Tutorial

Theory of cold atoms: Bose–Einstein statistics

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Abstract

This tutorial is the continuation of the previous tutorial part, published in (2013 Laser Phys. 23 062001), where the basic mathematical techniques required for an accurate description of cold atoms for both types of quantum statistics are expounded. In the present part, the specifics of the correct theoretical description of atoms obeying Bose–Einstein statistics are explained, including trapped Bose atoms. In the theory of systems exhibiting the phenomenon of Bose–Einstein condensation, there exists a number of delicate mathematical points, whose misunderstanding often results in principally wrong conclusions. This is why the consideration in the present tutorial is sufficiently detailed in order that the reader could clearly understand the underlying mathematics and would avoid confusions.

Keywords: Bose–Einstein condensate, thermodynamic stability, trapped atoms, superfluidity

1. Introduction

In the previous tutorial [1], the basic mathematical notions that are necessary for an accurate description of quantum systems composed of atoms or molecules are elucidated. That consideration has been done for the general case of atoms satisfying either Bose–Einstein or Fermi-Dirac statistics. The present tutorial is devoted to the consideration of specifics related to atomic systems of Bose–Einstein statistics. These systems exhibit the phase transition of Bose–Einstein condensation and the related superfluid transition. The theoretical description of Bose-condensed systems confronts several delicate points that are often misunderstood in literature, resulting in wrong conclusions. Among such misconceptions, it is possible to mention the following.

One assumes that the ideal Bose gas is a realistic object and can be a good approximation for Bose-condensed systems with weak interactions. However, this is not exactly correct, since the ideal Bose gas and an interacting Bose gas pertain to different classes of universality. Moreover, the uniform ideal Bose-condensed gas is unstable, being a pathological system with infinite compressibility. The ideal Bose-condensed gas can be stabilized inside a trap. But not each trap can stabilize the Bose-condensed gas. For instance, a three-dimensional harmonic trap does stabilize the ideal Bose-condensed gas, although the lower dimensional harmonic traps cannot make it stable.

Sometimes, in the literature it is possible to meet the statement that Bose–Einstein condensation does not necessarily require gauge symmetry breaking. But this is wrong, since there exist strict mathematical theorems proving that gauge symmetry breaking is a necessary and sufficient condition for Bose–Einstein condensation. As a consequence, a mean-field approximation of the Hartree–Fock type, where gauge symmetry is not broken, is not applicable to Bose-condensed systems, but the Hartree–Fock–Bogolubov approximation, with the broken gauge symmetry, is compulsory.

Neglecting the broken gauge symmetry leads to the appearance of thermodynamically anomalous particle fluctuations, when using the grand canonical ensemble, which one sometimes calls ‘grand canonical catastrophe’. However, there is no any catastrophe when correctly using the grand ensemble. Catastrophes arise only because of incorrect calculations.
Similarly, thermodynamically anomalous particle fluctuations in a Bose-condensed system formally occur in the Bogolubov approximation in any ensemble, whether grand canonical or canonical. This, however, is also caused by the incorrect use of the second-order, with respect to field operators, Bogolubov approximation to calculating the fourth-order operator products. Being in the frame of the applicability of the approximation order always leads to thermodynamically normal fluctuations.

There are discussions stating that canonical and grand canonical ensembles are not equivalent for Bose-condensed systems. This is again due to an incorrect use of the ensembles, for example, when one forgets to break gauge symmetry under Bose–Einstein condensation. Generally, it is necessary to employ representative ensembles, where all necessary restrictions, uniquely characterising the system, are taken into account. Then such representative ensembles are always equivalent in thermodynamic limit.

A very widespread mistake is the neglect of the so-called anomalous averages, when describing Bose-condensed systems, while retaining the normal averages corresponding to uncondensed atoms. The fact that such a neglect is principally inadmissible is evident, if one remembers that Bose–Einstein condensation is necessarily accompanied by gauge symmetry breaking, which is responsible for the appearance of the condensate fraction as well as of the anomalous averages. Therefore it should be logically clear that omitting one of the basic characteristics of the Bose-condensed system, while keeping the other, is principally wrong. Moreover, by direct calculations, it is straightforward to check that the anomalous averages, by the order of magnitude, are always larger, depending on temperature, than either the normal averages, representing the fraction of normal atoms, or than the condensate fraction. Thus omitting the larger terms, while keeping the smaller ones is mathematically wrong. Such a contradiction results in the system instability and in the incorrect description of the Bose–Einstein condensation transition.

One sometimes involves the Dirac representation of field operators, by defining a phase operator. This representation, unfortunately, is mathematically incorrect and can lead to wrong results.

Because of a number of misconceptions in the theoretical study of Bose-condensed systems, it looks important to give a thorough analysis of the mathematics providing the tools for a correct description of systems with Bose–Einstein condensate.

In the following parts, the knowledge of the previous tutorial [1] is assumed, because of which many definitions are not repeated here. Since the present paper is a tutorial, but not a review article, only the most important, from the point of view of the author, material is discussed. Also, no extensive citations of numerous literature are given, but only the publications directly related to the concrete points under consideration are cited.

Throughout the paper, the system of units is employed where the Planck constant \( \hbar \rightarrow 1 \) and the Boltzmann constant \( k_B \rightarrow 1 \).

