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Abstract

Full Text

Physics

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On the Application of the Variational Principle in Problems on a Binary Alloy and the Ising System

(Presented by Academician N. N. Bogolyubov, 14 XI 1956)

As was indicated in the preceding note ⁽²⁾, in order to determine the statistical sum of a binary alloy it is necessary to solve the auxiliary problem of an Ising antiferromagnet. In the present note, when applying N. N. Bogolyubov's variational principle ⁽¹⁾, a different division into parts of the Hamiltonian of the antiferromagnet ^{((2), (1))} will be made, consisting in the fact that some of the terms from $\mathcal{H}_1$ are transferred to $\mathcal{H}_0$, with the sole condition that $Z_0 = \text{Sp}\{\exp(-\mathcal{H}_0)\}$ be computable. Namely, $\mathcal{H}_0$ includes the interaction terms of groups of neighboring sites; the interaction between these groups and the interaction with distant neighbors remains in $\mathcal{H}_1$. The simplest choice of these groups is in the form of pairs of sites. For simplicity we neglect the interaction with distant neighbors, which can be taken into account analogously to ⁽²⁾. Apparently, increasing the number of sites in each of the groups included in $\mathcal{H}_0$ (as the next approximation, it is natural to choose groups each of which consists of a central site and a "shell" of all its nearest neighbors) will, at the cost of increasing the computational part, lead to an increasingly good approximation.

Let us agree to denote by the letter $\mathcal{H}$ the Hamiltonian divided by the temperature θ ; B is the magnetic field in units of the Bohr magneton, divided by θ ; N is the number of lattice sites; $E = e/\theta$ is the exchange integral divided by the temperature. We shall also assume that all lattice sites are equivalent and that opposite boundaries of the crystal are joined to one another. In accordance with what has been said, for the antiferromagnet we have

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \frac{1}{2}E \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i=1}^N \sigma_i, \quad (1)$$

$$\mathcal{H}_0 = \sum_{l=1}^{N/2} \mathcal{H}_{2l}, \quad \mathcal{H}_k = -(B - \beta_0)\sigma_k - (B - \beta_1)\sigma_{k+1} + \varepsilon\sigma_k\sigma_{k+1}.$$

Here β_0 and β_1 are variational parameters referring to two sublattices; ε is a parameter characterizing the effective interaction of a pair of nearest sites. It is easy to see that for $\varepsilon = 0$ the above choice of $\mathcal{H}_0$ coincides with formula (6) of

note ⁽²⁾. Proceeding in accordance with the method described earlier ^{((1), (4))}, after simple calculations we obtain:

$$\begin{aligned}
 -\frac{2}{N} \ln Z_{inf} = & 2 \ln 2 + \ln [\operatorname{ch} \gamma_0 \operatorname{ch} \gamma_1 \operatorname{ch} \varepsilon - \operatorname{sh} \gamma_0 \operatorname{sh} \gamma_1 \operatorname{sh} \varepsilon] \\
 & + \beta_0 \frac{\operatorname{th} \gamma_0 - \operatorname{th} \gamma_1 \operatorname{th} \varepsilon}{1 - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1 \operatorname{th} \varepsilon} + \beta_1 \frac{\operatorname{th} \gamma_1 - \operatorname{th} \gamma_0 \operatorname{th} \varepsilon}{1 - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1 \operatorname{th} \varepsilon} \\
 & + (E - \varepsilon) \frac{\operatorname{th} \varepsilon - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1}{1 - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1 \operatorname{th} \varepsilon} - E(c - 1) \frac{(\operatorname{th} \gamma_0 - \operatorname{th} \gamma_1 \operatorname{th} \varepsilon)(\operatorname{th} \gamma_1 - \operatorname{th} \gamma_0 \operatorname{th} \varepsilon)}{(1 - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1 \operatorname{th} \varepsilon)^2},
 \end{aligned}
 \tag{2}$$

where, for convenience, the notation $\gamma_0 = B - \beta_0$, $\gamma_1 = B - \beta_1$ has been introduced.

The variational parameters β_0 , β_1 , and ε are then determined from the system of transcendental equations:

$$\frac{\partial \ln Z_{inf}}{\partial \beta_0} = \frac{\partial \ln Z_{inf}}{\partial \beta_1} = \frac{\partial \ln Z_{inf}}{\partial \varepsilon} = 0.
 \tag{3}$$

As in notes ^(1,2), we shall regard Z_{inf} as an approximate expression for the statistical sum of an antiferromagnet.

