Section E. Phase Transitions and Diffusion Processes in Condensed Matter and Gases

NONPERTURBATIVE APPROACH TO SUPERFLUID BOSE SYSTEMS

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We study a superfluid Bose system with single-particle and pair condensates using a nonperturbative approach. The self-consistency equations for two order parameters are obtained from the principle of maximum entropy. They are analyzed numerically at zero temperature for dilute (gases of alkali-metal atoms) and dense (superfluid 4He) systems. It is shown that the pair condensate fraction is negligible for dilute systems and becomes dominant for dense systems. We shall construct the quasiparticle description of a Bose superfluid. Therefore, the statistical operator should be approximated by the general quadratic form (1) is chosen to satisfy the principle of maximum entropy.

\[ \rho = \exp(\Omega - F), \]
\[ F = a^\dagger A a + \frac{1}{2}(a B a + a^\dagger B^* a^\dagger) + a^\dagger C + C^* a, \] (1)

where we have omitted the repeated summation indices bearing in mind that, e.g., \( a^\dagger A a \equiv a^\dagger_p A_{pp} a^\dagger_p \) or \( a^\dagger C \equiv a^\dagger_p C_p \). Thermodynamic potential \( \Omega \) is found from the normalization condition \( \text{Sp} \rho = 1 \). The choice of \( \rho \) is based on the fact that it satisfies the principle of spatial correlation weakening and Wick’s rule applies to it [1, 2, 8]. This statistical operator can be used to describe the many-body system of interacting particles in the language of free particles (or quasiparticles). The coefficients in the quadratic form (1) are chosen to satisfy the principle of maximum entropy.

It is more convenient to characterize the state by the condensate amplitudes \( b_p, b^*_p \) and by the following correlation functions:

\[ f_{pp}^c = f_{pp'} - b^*_p b_p, \quad g_{pp'} = g_{pp'} - b^*_p b_p. \] (2)

A compact formulation of the theory is attained in terms of a two-row correlation matrix \( f^c \) containing both normal and anomalous correlation functions and a vector \( \psi \), whose components are the condensate amplitudes [1, 2]:

\[ f^c = \begin{pmatrix} f^c & -g^c \\ g^c & -1 - f^c \end{pmatrix}, \quad \psi = \begin{pmatrix} b \\ b^* \end{pmatrix}. \] (3)

We shall construct the quasiparticle description of a Bose superfluid. Therefore, the statistical operator should be approximated by the general quadratic form of creation and annihilation operators as well as linear terms in them [1, 2]:

\[ \rho = \exp(\Omega - F), \]
\[ F = a^\dagger A a + \frac{1}{2}(a B a + a^\dagger B^* a^\dagger) + a^\dagger C + C^* a, \] (1)

where we have omitted the repeated summation indices bearing in mind that, e.g., \( a^\dagger A a \equiv a^\dagger_p A_{pp} a^\dagger_p \) or \( a^\dagger C \equiv a^\dagger_p C_p \). Thermodynamic potential \( \Omega \) is found from the normalization condition \( \text{Sp} \rho = 1 \). The choice of \( \rho \) is based on the fact that it satisfies the principle of spatial correlation weakening and Wick’s rule applies to it [1, 2, 8]. This statistical operator can be used to describe the many-body system of interacting particles in the language of free particles (or quasiparticles). The coefficients in the quadratic form (1) are chosen to satisfy the principle of maximum entropy.

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\[ f^c = \begin{pmatrix} f^c & -g^c \\ g^c & -1 - f^c \end{pmatrix}, \quad \psi = \begin{pmatrix} b \\ b^* \end{pmatrix}. \] (3)
The state of thermodynamic equilibrium is determined by the maximum of entropy $S = -Sp\rho \ln \rho$ at fixed values of the total energy and total particle number. The solution of this variational problem is given by the following self-consistency equations [1,2]:

$$f^c = \left[ \exp(\beta(\hat{\varepsilon} - \hat{\mu}) - 1) \right]^{-1},$$

where

$$\hat{\varepsilon} = \left( \begin{array}{cc} \varepsilon & \Delta^* \\ -\Delta & -\hat{\varepsilon} \end{array} \right), \quad \hat{\mu} = \left( \begin{array}{c} \mu \\ 0 \end{array} \right), \quad \hat{\eta} = \left( \begin{array}{c} \eta \\ \eta^* \end{array} \right),$$

and

$$\eta_p = \frac{\partial E(f^c, \psi)}{\partial f^c_{cp}}, \quad \Delta_p = \frac{\partial E(f^c, \psi)}{\partial g^c_{cp}}.$$  \hspace{1cm} (6)

