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Abstract

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ON THE THEORY OF A PHASE TRANSITION IN A NONIDEAL BOSE GAS

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In paper (^{1}), starting from Bardin' s model Hamiltonian, asymptotically exact (as the volume of the system tends to infinity) expressions were obtained for the thermodynamic functions of a nonideal Fermi gas, which on the whole correctly describe the thermodynamic properties of superconductors. In view of the deep analogy between superconductivity and superfluidity, it is of interest to construct an analogous theory for a nonideal Bose gas, also based on a model Hamiltonian. This is all the more interesting because the existing microscopic theories of superfluidity proceed from the assumption that the number of elementary excitations is small and do not allow one to investigate the behavior of the system near the phase-transition point.

In the present paper we shall show that, for a model Hamiltonian of the form

$$H = E_0 + \sum_{k} \varepsilon(k) b_k^+ b_k + \sum_{k \neq k'} \frac{v(k-k')}{2V} b_k^+ b_k b_{k'}^+ b_{k'} +$$

$$+ \sum_{k \neq k'} \frac{v(k-k')}{2V} b_k^+ b_{-k}^+ b_{-k'} b_{k'}, \qquad (1)$$

$$E_0 = \frac{v(0)}{2V} N(N-1)$$

(where b_k are Bose operators; $\varepsilon(k) = k^2/2m - \mu$; μ is the chemical potential; $v(k)$ is the Fourier component of the interaction energy), the thermodynamic functions can be calculated asymptotically exactly for $V \to \infty$, $N \to \infty$, $v = V/N = \text{const}$.

Hamiltonian (1) differs from the complete Hamiltonian in that in it we have retained terms depending only on two indices. At the same time, (1) contains as a special case the Hamiltonian used in N. N. Bogolyubov's theory of superfluidity (^{2}). We note that in the work of Bruckner and Sawada (^{3}) a Hamiltonian of the same type as (1) was obtained, in which matrix elements of the scattering operator enter in place of $v(k)$. Therefore the methods used by us can also be applied to the Hamiltonian of paper $(^3)$.

Let us perform the canonical transformation of operators proposed in 1947 by N. N. Bogolyubov in the theory of superfluidity:

$$b_k = \lambda_k \beta_k + \mu_k \beta^+_{-k}, \qquad b^+_k = \lambda_k \beta^+_k + \mu_k \beta_{-k}, \qquad \lambda^2_k - \mu^2_k = 1, \quad k \neq 0, \tag{2}$$

where β_k and β^+_k are new Bose operators. We shall assume that the interaction is sufficiently small and that in the state $k = 0$ there is a macroscopically large-number of particles $N_0 \sim N$. Then, taking the operators b_0, b^+_0 and $b^+_0 b_0 = N_0$ to be c-numbers, we can write the Hamiltonian (1) in the form

$$H = H_0 + H_1,$$

$$H_0 = U + \sum_k E(k) \beta^+_k \beta_k + \sum_k Q(k) \left(\beta^+_k \beta^+_{-k} + \beta_{-k} \beta_k\right), \tag{3}$$

$$H_1 = \sum_{k \neq k'} \frac{v(k-k')}{2V} \left\{A^+_k A_{k'} + B_k B_{k'}\right\},$$

where

$$\begin{aligned} U = E_0 - \mu N_0 + \sum_k \left\{ \left[\varepsilon(k) + \frac{N_0}{V} v(k)\right] \mu^2_k + \frac{N_0}{V} v(k) \lambda_k \mu_k \right\} + \\ + \sum_{k \neq k'} \frac{v(k-k')}{2V} \left\{ \mu^2_k \mu^2_{k'} + \lambda_k \mu_k \lambda_{k'} \mu_{k'} (1 - 4\bar{n}_k \bar{n}_{k'}) - \right. \\ \left. - (\lambda^2_k + \mu^2_k)(\lambda^2_{k'} + \mu^2_{k'}) \bar{n}_k \bar{n}_{k'} \right\}, \end{aligned} \tag{4a}$$

$$E(k) = \varepsilon'(k)(\lambda^2_k + \mu^2_k) + 2\lambda_k \mu_k \left\{ \frac{N_0}{V} v(k) + \sum_{k' \neq k} \frac{v(k-k')}{V} \lambda_{k'} \mu_{k'} (1 + 2\bar{n}_{k'}) \right\},$$

$$Q(k) = \varepsilon'(k) \lambda_k \mu_k + (\lambda^2_k + \mu^2_k) \left\{ \frac{N_0}{2V} v(k) + \sum_{k' \neq k} \frac{v(k-k')}{2V} \lambda_{k'} \mu_{k'} (1 + 2\bar{n}_{k'}) \right\},$$