### 2. Basic notions

In this part, the main notions and specific characteristics of atomic systems, satisfying the Bose–Einstein statistics, are described, giving the general understanding of the peculiarities accompanying the phenomenon of Bose–Einstein condensation.

#### 2.1. Phenomenon of superfluidity

Probably, the most physically important property of Bose systems is the occurrence of superfluidity. Therefore, let us start the consideration from the problem of how this property could be quantified.

The occurrence of superfluidity implies the appearance of superfluid fraction of atoms

\[
n_s = \frac{N_s}{N},
\]

where \( N_s \) is the average number of superfluid atoms among the total number of atoms \( N \). This number \( N_s \) represents the average number of atoms, but is not related to particular atoms, since the latter are not distinguishable.

The system of atoms, without internal degrees of freedom, is characterized by the Hamiltonian

\[
H = \int \psi^\dagger(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu \right) \psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \phi(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}) \psi(\mathbf{r}') \, d\mathbf{r} \, d\mathbf{r}',
\]

in which the field operators satisfy Bose commutation relations and, generally, depend on time \( t \) that is not shown explicitly. Here \( U = U(\mathbf{r}) \) is an external potential.

The motion of the system is associated with the momentum operator

\[
\hat{\mathbf{P}} = \int \psi^\dagger(\mathbf{r})(-i\nabla)\psi(\mathbf{r}) \, d\mathbf{r},
\]

defining the observable quantity, the average system momentum

\[
\langle \hat{\mathbf{P}} \rangle \equiv \text{Tr} \hat{\rho} \hat{\mathbf{P}},
\]

where the statistical averaging is done with respect to a statistical operator \( \hat{\rho} \). For an equilibrium system, the latter is

\[
\hat{\rho} = \frac{e^{-\beta H}}{\text{Tr} e^{-\beta H}},
\]

with \( \beta = 1/T \) being the inverse temperature.

The property of superfluidity is related to the nontrivial response of the system with respect to a boost with velocity \( \mathbf{v} \). Under this boost, the field operator, in the laboratory frame, satisfies the Galilean transformation

\[
\psi(\mathbf{r}, t) = \psi(\mathbf{r} - \mathbf{v}t, t) \exp \left\{ i \left( \frac{m \mathbf{v} \cdot \mathbf{r} - \frac{mv^2}{2}t}{\beta} \right) \right\}.
\]

[1] Laser Phys. 26 (2016) 062001 Tutorial
Then the Hamiltonian for the moving system becomes
\[ H_c = H + \int \psi(\mathbf{r}) \left( -i \mathbf{v} \cdot \nabla + \frac{m v^2}{2} \right) \psi(\mathbf{r}) d\mathbf{r}, \]
and the momentum operator is
\[ \hat{P}_a = \hat{P} + m v \mathbf{v}. \]
The average momentum reads as
\[ \langle \hat{P}_a \rangle = \text{Tr} \hat{\rho} \hat{P}, \]
with the statistical operator
\[ \hat{\rho} = e^{-\beta H} / \text{Tr} e^{-\beta H}. \]
To find the number of particles nontrivially responding to the velocity boost,
\[ N_s \equiv \frac{1}{3m} \lim_{v \to 0} \frac{\partial}{\partial \mathbf{v}} \cdot \langle \hat{P} \rangle_v, \]
one needs the derivatives
\[ \frac{\partial}{\partial \mathbf{v}} \cdot \hat{P} = \sum_{\alpha=1}^3 \frac{\partial P^\alpha}{\partial v^\alpha} e^{-\beta H} \frac{\partial H}{\partial \mathbf{v}}. \]
The statistical operator, for small \( v \to 0 \), varies as
\[ \hat{\rho} \approx \hat{\rho} + \beta \left( \hat{\rho} \langle \hat{P} \rangle - \beta [ \hat{\rho}, \hat{P} ] \right) \mathbf{v}. \]
The average momentum of the moving system is
\[ \langle \hat{P}_a \rangle = \langle \hat{P} \rangle_v + m v N. \]
For small \( v \), we have
\[ \langle \hat{P}_a \rangle \approx \langle \hat{P} \rangle + \beta \left[ \langle \hat{P} \hat{\rho} \rangle - \beta \langle \hat{P} \hat{\rho} \rangle \langle \hat{\rho} \hat{P} \rangle \right], \]
and
\[ \frac{\partial}{\partial \mathbf{v}} \cdot \langle \hat{P} \rangle_v \approx -\beta \text{var}(\hat{P}), \]
where
\[ \text{var}(\hat{P}) = \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2. \]
In this way, the average numbers of superfluid and normal atoms, respectively, are
\[ N_s = N - \frac{\beta}{3m} \text{var}(\hat{P}), \quad N_n = \frac{\beta}{3m} \text{var}(\hat{P}), \]
so that the superfluid fraction is
\[ n_s = 1 - \frac{\beta}{3mN} \text{var}(\hat{P}). \]
In equilibrium
\[ \langle \hat{P} \rangle = 0, \quad \text{var}(\hat{P}) = \langle \hat{P}^2 \rangle. \]
Hence, we need to find the quantity
\[ \langle \hat{P}^2 \rangle = -\int \psi^*(\mathbf{r}) \nabla \psi(\mathbf{r}) \psi^*(\mathbf{r}_2) \nabla \psi(\mathbf{r}_2) d\mathbf{r}_2, \]
which can also be written as
\[ \langle \hat{P}^2 \rangle = \int \lim_{r_1 \to r_2, r_2 \to r_1} \nabla \cdot \nabla [\rho(\mathbf{r}_1, \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho(\mathbf{r}_1, \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2, \]
where
\[ \rho(\mathbf{r}, \mathbf{r}) \equiv \langle \psi^*(\mathbf{r}) \psi(\mathbf{r}) \rangle \]
and \( \rho_2 \) is the second-order density matrix (see [1]).
In the case of a uniform system, the field operators can be expanded over the plane waves,
\[ \psi(\mathbf{r}) = \sum_k a_k \varphi_k(\mathbf{r}), \quad \varphi_k(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i k \cdot \mathbf{r}}, \]
which yields
\[ \langle \hat{P}^2 \rangle = \sum_{k} (\mathbf{k} \cdot \mathbf{p})(\hat{\rho}_k \hat{\rho}_k) \quad (\hat{\rho}_k \equiv \hat{a}_k^\dagger \hat{a}_k). \]
Introducing the notation for the dissipated heat
\[ Q \equiv \frac{\text{var}(\hat{P})}{2mN}, \]
that for an equilibrium system reads as
\[ Q = \frac{\langle \hat{P}^2 \rangle}{2mN}, \]
we get the superfluid fraction
\[ n_s = 1 - \frac{2Q}{3T}. \]
Whether the considered system exhibits superfluidity or not depends on particular system properties yielding the nonzero dissipated heat. The existence of the latter essentially depends on the character of pair atomic correlations. Note that the Bose–Einstein statistics has not been used in deriving the above formulas. Hence, in principle, the effect of superfluidity is not prohibited for Fermi systems.