The quantities $\beta = 1/T$ and $\mu$ entering Eqs. (4), (5) are the reciprocal temperature and chemical potential, respectively. The matrix equation (4) has a form of the Bose distribution function if $\hat{\varepsilon}$ is interpreted as the operator of quasiparticle energy. Equation (5) has a structure of the well-known Gross-Pitaevskii equation [3,4] without external potential. However, the principle difference between these equations is that the energy of the system $E(f^c, \psi)$ depends not only on the condensate amplitudes but also on normal and anomalous correlation functions. The system of coupled Eqs. (4), (5) describe an inhomogeneous state of a Bose superfluid with single-particle and pair condensates if the energy functional is known.

For a homogeneous system, Eqs. (4), (5) are significantly simplified. In this case the correlation functions and condensate amplitudes are given by:

$$f^c_{pp'} = f^c_{p} \delta_{p',p}, \quad g^c_{pp'} = g^c_p \delta_{p,-p'}, \quad b_p = b_0 \delta_{p,0},$$

where $f^c_p = f^c_p$ and $g^c_p = g^c_{-p}$. Therefore, according to Eqs. (7), one finds

$$\varepsilon_{pp'} = \varepsilon_p \delta_{p',p}, \quad \Delta_{pp'} = \Delta_p \delta_{p,-p'},$$

where

$$\varepsilon_p = \frac{\partial E(f^c, \psi)}{\partial f^c_p}, \quad \Delta_p = \frac{\partial E(f^c, \psi)}{\partial g^c_p}.$$  \hspace{1cm} (9)

The correlation functions $f^c_p$ and $g^c_p$ are found to be [1,2,9]:

$$f^c_p = -\frac{1}{2} \xi_p E_p \coth \frac{\beta E_p}{2},$$

$$g^c_p = \frac{\Delta_p}{2E_p} \coth \frac{\beta E_p}{2},$$

where

$$\xi_p = \varepsilon_p - \mu, \quad E_p = \sqrt{\xi_p^2 - |\Delta_p|^2}.$$  \hspace{1cm} (11)

and $\xi_p$, $\Delta_p$ are given by Eqs. (10). The condensate amplitudes $b_0$ satisfy the following equation:

$$\frac{\partial E(f^c, \psi)}{\partial b^*_0} - \mu b_0 = 0.$$  \hspace{1cm} (13)

Equations (11)-(13) completely describe a homogeneous state of a Bose superfluid with single-particle and pair condensates for a given energy $E(f^c, \psi)$.

3. ENERGY FUNCTIONAL AND SELF-CONSISTENCY EQUATIONS

The subsequent analysis of the system can be done if we specify the energy functional $E(f^c, \psi)$. It can be constructed from the condensate energy functional $E(\psi) \equiv E(b_p, b^*_p) = E(0, \psi)$ according to the following formula [1,2]:

$$E(f^c, \psi) = Sp \rho H(a^+_p, a_p) = RE(\psi)$$  \hspace{1cm} (14)

with

$$R = \exp \left( \frac{\partial \varepsilon_p}{\partial b} f^c_p \partial \varepsilon_p + \frac{1}{2} \frac{\partial}{\partial b} \partial \varepsilon_p \right),$$

where $H(a^+_p, a_p)$ is a microscopic Hamiltonian. We have omitted the repeated summation indices, like in Eq. (1). We choose the condensate energy functional in the form of a binary interaction Hamiltonian,

$$E(\psi) = \sum_p \frac{\rho}{2m} b^*_p b_p + \frac{1}{2V} \sum_{p_1, p_2, p_3, p_4} \nu(p_1 - p_2) b^*_p b^*_q b_p b_q,$$

where $V$ is the volume of the system. Therefore, from Eqs. (14)-(16), we can obtain the explicit expression for $E(f^c, \psi)$ [9]. For the latter Eq. (13) becomes:

