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Abstract

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AN APPROXIMATE METHOD FOR CALCULATING THE MAGNETIZATION OF AN ISOTROPIC ANTIFERROMAGNET

(Presented by Academician N. N. Bogolyubov, 27 XI 1959)

In our work ([1]), with the aid of spectral representations of Green' s functions by the method of paper ([2]), we obtained formulas for the quantities of interest to us: the relative magnetization of each sublattice and the cosine γ of the angle between the sublattice magnetization vector and the direction of the magnetic field. We then investigated their solution for temperature $\tau = 0$. In the present paper we study these equations for $\tau \neq 0$. As was shown ([1]), because the vacuum is not determined by the condition $\Phi = 0$, it is necessary to consider simultaneously Green' s functions of the type $\ll h|l_h^+ \gg$, $\ll l_h^+|l_h^+ \gg$. It is easy to see that σ and γ can be written in the form (see ([1]), equations (7), (8))

$$\frac{1}{\sigma} = \frac{1}{(2\pi)^3} \int \frac{h\gamma - \sigma(2\gamma^2 - 1 + \gamma^2 Q/3)}{\varepsilon} \operatorname{cth} \frac{\varepsilon}{\tau}\, dv; \tag{1}$$

$$\frac{1}{\gamma} = \frac{2}{h} \left\{ \sigma - \frac{1}{(2\pi)^3} \int \frac{Q}{3} \left[\frac{h\gamma - \sigma(2\gamma^2 - 1 + Q/3)}{h\gamma - \sigma(2\gamma^2 - 1)(1 + Q/3)} \right]^{1/2} \operatorname{cth} \frac{\varepsilon}{\tau}\, dv \right\}, \tag{2}$$

where

$$\varepsilon = \sqrt{[h\gamma - \sigma(2\gamma^2 - 1 + Q/3)]\,[h\gamma - \sigma(2\gamma^2 - 1)(1 + Q/3)]},$$

$h = \mu H/|\bar{J}_{12}|$, $\tau = \theta/|\bar{J}_{12}|$, $Q = \cos x + \cos y + \cos z$, and the integrals are taken over the region $-\pi < x, y, z < \pi$ ($dv = dx\, dy\, dz$). We note that we restrict ourselves to taking into account interactions only between nearest neighbors.

To investigate the expansion at low temperatures, let us expand $\operatorname{cth} \frac{\varepsilon}{\tau}$ in a series in powers of $e^{-2\varepsilon/\tau}$ and calculate the integrals by the saddle-point method. We shall then use the iteration method with the solutions σ, γ for $\tau = 0$ as the zeroth approximation; as a result we obtain:

Case A. $h = 0$. In this case $\gamma = 0$, i.e., the spins of the two sublattices are oriented parallel,

$$\sigma = \sigma_0 \left\{ 1 - \sigma_0 a_1 \left(\frac{\tau}{\sigma_0}\right)^2 - \sigma_0(a_2 + \sigma_0 a_1^2)\left(\frac{\tau}{\sigma_0}\right)^4 - \right.$$

$$\left. -\sigma_0(a_3 + 4a_1 a_2 \sigma_0 + 2\sigma_0^2 a_1^3)\left(\frac{\tau}{\sigma_0}\right)^6 - \dots \right\}, \quad (3)$$

where

$$\sigma_0 = \frac{1}{J} = 0.865, \quad a_1 = \frac{3^{3/2}\zeta(2)}{2\pi^2} = \frac{3^{3/2}}{12}, \quad a_2 = \frac{9\sqrt{3}}{4\pi^2}\zeta(4) = \frac{\sqrt{3}}{40}\pi^2, \dots$$

and

$$J = \frac{1}{(2\pi)^3} \int \frac{dv}{\sqrt{1 - (Q/3)^2}}. \quad (4)$$

We note that spin-wave theory gives

$$\sigma = 2 - J - a_1\tau^2 - a_2\tau^4 - a_3\tau^6 - \dots, \quad (5)$$

where $a_1,\ a_2, \dots$ are determined from (4). The coefficients of τ^2 in both formulas coincide, but starting with τ^4 they begin to diverge.