2.2. Moment of inertia

The existence of a nontrivial response to a velocity boost should be connected with a nontrivial response to a rotation boost that also produces a velocity boost with the angular velocity \( \omega \).

The occurrence of quantum effects, such as superfluidity, happens when a quantum system behaves differently from a classical one. In classical mechanics, the angular momentum is
\[ \mathbf{L} = m \int (\mathbf{r} \times \mathbf{v}) \rho(\mathbf{r}) d\mathbf{r}, \]
where the linear velocity \( \mathbf{v} = \omega \times \mathbf{r} \) and \( \rho(\mathbf{r}) \) is the density distribution. The classical angular momentum takes the form
\[ \mathbf{L} = m \int (\mathbf{r} \times \omega) d\mathbf{r} \rho(\mathbf{r}) d\mathbf{r}. \]
Directing the axis \( z \) along the rotation axis, so that
\( \mathbf{e}_z = \frac{\mathbf{\hat{\omega}}}{{\mathbf{\omega}}} \) \((\mathbf{\omega} \equiv |\mathbf{\omega}|)\),
gives the z-component of the angular momentum
\[
L_z = m\omega \int (r^2 - z^2) \rho(r) dr,
\]
which can also be written as
\[
L_z = m\omega \int (r \times \mathbf{e}_z)^2 \rho(r) dr.
\]

The classical moment of inertia with respect to the rotation axis is defined by the derivative
\[
I_0 \equiv \lim_{\omega \to 0} \frac{\partial L_z}{\partial \omega}.
\]
Under a slow rotation, when \( \omega \to 0 \), the density \( \rho(r) \) does not change. Then the classical moment of inertia is
\[
I_0 = m \int (r \times \mathbf{e}_z)^2 \rho(r) dr.
\]

As examples, let us consider the case where \( \rho(r) = \rho = \) constant. Then, for a sphere of radius \( R \), the classical moment of inertia is \( I_0 = \frac{2mR^2}{5} \). For a cylinder of radius \( R \), we have \( I_0 = \frac{mR^2}{2} \).

In quantum theory, the local angular momentum operator is \( \mathbf{L}(r) \equiv -i \mathbf{r} \times \mathbf{\nabla} \). The total angular momentum operator reads as
\[
\mathbf{\hat{L}} \equiv \int \psi^*(r) \mathbf{L}(r) \psi(r) dr.
\]
The axial component of the angular momentum is
\[
\langle \mathbf{L}_z \rangle_\omega = \int \psi^*(r) \mathbf{L}_z(r) \psi(r) dr,
\]
where
\[
\mathbf{L}_z(r) = -i \mathbf{e}_z \cdot (r \times \mathbf{\nabla}) = -i \frac{\partial}{\partial \varphi},
\]
with the angle \( \varphi \) in the cylindrical system of coordinates. The statistical averages \( \langle \ldots \rangle_\omega \) in the rotating frame are taken with the Hamiltonian
\[
H_\omega \equiv H - \mathbf{\hat{\omega}} \cdot \mathbf{\hat{L}}.
\]
Then the average of an operator \( \mathbf{\hat{A}} \) is
\[
\langle \mathbf{\hat{A}} \rangle_\omega = \text{Tr} \hat{\rho}_\omega \mathbf{\hat{A}}, \quad \hat{\rho}_\omega \equiv \frac{e^{-\beta H_\omega}}{\text{Tr} e^{-\beta H_\omega}}.
\]
Thus the moment of inertia with respect to the rotation axis is
\[
I \equiv \lim_{\omega \to 0} \frac{\partial}{\partial \omega} \langle \mathbf{L}_z \rangle_\omega.
\]