$$b_0[n_0 (\nu(0) - \mu)] + \frac{b_0}{V} \sum_p f^c_p [\nu(0) + \nu(p)] +$$

$$+ \frac{b_0}{V} \sum_p g^c_p \nu(p) = 0,$$  \hspace{1cm} (17)

where we have employed Eqs. (8) and introduced the density of a single-particle condensate $n_0 = b_0^\dagger b_0 / V$. Next, Eqs. (10) allow one to find $\xi_p$ and $\Delta_p$ through the correlation functions $f^c_p = f^c_p$ and $g^c_p = g^c_{-p}$. The subsequent substitution of equilibrium correlation functions (11) into these quantities gives equations for $\xi_p = \varepsilon_p - \mu$ and $\Delta_p$. We should also eliminate the correlation functions in Eq. (17). After some algebraic manipulations, we come to the following system of coupled equations [9,10]:

$$\xi_p = \frac{\rho^2}{2m} - \mu + n_0 [\nu(0) + \nu(p)] -$$

$$- \frac{1}{2V} \sum_{p'} [\nu(0) + \nu(p + p')] \left( 1 - \frac{\xi_p}{E_p} \coth \frac{\beta E_p}{2} \right),$$

$$\Delta_p = \frac{1}{V} \nu(p) b^*_p - \frac{1}{2V} \sum_{p'} \nu(p + p') \frac{\Delta_p}{E_{p'}} \coth \frac{\beta E_{p'}}{2},$$

$$b_0 \left( 2n_0 (\nu(0) - \xi_p) - \frac{b^*_0}{b_0} \Delta_0 \right) = 0.$$  \hspace{1cm} (18)
The obtained equations have three types of solutions. The first, with zero values of \( n_0 \) and \( \Delta_p \), describes the normal state in which both condensates are absent. The second type of solution, with \( n_0 = 0 \) and \( \Delta_p \neq 0 \), breaks \( U(1) \) symmetry and describes the state with a pair condensate only (this condensate is similar to a condensation of Cooper pairs in a Fermi superfluid). Finally, the solution with \( n_0 \neq 0 \) and \( \Delta_p \neq 0 \) also characterizes the state with broken \( U(1) \) symmetry. However, in this state both single-particle and pair condensates exist. Note that the derived equations have no solution of the type \( \Delta_p = 0, n_0 \neq 0 \).

It is easy to see that the total particle number is given by:

\[
N(\hat{f}, \hat{\psi}) = \sum_p (f^c_p + b^\dagger_p b_p), \quad f^c_{pp} \equiv f^c_p.
\]  

Using Eqs. (11), we can find the total particle density:

\[
n = n_0 + n_{\text{pair}} + n_{\text{quas}},
\]  

where

\[
n_{\text{pair}} = \frac{1}{2V} \sum_p \left( \frac{\xi_p}{E_p} - 1 \right) \coth \frac{\beta E_p'}{2},
\]  

\[
n_{\text{quas}} = \frac{1}{2V} \sum_p \left( \coth \frac{\beta E_p'}{2} - 1 \right).
\]  

The first term in Eq. (20) is the particle density in a single-particle condensate, the second one is the pair condensate density, and the last term represents the contribution of quasiparticles. The obtained expression for the total particle density should be used to eliminate the chemical potential in Eqs. (18).

### 4. ZERO TEMPERATURE AND CONTACT INTERACTION

Here we study the system at zero temperature and with contact interaction between atoms, \( \nu(p) = \nu = \text{const} \). In this case Eqs. (18) are significantly simplified because the quasiparticle density turns to zero and \( \Delta_p \) does not depend on momentum, \( \Delta_p \equiv \Delta \). Moreover, the structure of equations allows us to consider \( b_0 \) and \( \Delta \) as real and positive quantities. In view of the aforesaid, we find the following system of coupled equations:

\[
\frac{\nu}{V} \sum_p \left( \frac{\xi_p}{E_p} - 1 \right) - \mu + \Delta = 0,
\]  

\[
\Delta \left( 1 + \frac{\nu}{2V} \sum_p \frac{1}{E_p} \right) - \nu n_0 = 0,
\]  

where

\[
\xi_p = p^2/2m + \alpha, \quad \alpha = 2\nu n_0 - \Delta.
\]  

