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Abstract

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AN APPROXIMATE METHOD FOR CALCULATING THE GROUND STATE OF AN ISOTROPIC ANTIFERROMAGNET

(Presented by Academician N. N. Bogolyubov on 24 X 1959)

Various variants of the "spin-wave" method have been applied by a number of authors (^{1}) to the development of the theory of antiferromagnetism. The assumption of a small deviation of the spin from its value in the ground state restricts the applicability of this method to the region of low temperatures. The only theory applicable in the region of high temperatures is the molecular theory of Néel (^{2}). However, the molecular theory cannot be regarded as satisfactory, since it is very crude, especially in the region of low temperatures. In works (^{3},^{4}), using spectral representations of Green' s functions by the method proposed by N. N. Bogolyubov and S. V. Tyablikov (^{3}), a formula was obtained for the magnetization of a ferromagnet over the entire temperature range. In the present work, with the aid of the same method, the theory of antiferromagnetism without allowance for anisotropy is considered. The formula obtained for the magnetization is valid for all temperatures. In this brief communication only the results for the ground state are presented.

Using the notation adopted in work (^{5}), we write the Hamiltonian of the system of an isotropic antiferromagnet as

$$\mathcal{H} = -\mu \sum H^\alpha S_f^\alpha - \mu \sum H^\alpha S_g^\alpha - \frac{1}{2} \sum J_{11}(f_1 - f_2) S_{f_1}^\alpha S_{f_2}^\alpha -$$

$$-\frac{1}{2} \sum J_{22}(g_1 - g_2) S_{g_1}^\alpha S_{g_2}^\alpha - \sum J_{12}(f - g) S_f^\alpha S_g^\alpha . \qquad (1)$$

We perform the transformation* from spin operators to Pauli operators

$$S_h^\alpha = \gamma_i^\alpha (1 - 2n) + A_i^\alpha b_h + \overset{*}{A}{}_i^\alpha b_h^+, \qquad (2)$$

where $h = f, g;\ i = 1$ for $h \in f,\ i = 2$ for $h \in g$. Under the assumption that $\langle b_h \rangle = 0$, γ^α have the meaning of the direction cosines of the spin, and

$$A^x = \frac{-\gamma^x\gamma^z - i\gamma^y}{\sqrt{(\gamma^x)^2 + (\gamma^y)^2}}, \qquad A^y = \frac{-\gamma^y\gamma^z + i\gamma^x}{\sqrt{(\gamma^x)^2 + (\gamma^y)^2}}, \qquad A^z = \sqrt{(\gamma^x)^2 + (\gamma^y)^2}. \tag{3}$$

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* This transformation is due to S. V. Tyablikov.

Substituting (2) into (1), we obtain the Hamiltonian in Pauli operators. Following the work of [3], we introduce the following Green' s functions

$$G^{(1)}_{hh'} \equiv \langle\langle b_h(t) \mid b^+_{h'}(t')\rangle\rangle = \theta(t-t')\langle[b_h(t),\, b^+_{h'}(t')]_-\rangle,$$

$$G^{(2)}_{hh'} \equiv \langle\langle b^+_h(t) \mid b^+_{h'}(t')\rangle\rangle = \theta(t-t')\langle[b^+_h(t),\, b^+_{h'}(t')]_-\rangle, \tag{4}$$

$$(h = f, g; \quad h' = f', g').$$

Using the equations of motion for b_h, b^+_h, we obtain chains of equations for the Green' s functions. To decouple these equations we assume that

$$\langle\langle n_{h_1}(t) b_{h_2}(t) \mid b^+_{h_3}(t')\rangle\rangle = \bar{n}_i \langle\langle b_{h_2}(t) \mid b^+_{h_3}(t')\rangle\rangle$$

$$\langle\langle n_{h_1}(t) b^+_{h_2}(t) \mid b^+_{h_3}(t')\rangle\rangle = \bar{n}_i \langle\langle b^+_{h_2}(t) \mid b^+_{h_3}(t')\rangle\rangle,$$

where $i = 1$ for $h_1 \in f$, $i = 2$ for $h_1 \in g$, $\bar{n}_i = \langle n_i\rangle$, and we assume that higher-order Green' s functions may be neglected. Then we obtain a system of closed equations for the Green' s functions (4). We shall seek their solutions in the form

$$G^{(i)}_{hh'}(t-t') = \int_{-\infty}^{\infty} G^{(i)}_{hh'}(E) e^{-iE(t-t')}\, dE, \qquad G^{(i)}_{hh'}(E) = \frac{1}{N}\sum_{(\nu)} e^{i(h-h',\nu)} K^{(i)}_{ll'}(\nu) \tag{5}$$

$$(i = 1, 2),$$

where $l = 1$ for $h \in f$, $l = 2$ for $h \in g'$; $l' = 1$ for $h' \in f$, $l' = 2$ for $h' \in g$; ν is a reciprocal-lattice vector. As a result we obtain a system of linear equations for $K^{(i)}_{ll'}$.