$$\varepsilon'(k) = \varepsilon(k) + \frac{N_0}{V} v(k) + \sum_{k' \neq k} \frac{v(k-k')}{V} \left(\mu^2_{k'} + (\lambda^2_{k'} + \mu^2_{k'}) \bar{n}_{k'}\right),$$

$$A_k = \lambda_k\mu_k\left(\beta_k^+\beta_k + \beta_{-k}^+\beta_{-k} - 2\bar{n}_k\right) + \lambda_k^2\beta_k\beta_{-k} + \mu_k^2\beta_k^+\beta_{-k}^+,$$

$$B_k = \lambda_k^2(\beta_k^+\beta_k - \bar{n}_k) + \mu_k^2(\beta_{-k}\beta_{-k}^+ - \bar{n}_k) + \lambda_k\mu_k(\beta_k\beta_{-k} + \beta_k^+\beta_{-k}^+) \tag{4b}$$

(everywhere $k, k' \neq 0$).

In the Hamiltonian (3) we have introduced, for the time being formally, the numbers $\bar{n}_k$, which cancel in the sum. As we shall see below, $\bar{n}_k$ have the meaning of mean occupation numbers.

Following paper (1), it is easy to verify that, as $V \to \infty$, the operator H_1 does not contribute to the thermodynamic functions if the mean values of the operators A_k and B_k over the grand Gibbs ensemble with Hamiltonian H_0 are equal to zero,

$$\bar{A}_k = \bar{B}_k = 0. \tag{5}$$

The thermodynamic potential then has the form

$$\Omega = -\theta \ln\left\{\mathrm{sp}\, e^{-H_0/\theta}\right\}. \tag{6}$$

We choose the parameters of the canonical transformation (2) from the condition of diagonalizing H_0, setting $Q(k) = 0$. In this case, according to (5) and (4b),

$$\bar{n}_k = \overline{\beta_k^+\beta_k} = \left(e^{E(k)/\theta} - 1\right)^{-1}.$$

Now put

$$C(k) = \frac{N_0}{V}v(k) + \sum_{k' \neq k}\frac{v(k-k')}{V}\lambda_{k'}\mu_{k'}(1 + 2\bar{n}_{k'}). \tag{7}$$

and write the equation $Q(k) = 0$ in the form

$$2\varepsilon'(k)\lambda_k\mu_k + (\lambda_k^2 + \mu_k^2)C(k) = 0. \tag{8}$$

From (8), taking (2) into account, we obtain

$$\lambda_k^2 = \frac{1}{2}\left(1 + \frac{\varepsilon'(k)}{\sqrt{\varepsilon'^2(k) - C^2(k)}}\right); \qquad \mu_k^2 = \frac{1}{2}\left(-1 + \frac{\varepsilon'(k)}{\sqrt{\varepsilon'^2(k) - C^2(k)}}\right), \tag{9}$$

where

$$\varepsilon'(k) = \varepsilon(k) + S(k), \tag{10}$$

$$S(k) = \frac{N_0}{V}\nu(k) + \sum_{k'\neq k} \frac{\nu(k-k')}{V}\left\{\mu_{k'}^2 + (\lambda_{k'}^2 + \mu_{k'}^2)\,\bar{n}_{k'}\right\}.$$

Taking (7), (9), and (10) into account, for $C(k)$, $S(k)$, and N_0 we obtain the system of equations

$$C(k) = \frac{N_0}{V}\nu(k) - \sum_{k'\neq k} \frac{\nu(k-k')}{2V}\frac{1+2\bar{n}_{k'}}{E(k')}C(k'); \tag{11}$$

$$S(k) = \frac{N_0}{V}\nu(k) + \sum_{k'\neq k} \frac{\nu(k-k')}{2V}\left\{\frac{(\varepsilon(k') + S(k'))(1+2\bar{n}_{k'})}{E(k')} - 1\right\}; \tag{11a}$$

$$N = N_0 + \sum_{k\neq 0} \frac{1}{2}\left\{\frac{(\varepsilon(k) + S(k))(1+2\bar{n}_k)}{E(k)} - 1\right\}, \tag{11b}$$

where the energy of an elementary excitation is equal to

$$E(k) = \frac{\varepsilon'(k)}{\lambda_k^2 + \mu_k^2} = \sqrt{\left(\varepsilon(k) + S(k)\right)^2 - C^2(k)}. \tag{12}$$

We choose the chemical potential from the condition of a minimum with respect to N_0 of the thermodynamic potential (6). We obtain $\mu = S(0) + C(0) - 2\frac{N_0}{V}\nu(0)$.