The magnetization per particle from (2) and (3) is determined by the expression:

$$M = \frac{1}{2} \frac{(\operatorname{th} \gamma_0 + \operatorname{th} \gamma_1)(1 - \operatorname{th} \varepsilon)}{1 - \operatorname{th} \gamma_0 \operatorname{th} \gamma_1 \operatorname{th} \varepsilon}.
 \tag{4}$$

In order to avoid cumbersome calculations, let us consider the application of the results obtained to a 50% binary alloy, using relations (2) and (4) of note ⁽²⁾. Setting $M = 0$, we obtain from equations 3) and (4):

$$B = 0; \quad \gamma_0 = -\gamma_1 = \gamma; \quad \varepsilon = E = \frac{e}{\theta}.
 \tag{5}$$

The mean thermodynamic energy per particle of the alloy, determined by relation (20) of work ⁽²⁾, will have the form:

$$\overline{E} = \frac{\varepsilon_0}{8} - \frac{e}{2} \frac{c \operatorname{th}^2 \gamma (1 + \operatorname{th} E)^2 + \operatorname{th} E (1 - \operatorname{th}^2 \gamma)^2}{(1 + \operatorname{th}^2 \gamma \operatorname{th} E)^2},
 \tag{6}$$

where c is the number of nearest neighbors for the given lattice; ε_0 is a constant. The quantity γ is determined from the equation

$$\gamma = E(c-1) \frac{\text{th} \gamma (1 + \text{th} E)}{1 + \text{th}^2 \gamma \text{th} E}. \quad (7)$$

From this equation it follows, in particular, that at temperature $\theta > \theta_0$ the quantity $\gamma = 0$, while the critical temperature θ_0 is determined by the equation:

$$1 = E_0(c-1)(1 + \text{th} E_0), \quad (8)$$

where $E_0 = e/\theta_0$.

Thus, in contrast to the results of ⁽²⁾, we have that for $\theta > \theta_0$ the mean energy and the heat capacity of the alloy, calculated in units of Boltzmann's constant, are functions of temperature:

$$\bar{E} = \frac{\varepsilon_0}{8} - \frac{e}{2} \text{th} \frac{e}{\theta}, \quad (9)$$

$$C = \frac{\partial \bar{E}}{\partial \theta} = \frac{e^2}{2\theta^2} \left(1 - \text{th}^2 \frac{e}{\theta}\right). \quad (10)$$

The value of the heat capacity at the point θ_0 from the left can be obtained from (6)–(3):

$$C = \frac{[2(c-1)E_0 - 1](6 + 4E_0) + 3(c-1)}{2(c-1)[3 - 2(c-1)E_0]}. \quad (11)$$

In the case of a simple cubic lattice, the numerical solution of equation (8) gives the value $E_0 \simeq 0.171$; then the value of the heat capacity to the left of the Curie point is $C \simeq 1.535$, and to the right, according to formula (10), $C \simeq 0.0142$, so that the jump in heat capacity only slightly exceeds the magnitude of the jump that follows from the Bragg–Williams theory (see also ⁽²⁾). It should also be noted that the values of E_0 obtained from (8) and formula (11) of work ⁽²⁾ are quantities of the same order; for example, for $c = 6$, according to formula (11) of work ⁽²⁾, we have $E_0 = 1.166$.

Applying the scheme set forth above to the Ising ferromagnetic system, we obtain for the average magnetic moment of a particle a formula which, from the point of view of the variational principle (1), is an improvement of the Weiss formula:

$$M = \frac{1}{N} \frac{\partial \ln Z}{\partial B} = \text{th}(B + J(c-1)M) \frac{1 + \text{th} J}{1 + \text{th}^2(B + J(c-1)M) \cdot \text{th} J}, \quad (12)$$

where J is the exchange integral divided by the temperature θ . The equation for the critical temperature θ_0 is analogous to (8):

$$1 = J_0(c-1)(1 + \text{th } J_0). \quad (13)$$

In the practically realizable case $B \ll 1$, for $\theta > \theta_0$ we obtain for the magnetic susceptibility

$$\chi \simeq \frac{1 + \text{th } J}{\theta - \theta_0 J_0(c-1)(1 + \text{th } J)}, \quad (14)$$

in contrast to the Curie-Weiss law (see also (1)):

$$\chi \simeq \frac{1}{\theta - \theta_0}.$$

Putting $B = 0$ in (12), we obtain the equation for the spontaneous magnetization as a function of temperature. Direct calculation for temperatures $\theta/\theta_0 = 1; 0.9; 0.8; 0.7; 0.6$ leads, respectively, to the values $M = 0.0; 0.533; 0.718; 0.838; 0.912$, which are somewhat larger than the quantities obtained from Weiss theory: $M = 0.0; 0.525; 0.710; 0.828; 0.907$.

The relations for the energy and heat capacity of the Ising ferromagnet are analogous to (9)–(11).

Under an analogous consideration of the Heisenberg model, instead of (12), for the susceptibility one obtains the more complicated expression

$$M = \text{th } \gamma \frac{1 + \text{th } J}{1 + \text{th } J \cdot \text{th}^2 \gamma + e^{-J} \text{th } J \cdot \text{sh } J \cdot (1 - \text{th}^2 \gamma)},$$

where $\gamma = B + J(c-1)M$.

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

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