In what follows we assume that $J_{11} = J_{22} = J$, $\bar{n}_1 = \bar{n}_2 = \bar{n}$, and $H^x = H^y = 0$, $H^z = H$, $\gamma_1^x = -\gamma_2^x = \sqrt{1-\gamma^2}$, $\gamma_1^z = \gamma_2^z = \gamma$, $\gamma_1^y = \gamma_2^y = 0$. In this case one can verify that $K_{11}^{(1)} = K_{22}^{(1)}$, $K_{21}^{(1)} = K_{12}^{(1)}$, $K_{11}^{(2)} = K_{22}^{(2)}$, $K_{21}^{(2)} = K_{12}^{(2)}$, and the solutions for them can easily be found. Following the principal formula of [3] and taking into account the relations [5] $J_{12}(\pi b - \nu) = -J_{12}(\nu)$, $J(\pi b - \nu) = J(\nu)$, ($J(\nu)$ is the Fourier component of the exchange integral), after passing from the sum to an integral we obtain the formulas

$$\langle b_{h_1} b_{h_2}^+ \rangle = \frac{\sigma}{2}\delta_{h_1 h_2} + \frac{\sigma}{2}\frac{v}{(2\pi)^3}\int e^{i(h_1-h_2,\nu)}\frac{F_\nu + 2\gamma^2\sigma J_{12}}{E_\nu}\,\mathrm{cth}\,\frac{E_\nu}{2\theta}\,d\nu,$$

$$\langle b_f^+ b_g^+ \rangle = \frac{\sigma}{2}\frac{v}{(2\pi)^3}\int e^{i(g-f,\nu)}\frac{2(1-\gamma^2)\sigma J_{12}}{E_\nu}\,\mathrm{cth}\,\frac{E_\nu}{2\theta}\,d\nu, \tag{6}$$

where v is the volume of the elementary cell; $\sigma = 1 - 2\bar{n}$;

$$F_\nu = 2[\mu H\gamma + \sigma(\bar{J} - J + (2\gamma^2 - 1)\bar{J}_{12})],$$

$$E_\nu = 2\{[\mu H\gamma + \sigma(\bar{J} - J) + \sigma((2\gamma^2 - 1)\bar{J}_{12} + J_{12})]\times$$

$$\times[\mu H\gamma + \sigma(\bar{J} - J) + \sigma(2\gamma^2 - 1)(\bar{J}_{12} + J_{12})]\}^{1/2}.$$

Substituting $h_1 = h_2$ into the first formula (6), we obtain

$$\frac{1}{\sigma} = \frac{v}{(2\pi)^3}\int \frac{F_z + 2\gamma^2\sigma J_{12}}{E_v}\,\mathrm{cth}\,\frac{E_v}{2\theta}\,dv. \tag{7}$$

Suppose that the mean value of an odd number of Pauli operators is equal to zero and $\langle n_h n_{h'} \rangle \cong \bar{n}^2$. From the condition for the minimum of the free energy $\left\langle \frac{\partial \mathcal{H}}{\partial \gamma} \right\rangle = 0$ and (6) we obtain

$$\frac{1}{\gamma} = \frac{2}{\mu H}\left\{\frac{v}{(2\pi)^3}\int \frac{F_v + 2\sigma J_{12}}{E_v}\,\mathrm{cth}\,\frac{E_v}{2\theta}\,dv - \overline{J}_{12}\sigma\right\} \tag{8}$$

and the expression for the mean energy

$$E = -N\mu H\gamma - N\sigma^2(\mu H\gamma + \overline{J} + (2\gamma^2 - 1)\overline{J}_{12}) -$$

$$-2\sigma N\frac{v}{(2\pi)^3}\int J\,\frac{F_v + 2\gamma^2\sigma J_{12}}{E_v}\,\mathrm{cth}\,\frac{E_v}{2\theta}\,dv -$$

$$-2\sigma N\frac{v}{(2\pi)^3}\int J_{12}\,\frac{2(1-\gamma^2)2\sigma J_{12}-\gamma^2(F_v+2\gamma^2\sigma J_{12})}{E_v}\,\mathrm{cth}\,\frac{E_v}{2\theta}\,dv. \tag{9}$$

For simplicity, let us consider a simple cubic lattice and take $J_{12}=-|J_{12}|$, $J=0$. To study the ground state we put $\theta=0$ in (7), (8), and (9). Let us introduce the dimensionless quantity $h=\frac{\mu H}{|J_{12}|}$; then, after some calculations, we obtain the solutions A and B.