Case B. $h \simeq 0$ $(0 < h < 1)$. For simplicity we shall restrict ourselves to only the first two terms of the expansion in temperature:

$$\sigma = \sigma_0 + \sigma_1 h^2 \ln h + O(h^2) + [\sigma_0' + (h^2 \ln h)]\tau^2 + \dots; \quad (6)$$

$$\gamma = \gamma_1 h + \gamma_2 h^3 \ln h + O(h^3) + [\gamma_1' h + O(h^3 \ln h)]\tau^2 + \dots, \quad (7)$$

where $\sigma_0,\ \sigma_1,\ \gamma_1,\ \gamma_2$ are determined by formulas (10), (11) of work [1], and

$$\sigma_0' = -\frac{3^{3/2}\zeta(2)}{4\pi^2} = -\frac{3^{3/2}}{12}, \qquad \gamma_1' = \frac{3^{3/2}}{\pi^2}\zeta(2)\gamma_1^2\left(1 - \frac{1}{\sigma_0^2}\right) = \frac{\sqrt{3}}{2}\gamma_1^2\left(1 - \frac{1}{\sigma_0^2}\right).$$

Case C. $h \simeq 2$ and $h < 2$ $(0 < \eta \equiv 2 - h < 2)$. As was noted in [1], at $\tau = 0$, when h approaches the value $h = 2$, a transition occurs to a state with ferromagnetic spin arrangement. The same situation also takes place for $\tau \neq 0$. For this region we have:

$$\sigma = 1 + \sigma_1 \eta + \sigma_2 \eta^{3/2} + O(\eta^2 \ln \eta) + [\sigma_0' + O(\eta)]\tau^{3/2} + \dots; \tag{8}$$

$$\gamma = 1 + \gamma_1 \eta + \gamma_2 \eta^{3/2} + O(\eta^2 \ln \eta) + O(\eta)\tau^{3/2} + \dots, \tag{9}$$

where $\sigma_1,\ \sigma_2,\ \gamma_1,\ \gamma_2$ are determined by formulas (13), (14) of work [(1)], and

$$\sigma_0' = -\frac{1}{4}\left(\frac{3}{\pi}\right)^{3/2} \zeta\left(\frac{3}{2}\right).$$

Let us note that $\gamma_1 < 0$, and therefore at sufficiently low temperatures γ cannot exceed 1. When $\gamma = 1$, the substance passes into the ferromagnetic state (parallel orientation of the spins in both sublattices).

Case D. $h > 2,\ \gamma = 1$. The substance behaves like a ferromagnet.

$$\sigma = 1 - a_1 \tau^{3/2} - a_2 \tau^{5/2} - \frac{a_1^2}{2}\tau^{6/2} - a_3 \tau^{7/2} - \dots, \tag{10}$$

where

$$a_1 = \frac{1}{4}\left(\frac{3}{\pi}\right)^{3/2} \varphi\left(\frac{3}{2}, x\right), \qquad a_2 = \frac{9}{64}\left(\frac{3}{\pi}\right)^{3/2} \varphi\left(\frac{5}{2}, x\right),$$

$$a_3 = \frac{33}{128}\frac{1}{6}\times\frac{3^{7/2}}{\pi^{3/2}}\varphi\left(\frac{7}{2}, x\right) \quad \text{and} \quad \varphi(s, x) = \sum_{n=1}^{\infty}\frac{e^{-nx}}{n^s}, \qquad x = \frac{2}{\tau}(h - 2\sigma) \simeq \frac{2}{\tau}(h-2).$$

When $h \to 2$ $(h \geq 2)$, then $x \to 0$, $\varphi(s, x) = \zeta(s)$, and

$$\sigma = 1 - \frac{1}{4}\left(\frac{3}{\pi}\right)^{3/2} \times \zeta\left(\frac{3}{2}\right)\tau^{3/2} - \dots,$$

which coincides with the result of the limiting transition $h \to 2$ $(h \leq 2)$ for case C. It is important to note that here, in contrast to work [(3)], at $h = 2$ σ does not undergo a jump

$$\Delta\sigma = \frac{1}{3}\left(\frac{3}{\pi}\right)^{3/2} \zeta\left(\frac{3}{2}\right)^{(3)}$$

