

In the ideal model one can define another orthogonal system

$$|a\rangle = \prod_{\lambda} [(a_{\lambda}!)^{-1/2} (\alpha_{\lambda}^*)^{a_{\lambda}}] |0\rangle, \quad (17)$$

where α_{λ}^* are defined as follows:

$$\alpha_{\lambda}^* = N^{-1/2} \sum_j \exp(i\lambda j) \eta_j^* \quad (18)$$

and satisfy the relations

$$[\alpha_{\lambda} \alpha_{\mu}^*] = \delta_{\lambda\mu}, \quad \alpha_{\lambda}^* \alpha_{\lambda} = a_{\lambda}. \quad (19)$$

The sum of states is expressed in the ideal model as

$$Z = e^{-\beta E_0} \sum_{ab} U_{ba} V_{ab}, \quad (20)$$

where

$$U_{ba} = \langle b | \exp[-\beta(\mathcal{H} - E_0)] | a \rangle,$$

$$V_{ab} = \sum_u \langle a | u \rangle E_u \langle u | b \rangle; \quad (21)$$

$$E_u = \prod_j E(u_j); \quad (22)$$

$$E(u) = 1 \text{ for } u = 0, 1, \dots, 2S; \quad E(u) = 0 \text{ for } u > 2S.$$

The expression V_{ab} represents the effect of the kinematic interaction. The physical states of our system correspond to a set (u) of numbers u_j , in which the u_j take the values $0, 1, \dots, 2S$. The sum of states of our system can be represented in the form

$$Z = Z_T - Z_1, \quad (23)$$

where Z_T extends over states with arbitrary u_j , while Z_1 only over states with $u_j > 2S$. The sum Z_1 contains the factor $e^{-T_c/T}$ (T_c is the Curie temperature). Therefore, in the expansion of the free energy in powers of T , the terms taking account of the kinematic interaction may be omitted. To compute U_{ba} , we represent $\exp[-\beta(\mathcal{H} - E_0)]$ in the form of a series:

$$\begin{aligned} & \exp[-\beta(\mathcal{H} - E_0)] = \\ & = \sum_{m=0}^{\infty} (-1)^m \int_0^{\beta} d\beta_1 \dots \int_0^{\beta_{m-1}} d\beta_m \exp[(\beta_1 - \beta)\mathcal{H}_1] \mathcal{H}_2 \dots \mathcal{H}_2 \exp(-\beta_m \mathcal{H}_1), \end{aligned} \quad (24)$$

where

$$\mathcal{H}_1 = \sum_{\lambda} (L + \varepsilon_{\lambda}) \alpha_{\lambda}^* \alpha_{\lambda}, \quad \mathcal{H}_2 = \mathcal{H} - E_0 - \mathcal{H}_1. \quad (25)$$

To compute the sums we shall apply Feynman's graph method. For the free energy per atom we obtain

$$F = -\mu H^z S - \frac{1}{2} (I + \delta I \cos^2 \theta) \gamma_0 S^2 - kT \{ Z_{1/2}(\beta L) \theta a'^{3/2} + 3/4 \pi \nu Z_{7/2}(\beta L) \theta a'^{5/2} + \left(\frac{3\pi\nu}{4S} \right) [Z_{5/2}(\beta L)]^2 \theta a'^4 \} - \delta I \gamma_0 \quad (26)$$

where

$$\theta' = \frac{3kT}{2\pi I' \gamma_0 \nu}, \quad \nu = \frac{a^2}{v^{2/3}}, \quad Z_n(x) = \sum_{j=1}^{\infty} j^{-n} e^{-jx}.$$

Expanding $Z_n(\beta L)$ in powers of $\delta I/kT$ and θ' in powers of $\delta I/I$, we obtain for the free energy

$$F = F_0 + F_A,$$

where F_A is the free energy of anisotropy:

$$F_A = -1/2 \delta I \gamma_0 \cos^2 \theta \{ S^2 - 3S Z_{3/2}(\beta L') \theta^{3/2} - 5S Z_{5/2}(\beta L') \theta^{5/2} + 3[Z_{3/2}(\beta L')]^2 \theta^3 \}, \quad (27)$$

$$L' = \mu H^z, \quad \theta = \frac{3kT}{2\pi I S \gamma_0 \nu} = \frac{T}{2\pi T_c}.$$

The term with $\theta^{3/2}$ corresponds to Bloch's approximation and agrees with the results of (3); the term with $\theta^{5/2}$ appears because of the discreteness of the crystal lattice and the dependence of the spin-wave energy on δI . The term with θ^3 represents the dynamical interaction of spin waves. In the temperature

range up to $T = 1/4T_c$, the term representing the dynamical interaction does not exceed 4% (for $S = 1/2$) and 2% (for $S = 1$) of the term corresponding to Bloch's approximation. The small magnitude of the dynamical interaction shows that spin-wave theory is applicable to this temperature range.

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