A. Solution for $h\ll 1$:

$$\sigma=\sigma_0+\sigma_1 h^2\ln h+O(h^2); \tag{10}$$

$$\gamma=\gamma_1+\gamma_2 h^3\ln h+O(h^3); \tag{11}$$

$$E=N|\overline{J}_{12}|(e_1+e_2h^2\ln h+O(h^2)), \tag{12}$$

where

$$\sigma_0=\frac{1}{J}=0.865;\qquad \sigma_1=-\frac{\sqrt{2}}{4}\,A\,\frac{J^2(1+2J(J-I))}{(1+J(J-I))^2}=-0.168;$$

$$\gamma_1=\frac{J}{2(1+J(J-I))}=0.445;\qquad \gamma_2=-\frac{\sqrt{2}}{4}\,A\,\frac{J^4}{(1+J(J-I))^2}=-0.108;$$

$$e_1=-\frac{1}{J}\left\{\frac{1}{J}+2(J-I)\right\}=-1.186;$$

$$e_2=-2\{\sigma_0\sigma_1+\sigma_1(J-I)+\sqrt{2}\,A\gamma_1(1-\sigma_0\gamma_1)\}=0.01;$$

$$A=\frac{6^{3/2}}{\pi^3}\frac{\pi}{4};\qquad J=\frac{1}{(2\pi)^3}\int_\Gamma\frac{dv}{\sqrt{1-(Q/3)^2}},\qquad I=\frac{1}{(2\pi)^3}\int_\Gamma\sqrt{1-(Q/3)^2}\,dv$$

($dv=dx\,dy\,dz$; Γ is the region $-\pi<x,y,z<\pi$; $Q=\cos x+\cos y+\cos z$).

We note that spin-wave theory gives the values $\sigma_0=2-J=0.844$, $e_1=2I-3=-1.194$.

B. Solution for $2-h \gtreqless 0$:

$$\sigma = 1 + \sigma_1(2-h) + \sigma_2(2-h)^{3/2} + O((2-h)^2 \ln(2-h)); \tag{13}$$

$$\gamma = 1 + \gamma_1(2-h) + \gamma_2(2-h)^{3/2} + O((2-h)^2 \ln(2-h)); \tag{14}$$

$$E = N|\bar{J}_{12}|\{-3 + e_1(2-h) + e_2(2-h)^{3/2} + O((2-h)^2 \ln(2-h))\}, \tag{15}$$

where

$$\sigma_1 = \frac{K(1-K)}{2K^2-5K+4} = -0.770; \qquad \gamma_1 = \frac{K-2}{2(2K^2-5K+4)} = -0.238;$$

$$\sigma_2 = \frac{2\sqrt{2}A\left(-13K^{3/2}+6K^{1/2}+8K^{-1/2}\right)}{3(2K^2-5K+4)^{1/2}} = -3.54;$$

$$\gamma_2 = \frac{2\sqrt{2}A\left(7K^{3/2}-8K^{1/2}-4K^{-1/2}\right)}{3(2K^2-5K+4)^{1/2}} = 6.65;$$

$$e_1 = 2 - 2\sigma_1 - 2(1-K)\left(\frac{1}{2} + \sigma_1 + 3\gamma_1\right) = 2.52;$$

$$e_2 = -2\sigma_2 - \frac{8}{3}A\,\frac{(2\gamma_1+2\sigma_1+1)}{\sqrt{-2-4\sigma_1-8\gamma_1}} - 2(1-K)(\sigma_2+3\gamma_2) = 17.4;$$

$$K = \frac{1}{(2\pi)^3}\int_\Gamma \frac{dv}{1-Q/3}.$$

When $h \gtreqless 2$, $\gamma = 1$, and the substance behaves as a ferromagnet. In conclusion, the author expresses his deep gratitude to S. V. Tyablikov, and also to T. Shiklosh for valuable discussions.

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CITED LITERATURE

1. *Antiferromagnetism*, collected volume, Foreign Literature Publishing House, 1956.
2. L. Neel, Ann. de Phys., 134 (1948).
3. N. N. Bogolyubov, S. V. Tyablikov, DAN, 126, 53 (1959).
4. S. V. Tyablikov, Ukr. Math. Journal, 11, No. 3 (1959).
5. S. V. Tyablikov, Fiz. Met. i Metalloved., 2, 193 (1956).
6. P. W. Anderson, Phys. Rev., 86, 693 (1952).

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