The spectrum of single-particle excitations has the form:

\[
E_p = \sqrt{(p^2/2m + \alpha)^2 - \Delta^2}.
\]  

As we see, it exhibits a gap which is given by the following expression:

\[
\delta = \sqrt{\alpha^2 - \Delta^2} = \sqrt{4\nu n_0 (\nu n_0 - \Delta)}.
\]  

The total particle density at \( T = 0 \), according to Eqs. (20)-(22), becomes

\[
n = n_0 + n_{\text{pair}} = n_0 + \frac{1}{2V} \sum_p \left( \frac{\xi_p}{E_p} - 1 \right).
\]  

The comparison of Eq. (28) with Eq. (23) yields the expression for the chemical potential:

\[
\mu = \Delta - 2\nu(n_0 - n).
\]  

Now we return to the coupled Eqs. (23,24). First, let us eliminate the chemical potential in Eq. (23) using Eq. (29). Then we replace the summation by integration over the variable \( x = p^2/2m \) in both equations. The integral that appears in Eq. (24) diverges at the upper limit. The physical reason of this divergence is that we have taken a delta-like contact potential with zero radius of interparticle interaction. In order to remove the divergence, we introduce a typical length scale \( r_0 \) for the range of interaction. In subsequent numerical computations, we will assume that \( r_0 \) coincides with the value of a repulsive core of the interaction potential which is typically equal to a few angstroms. When integrating over the variable \( x \), having the dimension of energy, we will cut off the divergence by \( x_0 = (\hbar k_0)^2/2m = \hbar^2/2mr_0^2 \). In addition, it is convenient for numerical analysis to introduce the following dimensionless quantities: \( \bar{x} = x/x_0, \bar{\Delta} = \Delta/x_0, \bar{\alpha} = \alpha/x_0, \bar{n}_0 = n_0 r_0^3, \bar{n} = n r_0^3 \) and to consider \( \bar{\alpha} = 4g\bar{n}_0 - \bar{\Delta} \) as the sought quantity, instead of \( \bar{n}_0 \). Consequently, Eqs. (23,24) in dimensionless form are written as

\[
\bar{n} = \bar{\alpha} + \bar{\Delta}/4g + \frac{1}{8\pi^2} \int_0^\infty d\bar{x} \sqrt{\bar{x}} \left( \frac{\bar{x} + \bar{\alpha}}{\sqrt{(\bar{x} + \bar{\alpha})^2 - \bar{\Delta}^2}} - 1 \right), \quad \bar{\Delta} \frac{\bar{\Delta}}{\bar{\alpha}} \left( 1 + \frac{g}{2\pi^2} \int_0^1 d\bar{x} \frac{\sqrt{\bar{x}}}{\sqrt{(\bar{x} + \bar{\alpha})^2 - \bar{\Delta}^2}} \right) = 1,
\]  

where \( g = (\nu m \sqrt{2\pi \alpha m / \hbar^3}) = (\nu m / \hbar^2 r_0) \) is a dimensionless coupling constant and \( \nu \) is related to s-wave scattering length \( a \) by the well-known expression \( \nu = 4\pi a^2/\alpha \). We see that the dimensionless coupling constant is determined by the ratio of the scattering length to radius of interaction potential:

\[
g = 4\pi a/r_0.
\]  

Equation (30) reflects the fact that the total particle density is the sum of the particle densities in single-particle and pair condensates (the first and second terms, respectively).
5. NUMERICAL ANALYSIS