Nontrivial response to the rotation boost arises, when the quantum moment of inertia differs from the classical one. This defines the superfluid fraction
\[
n_s \equiv 1 - \frac{l}{I_0},
\]
Invoking the formulas of parametric variation [1], we have
\[
\frac{\partial H_\omega}{\partial \omega} = -\mathbf{\hat{L}}_\omega, \quad \frac{\partial}{\partial \omega} \langle \mathbf{L}_z \rangle_\omega = \beta \text{var}(\mathbf{\hat{L}}_\omega).
\]
In an equilibrium non-rotating system,
\[
\lim_{\omega \to 0} \langle \mathbf{L}_z \rangle_\omega = 0.
\]
Then the moment of inertia (17) becomes
\[
I = \lim_{\omega \to 0} \frac{\partial}{\partial \omega} \langle \mathbf{L}_z \rangle_\omega = \beta \langle \mathbf{L}_z^2 \rangle.
\]
Here in the right-hand side, the average \( \langle \ldots \rangle \) is taken with respect to the Hamiltonian \( H \) of a system at rest, which leads to the expression
\[
\langle \mathbf{L}_z^2 \rangle = \int \langle \psi^*(r_1) \mathbf{L}_z(r_1) \psi(r_1) \psi^*(r_2) \mathbf{L}_z(r_2) \psi(r_2) \rangle dr_1 dr_2.
\]
In terms of density matrices, this can be written as
\[
\langle \mathbf{L}_z^2 \rangle = -\int \lim_{\gamma \to 1} \lim_{\gamma \to 0} \frac{\partial^2}{\partial \gamma \partial \gamma} \langle \psi^*(r_1) \mathbf{L}_z(r_1) \psi(r_1) \psi^*(r_2) \mathbf{L}_z(r_2) \psi(r_2) \rangle dr_1 dr_2.
\]
In this way, we come to the superfluid fraction
\[
n_s = 1 - \frac{\langle \mathbf{L}_z^2 \rangle}{I_0 T}.
\]
Note again that the Bose–Einstein statistics is not used in the derivation of the above formulas. Hence superfluidity is not prohibited for Fermi systems. The importance of pair correlations is also evident.

The response to the rotation boost is related to the response to the velocity boost, so that the previous definition (12) is equivalent to definition (19). To show this, let us take a cylindrical annulus of radius \( R \), width \( \delta \ll R \), height \( L \), and volume \( V \equiv 2\pi RL \delta \). Then the classical moment of inertia is \( I_0 \equiv mNR^2/2 \).

When \( R \to \infty \), then the elementary length, in the direction \( \mathbf{e}_y \) perpendicular to the radius, is \( dl = Ld\varphi \), so that
\[
\mathbf{L}_z(r) \equiv -iR \frac{\partial}{\partial l},
\]
and we get
\[
\langle \mathbf{L}_z^2 \rangle \approx R^2 \int \lim_{\gamma \to 1} \lim_{\gamma \to 0} \frac{\partial^2}{\partial \gamma \partial \gamma} \langle \rho(r_1, r_2) \delta(r_1 - r_2) + \rho^*(r_1, r_2, r_3, r_4) \rangle dr_1 dr_2.
\]
Therefore
\[
\langle \mathbf{L}_z^2 \rangle \approx R^2 \langle \mathbf{P}_f^2 \rangle,
\]
where \( \mathbf{P}_f \equiv \mathbf{e}_y \cdot \mathbf{\hat{P}}. \) As a result, the superfluid fraction (19) transforms into
\[
n_s \simeq 1 - \frac{\langle \mathbf{P}_f^2 \rangle}{mN T}.
\]
The same formula follows from the previous definition (12), if the velocity boost \( \mathbf{v} \) is taken along the direction \( \mathbf{e}_z \), when \( \mathbf{v} = \mathbf{v e}_z \).
2.3. Bose–Einstein condensation

Bose systems exhibit the phase transition of Bose–Einstein condensation. Before discussing the relation between Bose–Einstein condensation and superfluidity, let us study the peculiarities of the Bose condensation transition.

Historically, Bose–Einstein condensation was first considered for an ideal uniform Bose gas (see, e.g. [2, 3]). The non-interacting gas is described by the Hamiltonian

\[ H = \int \psi^*(r) \left( -\frac{\nabla^2}{2m} - \mu \right) \psi(r) \, dr. \]  

(21)

Assuming spinless particles and expanding the field operator over the plane waves,

\[ \psi(r) = \sum_k a_k \varphi_k(r), \quad \varphi_k(r) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}}, \]

we get

\[ H = \sum_k \omega_k a_k^\dagger a_k, \quad \omega_k = \frac{k^2}{2m} - \mu. \]  

(22)

The chemical potential \( \mu \) is defined from the normalization to the total number of particles

\[ N = \sum_k n_k, \]  

(23)

with the momentum distribution

\[ n_k = \langle a_k^\dagger a_k \rangle = (e^{\beta \omega_k} - 1)^{-1}. \]

The latter, by definition, is non-negative, \( n_k \geq 0 \), which requires that \( \omega_k \geq 0 \), hence \( \mu \leq 0 \). The dangerous point is where \( \min_k \omega_k = 0 \). If the minimum occurs at \( k = 0 \), then \( \mu = 0 \).