Proceeding from the assumption that the interaction is small, we shall solve equations (11) by the method of iterations. As a result of the first iteration we obtain:

$$C(k) = \frac{N_0}{V}\nu(k); \quad S(k) = \frac{N_0}{V}\nu(k) + \frac{1}{(2\pi)^2}\int_0^\infty \bar{\nu}(k,k')\left\{\operatorname{cth}\frac{{k'}^2}{4m\theta} - 1\right\}{k'}^2\,dk', \tag{13}$$

$$\frac{N_0}{N} = 1 - \left(\frac{\theta}{\theta_{\text{cr}}}\right)^{3/2}, \tag{14}$$

where

$$\bar{\nu}(k,k') = \frac{1}{2}\int_{-1}^{1} \nu\left(k^2 + {k'}^2 - 2kk'\mu\right)^{1/2} d\mu, \quad (2m\theta_{\text{cr}})^{3/2} = \frac{(2\pi)^2}{v\alpha},$$

$$\alpha = \int_0^\infty \left(\operatorname{cth}\frac{x^2}{2} - 1\right) x^2\, dx.$$

The second iteration gives terms $\sim \nu^{3/2}$. However, the following terms of the expansion are unreliable (the introduction of a condensate is valid only for a small interaction), and we shall confine ourselves here to the first iteration, extrapolating the solution (13) to the point $\theta = \theta_{\text{cr}}$. Substituting (13) into (12), we obtain the spectrum of elementary excitations in the form

$$E(k) = \sqrt{\varepsilon^*(k)\left\{\varepsilon^*(k) + 2\frac{N_0}{V}\nu(k)\right\}}, \tag{15}$$

where

$$\varepsilon^*(k) = \frac{k^2}{2m} + \frac{1}{(2\pi)^2}\int_0^\infty [\bar{\nu}(k,k') - \nu(k')]\left\{\operatorname{cth}\frac{{k'}^2}{4m\theta} - 1\right\}{k'}^2\, dk'.$$

The spectrum (15) satisfies L. D. Landau' s criterion of superfluidity (^{4}) for $\theta < \theta_{\text{cr}}$, and does not satisfy it for $\theta = \theta_{\text{cr}}$. Consequently, at the point $\theta = \theta_{\text{cr}}$ the Bose gas passes from a nonsuperfluid state into a superfluid one. At $\theta = 0$, expression (15) coincides with the spectrum of elementary excitations previously established by N. N. Bogolyubov (^{2}).

Let us now consider the thermodynamic properties of the nonideal Bose gas. Taking (3) and (8) into account, we write the thermodynamic potential (6) in the form

$$\Omega = U + \theta\sum_k \ln(1 - e^{-E(k)/\theta}). \tag{16}$$

When differentiating (16) with respect to temperature, the quantities U and $E(k)$ may be regarded as constant, since the increments of the parameters λ_k and μ_k due to (8) make no contribution to the increment of the thermodynamic potential.

At the phase-transition point $\theta = \theta_{\text{cr}}$, the entropy is continuous, since N_0 and $C(k)$ then vanish. It is easy to verify that for $\theta = \theta_{\text{cr}}$ the heat capacity has a finite jump. We have:

$$\mathcal{C} = \theta\frac{dS}{d\theta} = -\theta\frac{\partial^2\Omega}{\partial\theta^2} - \theta\sum_k \frac{\partial^2\Omega}{\partial E(k)\,\partial\theta}\,\frac{\partial E(k)}{\partial\theta}. \tag{17}$$

The first term in (17) is continuous at $\theta = \theta_{\text{cr}}$. The second gives a jump of the heat capacity equal to

$$\frac{\Delta\mathcal{C}}{\mathcal{C}_{\text{n}}} \simeq \frac{3}{2}\frac{\nu(0)}{v\theta_{\text{cr}}}\gamma, \qquad \gamma = \int_0^\infty \frac{e^{x^2}x^4\,dx}{(e^{x^2}-1)^2} \Bigg/ \int_0^\infty \frac{e^{x^2}x^6\,dx}{(e^{x^2}-1)^2} \simeq 0.24, \tag{18}$$

where $\mathcal{C}_{\text{n}}$ is the heat capacity of the gas in the normal state at $\theta = \theta_{\text{cr}}$. Thus, starting from the solution (13), we have arrived at the conclusion that the nonideal Bose gas at the temperature $\theta = \theta_{\text{cr}}$ undergoes a second-order phase transition. The derivative of the heat capacity at the point $\theta = \theta_{\text{cr}}$ tends to infinity proportionally to $(1 - \theta^{3/2}/\theta_{\text{cr}}^{3/2})^{-1/2}$, and the critical point is a cusp point of the heat-capacity curve. These features of the behavior of the Bose gas are in agreement with the properties of He II.

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