A. Dilute gases with a condensate. Bose-Einstein condensation in dilute atomic gases was first realized in 1995 [11–13]. The particle density in condensed atomic cloud is $n \sim 10^{13} \ldots 10^{15} \text{cm}^{-3}$. Then the corresponding dimensionless density $\tilde{n}$, which enters Eq. (30), is of the order $10^{-11} \ldots 10^{-9}$, where we have taken $r_0 \approx 3\text{Å}$. The atomic interaction in such dilute systems is usually modeled by the contact interaction potential expressed through the scattering length $a$. For $^{87}\text{Rb}$ and $^{23}\text{Na}$, the scattering lengths are $90\,a_0$ and $19.1\,a_0$, respectively, where $a_0 \approx 0.53\text{Å}$ is the Bohr radius [14]. From Eq. (32), we can find the values of dimensionless coupling constant: $g \approx 200$ for $^{87}\text{Rb}$ and $g \approx 42$ for $^{23}\text{Na}$. The numerical analysis of Eqs. (30), (31) is presented in Figs. 1 and 2. Figure 1 shows the dependencies of the pair condensate fraction $\tilde{n}_{\text{pair}}/\tilde{n}$ on the coupling constant $g$ for the indicated above values of the total particle density. From this figure we can conclude that the pair condensate fraction is several orders less than the single-particle condensate fraction. Therefore, the dilute systems are described by the Gross-Pitaevskii equation with a high level of accuracy [3,4,14]. Moreover, in the limit $g \to 0$, the pair condensate fraction tends also to zero and, thereby, $n_0 \to n$. Figure 2 demonstrates the dimensionless energy gap $\tilde{\delta} = \delta/x_0$ as a function of the coupling constant $g$ for various values of the total density. We see that at small densities, the gap remains small even for large values of the coupling constant. Its value tends to zero as the coupling constant tends to zero. In the limit $g \to 0$ we obtain the gapless Bogolyubov spectrum [15].

B. Superfluid $^4\text{He}$. A superfluid $^4\text{He}$ represents a dense system in which Bose-Einstein condensation is also manifested. However, the experiments on inelastic neutron scattering [5–7] predict the single-particle condensate density to be less than 10%. Here we analyze the derived self-consistency equations at helium density, $n \approx 2.18 \cdot 10^{22} \text{cm}^{-3}$. The interaction potential of helium has a strong short-range repulsion whose radius is $r_0 \approx 2.55\text{Å}$, followed by a weak intermediate range attraction. Therefore, the dimensionless density entering Eq. (30) is $\tilde{n} \approx 0.36$. The scattering length $a$ for $^4\text{He}$ atoms varies from $46.1\text{Å}$ to $100\text{Å}$ depending on the used interaction potential [16]. Thus, according to Eq. (32), the dimensionless coupling constant $g$ lies in the interval from 227 to 492.

Figure 3 shows the behavior of the pair condensate fraction depending on the coupling constant at helium density. It significantly exceeds the single-particle condensate fraction. For the indicated above
values of the coupling constant, the pair condensate fraction is about 90...95%. This means that the single-particle condensate fraction is just about 5...10%. This fact agrees with the condensate fraction in a superfluid $^4$He measured in experiments [5–7].

Figure 4 presents the dependence of the dimensionless energy gap $\delta = \delta / x_0$ in the single-particle excitation spectrum on $g$ at helium density. For example, at $g = 227$ we have $\delta \approx 13.45$ or in the temperature units $\delta \approx 12.5$ K. Note that it is somewhat greater than the value of the roton gap $\Delta_{\text{max}} \approx 8.65$ K and less than the maxon energy $\Delta_{\text{max}} \approx 14$ K.

References


НЕПЕРТУРБАТИВНЫЙ ПОДХОД К СВЕРХТЕКУЧИМ БОЗЕ-СИСТЕМАМ

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На основе непертurbативного подхода изучается сверхтекучая бозе-система с одночастичным и парным конденсатом. Из принципа максимума энтропии найдены уравнения самосогласования для двух параметров порядка. Они проанализированы численно при нулевой температуре для разреженных (газы атомов нежелезных металлов) и плотных (сверхтекучий $^4$He) систем. Показано, что доля парного конденсата преобладающая мала для разреженных систем и становится преобладающей для плотных.

НЕПЕРТУРБАТИВНЫЙ ПОДХОД ДО НАДПЛИННЫХ БОЗЕ-СИСТЕМ

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На основе непертurbативного подхода включается надплиинная бозе-система с одночастичным и парным конденсатом. Из принципа максимума энтропии найдены уравнения самосогласования для двух параметров порядка. Они проанализированы численно при нулевой температуре для разреженных (газы атомов нежелезных металлов) и густых (надплиинный $^4$He) систем. Показано, что доля парного конденсата ёст нехтново малов для разреженных систем и задача преобладающей для густых систем.