The behaviour of \( \mu \) with varying temperature is described by the derivatives

\[ \frac{\partial \mu}{\partial T} + \frac{\partial \mu}{\partial N} \frac{\partial N}{\partial T} = 0, \quad \frac{\partial \mu}{\partial T} = -\frac{\partial N/\partial T}{\partial N/\partial \mu}, \]

\[ \frac{\partial \mu}{\partial T} = -\frac{\sum_k \beta \omega_k n_k (1 + n_k)}{\sum_k n_k (1 + n_k)}, \quad \frac{\partial \mu}{\partial T} \leq 0. \]

This shows that \( \mu \) increases with decreasing \( T \), so that at a critical temperature \( T_c \) it touches zero, \( \mu = 0 \). Since \( \mu \) cannot be positive, it remains zero everywhere below the critical temperature, \( T \leq T_c \). To satisfy the normalization condition (23), in the sum for \( N \), it is necessary to separate the term \( N_0 \) corresponding to the number of condensed atoms. Then normalization (23) changes to

\[ N = N_0 + N_1, \quad N_i = \sum_{k=0} n_k. \]  

(24)

Therefore the total density is the sum of the density of condensed atoms \( \rho_0 \) and of the density of uncondensed atoms \( \rho_1 \):

\[ \rho = \rho_0 + \rho_1, \quad \rho_0 = \frac{N_0}{V}, \quad \rho_1 = \frac{N_1}{V}. \]  

(25)

Respectively, the fractions of condensed and uncondensed atoms satisfy the normalization condition

\[ n_0 + m_1 = 1, \quad n_0 \equiv \frac{N_0}{N_1}, \quad m_1 \equiv \frac{N_1}{N}. \]  

(26)

At the critical temperature \( T_c \), one has \( N_1 = N, \ N_0 = 0, \rho_0 = 0 \), and \( \rho_1 = \rho \). For a macroscopically large system with volume \( V \), it is admissible to replace the summation over momenta by the related integration, which in a three-dimensional space reads as

\[ \sum_k \longrightarrow V \int \frac{dk}{(2\pi)^3}. \]

Then the density of uncondensed atoms, coinciding at the critical temperature with the total atomic density, is

\[ \rho = \int n_k \frac{dk}{(2\pi)^3} \quad (T = T_c). \]

This yields

\[ \rho = \frac{4\pi}{(2\pi)^3} \int_0^\infty \frac{k^2dk}{\exp(\beta k^2/2m) - 1} = \frac{\pi}{4} \frac{2mT_c}{\pi^2} \Gamma \left( \frac{3}{2} \right) \left( \frac{3}{2} \right). \]  

(27)

Here \( \Gamma(x) \) is the gamma function

\[ \Gamma(x) \equiv \int_0^\infty t^{x-1}e^{-t} \, dt \quad (\text{Re} \, x > 0) \]

and \( \zeta(x) \) is the Riemann zeta function

\[ \zeta(x) = \frac{1}{\Gamma(x)} \int_0^\infty t^{x-1} \, dt = \sum_{n=1}^\infty \frac{1}{n^x} \quad (\text{Re} \, x > 1). \]

In particular, \( \Gamma(3/2) = \sqrt{\pi}/2 \) and \( \zeta(3/2) = 2.61238 \). This gives the critical temperature

\[ T_c = \frac{2\pi}{m} \left[ \frac{\rho}{\zeta(3/2)} \right]^{2/3}. \]  

(28)

The density of condensed atoms plays the role of the order parameter. Since this density, at the transition temperature, continuously deviates from zero, Bose–Einstein condensation is a second-order phase transition [1].

Bose–Einstein condensation is characterized by the arising macroscopic number of particles in a lowest single-particle state:

\[ N_0 \equiv \lim_{k \to 0} n_k, \quad N_0 \sim N. \]  

(29)

From the expression for \( n_k \), it follows that the appearance of a macroscopic number of particles in a single-particle quantum state can occur when the single-particle spectrum \( \omega_k \equiv \omega(k) \) touches zero at a point labelled by a momentum \( k_0 \):

\[ \omega(k_0) \equiv \min_k \omega(k) = 0. \]  

(30)

In general, \( k \) is a set of quantum numbers labelling single-particle quantum states \( \varphi_k \). When \( k \) is a momentum and \( k_0 = 0 \), then \( \mu = \omega(k) / 2m = 0 \).

Let us consider whether Bose–Einstein condensation can happen in other dimensions. In one-dimensional real space,
$d = 1$, the existence of a critical temperature $T_c$ would require that at this temperature

$$
\rho \equiv 2 \int_0^\infty n_k \frac{dk}{2\pi} = \frac{mT_c}{2\pi} \sqrt{\Gamma(1/2)\zeta(1/2)},
$$

where the representation $\Gamma(1/2) = \sqrt{\pi}$ is taken into account.