and that the quantity σ in equation (8) does not exceed the value $\sigma = 1$. Finally, for the magnetization M and the susceptibility χ of the sample we obtain the following expressions, for example, for case B:

$$M = 2N\sigma\gamma = 2N\{\sigma_0\gamma_1 h + (\sigma_0\gamma_2 + \sigma_1\gamma_1)h^3 \ln h + O(h^3) +$$

$$+[\sigma_0'\gamma_1' h + O(h^3 \ln h)]\tau^2 + ...\}; \tag{11}$$

$$\chi = \frac{\partial M}{\partial H} = \frac{2N\mu}{|J_{12}|}\{\sigma_0\gamma_1 + 3(\sigma_0\gamma_2 + \sigma_1\gamma_1)h^2 \ln h + O(h^3) +$$

$$+[\sigma_0'\gamma_1' + O(h^2 \ln h)]\tau^2 + ...\}; \tag{12}$$

it is not difficult to obtain formulas for M and χ in the other cases as well.

For the investigation of the expansion at high temperatures we shall restrict ourselves only to the case of a pure antiferromagnetism ($\gamma = 0$). In this case, instead of (1) and (2), we have:

$$\frac{1}{\sigma} = \frac{1}{(2\pi)^3} \int \frac{2}{\sqrt{1-(Q/3)^2}} \operatorname{cth} \frac{\sigma}{\tau} \sqrt{1 - \left(\frac{Q}{3}\right)^2}\, dv. \tag{13}$$

Since σ tends to zero as τ tends to the Néel point, one may expand $\operatorname{cth} \frac{\sigma}{\tau}\sqrt{1-\left(\frac{Q}{3}\right)^2}$ in powers of σ/τ. Solving equation (11) approximately near the Néel point, we obtain

$$\frac{\sigma}{\tau} = \zeta \left\{1 + \frac{1}{36}\zeta^2 - \frac{6.5}{1000}\zeta^4 + \cdots\right\}, \tag{14}$$

where

$$\zeta = \sqrt{\frac{3(1-K\tau)}{\tau}}, \qquad K = \frac{1}{(2\pi)^3}\int \frac{dv}{1-Q/3}.$$

The Néel temperature τ_N is determined, obviously, as $\tau_N = 1/K = 0.66$. Near the Néel point, σ varies proportionally to $\sqrt{\tau_N - \tau}$ (as in a ferromagnet near the Curie point ([4,5])); this agrees with the result of the Néel molecular-field method ([6]). An indication of such a dependence of σ on temperature is also found in ([7]).

It is of interest to study the boundary separating the regions of the antiferromagnetic and ferromagnetic states. The equation for the boundary is obtained by substituting $\gamma = 1$ in (1) and (2):

$$\frac{1}{\sigma} = \frac{1}{(2\pi)^3}\int \operatorname{cth} \frac{h - \sigma(1+Q/3)}{\tau}\, dv; \tag{15}$$

$$\frac{h}{2} = \sigma - \frac{1}{(2\pi)^3} \int \frac{Q}{3} \operatorname{cth} \frac{h - \sigma(1 + Q/3)}{\tau} \, dv. \tag{16}$$

In the region of low temperatures the equation for the boundary has the form

$$h = 2 - A_1 \tau^{3/2} - A_2 \tau^{5/2} - A_3 \tau^{6/2} - A_4 \tau^{7/2} - A_5 \tau^{8/2} - \cdots, \tag{17}$$

where

$$A_1 = \left(\frac{3}{\pi}\right)^{3/2} \zeta\left(\frac{3}{2}\right), \qquad A_2 = \frac{3}{16}\left(\frac{3}{\pi}\right)^{3/2} \zeta\left(\frac{5}{2}\right), \qquad A_3 = \frac{9}{4}\frac{1}{\pi^3}\zeta^2\left(\frac{3}{2}\right),$$

$$A_4 = \frac{135}{1024}\left(\frac{3}{\pi}\right)^{3/2} \zeta\left(\frac{7}{2}\right), \qquad A_5 = \frac{3}{16}\left(\frac{3}{\pi}\right)^{3} \zeta\left(\frac{3}{2}\right)\zeta\left(\frac{5}{2}\right).$$

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