The representations for the Riemann $\zeta$ function, used above, assumed that its argument satisfies the condition $\text{Re} \ x > 1$. To define the function $\zeta(x)$ for $x < 1$, it is possible to resort to an analytical continuation of $\zeta(x)$ to the entire complex plane, except $x = 1$. This analytical continuation is

$$
\zeta(x) = \frac{1}{1-2^{1-x}} \sum_{n=0}^\infty \frac{1}{2^{n+1}} \sum_{m=0}^n \frac{(-1)^m C_n^m}{(1+m)^x},
$$

where the binomial coefficients are the combinations of $m$ from $n$,

$$
C_n^m \equiv \binom{n}{m} = \frac{n!}{(n-m)!m!}.
$$

From this analytical continuation, it follows that $\zeta(x) < 0$ for $x < 1$. For instance, $\zeta(1/2) = -1.460 35$. Since $\rho > 0$, but $\zeta(1/2) < 0$, the temperature $T_c$ does not exist. In one-dimensional space, there is no Bose condensation at any temperature.

Consider now the general case of a $d$-dimensional space. For macroscopically large systems, the summation over momenta is replaced as

$$
\sum_k \rightarrow V \int \frac{dk}{(2\pi)^d}.
$$

In spherical coordinates,

$$
dk \rightarrow \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1}dk,
$$

with $k \equiv |k|$. The system density is given by the integral

$$
\rho = \frac{2}{(4\pi)^{d/2}\Gamma(d/2)} \int_0^\infty n_k k^{d-1}dk.
$$

At $T = T_c$, when $\mu = 0$, we get

$$
\rho = \left(\frac{mT_c}{2\pi}\right)^{d/2} \zeta(d/2),
$$

which results in the critical temperature

$$
T_c = \frac{2\pi}{m} \left(\frac{\rho}{\zeta(d/2)}\right)^{2/d}.
$$

We know that for $d = 1$ there is no condensation at any temperature. For $d = 2$, we have $\Gamma(1) = 1$ and the $\zeta$ function behaves as

$$
\zeta(x) \approx \gamma + \frac{1}{x-1} \quad (x \rightarrow 1),
$$

where the Euler–Mascheroni constant $\gamma = 0.577 216$. Therefore $\zeta(x) \rightarrow \infty$ when $x \rightarrow 1 + 0$. This means that $T_c = 0$ for $d = 2$. Thus in a two-dimensional space, Bose–Einstein condensation can happen only at $T = 0$.

Finite condensation temperatures, for a uniform ideal Bose gas, exist only for spatial dimensions $d > 2$.

2.4. Condensation conditions

Bose–Einstein condensation can occur not only in an ideal Bose gas, but also in interacting systems. What would be general conditions for the possibility of this phenomenon? A reasonable expected condition of Bose–Einstein condensation is a low temperature, when the temperature wavelength

$$
\lambda_T \equiv \frac{2\pi}{\rho \lambda^3} \begin{cases}
\rho^3 \lambda^2 > 1 & \text{if } d = 1, 2,
\rho^3 \lambda^2 > 1 & \text{if } d > 2.
\end{cases}
$$

For example, in the case of a three-dimensional ideal Bose gas, considered in the previous section, $\rho^3 \lambda^2 = (3/2) = 2.612$. Since Bose–Einstein condensation implies a macroscopic occupation of a lowest single-particle energy level, while atomic interactions tend to disperse the particles over higher levels, one should expect that other conditions, favourable for Bose condensation, are connected with the weak influence of atomic interactions. Such a condition is the low-density condition, when the mean interatomic distance $a$ is larger than the effective radius of atomic interactions $r_0$, that is

$$
r_0 \ll 1, \quad \rho a^3 \ll 1.
$$

This condition should facilitate the appearance of condensate, but it is not compulsory.

The other condition that should facilitate the occurrence of Bose condensation is the condition of weak interactions, when the atomic scattering length $a_i$ is shorter than the mean distance $a$,

$$
\frac{|a_i|}{a} \ll 1, \quad \rho |a_i|^3 \ll 1.
$$

Let us emphasize that conditions (35) and (36) make the condensation easier. However, if they do not hold, it does not necessarily mean that the condensation is impossible. Just it may happen at a lower temperature and the condensate fraction will be smaller.

The mathematical formalization of condensation conditions can be done in several ways. The first evident condition is the Bose–Einstein condition requiring that the number of condensed particles $N_0 = \langle a_0^2 a_0 \rangle$ be macroscopic. This means that in thermodynamic limit it should be:

$$
\lim_{N \rightarrow \infty} \frac{N_0}{N} > 0.
$$

Note that for finite systems $N_0 \sim N$ and the phase transition becomes a crossover [1].
A general condition of Bose condensation was formulated by Penrose and Onsager [4]. They clarified what has to be understood as single-particle states. The latter are defined as the eigenstates of the eigenproblem
\[ \int \rho(r', r') \varphi_k(r') \, dr' = n_k \varphi_k(r) \tag{38} \]
for the single-particle density matrix \( \rho(r, r') \equiv \langle \psi^\dagger(r') \psi(r) \rangle \). Generally, \( k \) is a set of quantum numbers labelling the single-particle states. The field operators can be expanded over the basis of these states,
\[ \psi(r) = \sum_k a_k \varphi_k(r). \]
The density matrix is representable as the expansion
\[ \rho(r, r') = \sum_k n_k \varphi_k(r) \varphi_k^\dagger(r'), \tag{39} \]
where \( n_k = \langle a_k^\dagger a_k \rangle \). The eigenstates \( \varphi_n(r) \) of the single-particle density matrix, allowing for the diagonal expansion (39), are called natural orbitals [5].

The Penrose–Onsager condition tells us that Bose condensation occurs, when the largest eigenvalue of the density matrix is macroscopic, that is when
\[ N_0 \equiv \sup_k n_k \sim N. \tag{40} \]
This largest eigenvalue is identified with the number of condensed atoms. Then expansion (39) can be written in the form
\[ \rho(r, r') = N_0 \varphi_0(r) \varphi_0^\dagger(r') + \sum_{k=0}^{N_0} n_k \varphi_k(r) \varphi_k^\dagger(r'). \tag{41} \]

The Yang criterion of condensation [6]
\[ \lim_{|r-r'| \to \infty} \rho(r, r') = \rho_0 > 0 \tag{42} \]
requires the existence of the off-diagonal long-range order, with the limit \( \rho_0 \) being the condensate density. This is a good criterion for uniform systems, when
\[ \varphi_0(r) = \frac{1}{\sqrt{V}}, \quad \rho(r, r') \longrightarrow \frac{N_0}{V} = \rho_0. \]
But the Yang criterion is not suitable for finite and for nonuniform systems. This is because for a confined system \( \varphi_k(r) \to 0 \) as \( r \to \infty \). Hence the limit \( \rho(r, r') \to 0 \) for \( |r - r'| \to \infty \).

Quantification of the order, arising under the Bose–Einstein condensation, can be conveniently done with the help of the order indices [5, 7]. For this purpose, we can consider
\[ \hat{\rho}_n = [\rho_n(r_0, \ldots, r_n, r_0', \ldots, r_n')] \]
as a matrix with the elements
\[ \rho_n(r_0, \ldots, r_n, r_0', \ldots, r_n') = \langle \psi^\dagger(r_n') \ldots \psi^\dagger(r_0') \psi(r_n) \ldots \psi(r_0) \rangle. \]
The order index of the matrix \( \hat{\rho}_n \) is defined as
\[ \omega(\hat{\rho}_n) = \frac{\ln ||\hat{\rho}_n||}{\ln |\text{Tr} \hat{\rho}_n|}. \tag{43} \]
Here \( || \cdot || \) means an operator norm. For a semipositive matrix, \( ||\hat{\rho}_n|| \leq |\text{Tr} \hat{\rho}_n| \). Then \( \omega(\hat{\rho}_n) \leq 1 \). For a large number of atoms \( N \gg 1 \), one has \( \ln \text{Tr} \hat{\rho}_n \approx n \ln N \). Keeping in mind the Hermitian norm gives \( ||\hat{\rho}_n|| = N_0 \) and \( ||\hat{\rho}_n|| \sim N_0^n \), which is correct if there exists \( N_0 \gg 1 \).

In the case of a finite system,
\[ \omega(\hat{\rho}_n) = \frac{\ln N_0}{\ln N}. \tag{44} \]
This tells us that \( N_0 = N^{\omega(\hat{\rho}_n)} \).

With the help of the order indices, it is straightforward to classify different types of order. Thus, when \( \omega(\hat{\rho}_n) < 0 \), there is no order. If \( \omega(\hat{\rho}_n) = 0 \), there can be short-range order. When \( 0 < \omega(\hat{\rho}_n) < 1 \), there occurs mid-range order. And for \( \omega(\hat{\rho}_n) = 1 \), long-range order is present. This classification suits for any system.

Bogolubov [8, 9] connected Bose condensation with global gauge symmetry breaking. He noticed that in the field-operator expansion
\[ \psi(r) = \sum_k a_k \varphi_k(r), \]
one can separate out the condensate term getting
\[ \psi(r) = a_0 \varphi_0(r) + \psi_1(r), \quad \psi_1(r) \equiv \sum_{k=0}^{N_0} a_k \varphi_k(r). \]

In thermodynamic limit, the first operator term in \( \psi(r) \) can be replaced by a function,
\[ a_0 \varphi_0(r) \longrightarrow \eta(r). \]
Equivalently, it is possible to employ the Bogolubov shift
\[ \psi(r) = \eta(r) + \psi_1(r), \tag{45} \]
where \( \eta(r) \) plays the role of a condensate wave function normalized to the number of condensed atoms
\[ N_0 = \int |\eta(r)|^2 \, dr. \]
The condition of quantum-number conservation requires that
\[ \langle \psi_1(r) \rangle = 0. \tag{46} \]
The condensate wave function
\[ \eta(r) = \langle \psi(r) \rangle = \langle \eta(r) + \psi_1(r) \rangle \tag{47} \]
is zero in the normal thermodynamic phase and becomes non-zero after Bose condensation, when \( N_0 > 0 \). That is, the condensate wave function can be treated as an order parameter.

The Bogolubov shift (45) leads to global gauge symmetry breaking. However this does not contradict to the experimental setup, where the average number of atoms is conserved [10].

2.5. Uncondensed gas
The properties of the ideal Bose gas above the condensation temperature have been described in many publications [11–16]. For completeness, we give here a brief account of the results related to the ideal Bose gas, which can be useful in the following.

An important notion in characterizing Bose gas is the Bose–Einstein integral function
\[ g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{z u^{n-1}}{e^u - z} \, du. \]  
(48)

This function is finite for \( n \geq 0 \), while diverges for \( n < 0 \), if \( z < 1 \). It is such that \( g_0(z) \equiv 0 \), when \( z \leq 1 \). And \( \Gamma(n) \equiv 1/n \), if \( n \to 0 \).

In applications, \( z \) denotes the fugacity
\[ z \equiv e^\beta \mu. \]  
(49)

And the dimensionless variable \( u \equiv \beta k^2/2m \) is used. Then, since \( \omega_k = k^2/2m - \mu \), one has \( e^{\beta \omega_k} = e^{\beta \mu} \).

Differentiating and integrating by parts yields the relation
\[ \frac{\partial}{\partial z} g_n(z) = \frac{1}{z} g_{n-1}(z), \]
valid for all \( n \).

If \( |z| \leq 1 \), then the Bose–Einstein function can be written as
\[ g_n(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^n} \quad (|z| \leq 1, n > 0). \]

For \( \text{Re } n > 1 \), it is called the polylogarithmic function. And
\[ g_n(1) = \zeta(n) \quad (n > 1). \]

In low orders, one has
\[ g_0(z) = \frac{z}{z-1}, \quad g_1(z) = -\ln(1 - z) \quad (|z| < 1). \]

When approaching the condensation temperature from above, \( \mu \to 0 \) and \( z \to 1 \). Then the quantity
\[ \alpha \equiv -\ln z = -\beta \mu \]
tends to zero. The derivative with respect to fugacity can be transformed into
\[ \frac{\partial}{\partial \alpha} g_n(e^{-\alpha}) = -g_{n-1}(e^{-\alpha}). \]

There exists the Robinson representation
\[ g_n(e^{-\alpha}) = \Gamma(1-n)\alpha^{n-1} + \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} (\zeta(n-j)\alpha^j) \]  
(50)

that is valid for all \( n \) on the complex plane, except integers \( n = 1, 2, 3, \ldots \), since the values of \( \Gamma(0), \Gamma(-1), \Gamma(-2) \), etc diverge. This representation is especially convenient when \( \alpha \to 0 \).

For integer \( n \), one has
\[ g_n(e^{-\alpha}) = (-1)^{n-1} \alpha^{n-1} \left( \sum_{j=0}^{n-1} \frac{1}{j!} (\zeta(n-j)\alpha^j) \right) + \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} (\zeta(n-j)\alpha^j) \]  
\( (n = 1, 2, 3, \ldots) \),

with
\[ \lim_{n \to 1} \frac{1}{n!} \sum_{j=1}^{n-1} \zeta(n-j) \alpha^j = 0. \]

From here \( g_n(1) = \zeta(n) \) for \( n > 1 \).

Using the Robinson representation and the values
\[ \Gamma\left(\frac{3}{2}\right) = \frac{4\sqrt{\pi}}{3}, \quad \Gamma\left(-\frac{1}{2}\right) = -2\sqrt{\pi}, \quad \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \]

\[ \zeta\left(\frac{1}{2}\right) = -1.46035, \quad \zeta\left(\frac{3}{2}\right) = 2.61238, \quad \zeta\left(\frac{5}{2}\right) = 1.34149, \]

for \( z \to 1 \), one gets
\[ g_{3/2}(z) \approx \Gamma\left(-\frac{3}{2}\right) \alpha^{3/2} + \zeta\left(\frac{3}{2}\right), \]
\[ g_{3/2}(z) \approx \Gamma\left(-\frac{1}{2}\right) \alpha^{1/2} + \zeta\left(\frac{3}{2}\right), \]
\[ g_{3/2}(z) \approx \Gamma\left(\frac{1}{2}\right) \alpha^{-1/2} + \zeta\left(\frac{3}{2}\right). \]

Above the condensation temperature, \( T > T_c \), when \( n_0 = 0 \), one has
\[ N = \frac{2V}{\sqrt{\pi} \lambda_T^2} \int_0^\infty \frac{z \sqrt{u} \, du}{e^u - z} = \frac{V}{\lambda_T^2} g_{3/2}(z), \]

which defines \( \mu \). This can be rewritten in the compact form
\[ \rho \lambda_T^3 = g_{3/2}(z). \]  
(51)

At high temperatures \( T > T_c \), where \( z \ll 1 \), we get \( g_n(z) \approx z \) and \( z \approx \rho \lambda_T^3 \). Then \( \mu \approx T \ln(\rho \lambda_T^3) \). In the limit \( T \to \infty \), one has \( \rho \lambda_T^3 \to 0 \), hence \( \mu \to -\infty \).

Close to the condensation temperature, when \( T \to T_c \), with \( z \to 1 \), and \( \alpha \to +0 \), the use of the Robinson representation for \( g_{3/2}(z) \) gives
\[ \rho \lambda_T^3 \approx -2\sqrt{\pi} \alpha^{1/2} + \zeta\left(\frac{3}{2}\right), \]  
(52)

where \( \lambda_T = \sqrt{2\pi/mT} \). Taking into account that
\[ \rho \lambda_T^3(T_c) = \zeta\left(\frac{3}{2}\right), \]

it is also possible to write
\[ \rho \lambda_T^3 \approx \zeta\left(\frac{3}{2}\right) \left(\frac{T_c}{T}\right)^{3/2}, \]  
(53)

Also, since
\[ \alpha^{1/2} \approx \zeta(3/2) \left[ 1 - \left(\frac{T_c}{T}\right)^{3/2} \right], \]

and \( \alpha = -\beta \mu \), we find
\[ \mu \approx -T \zeta(3/2) \left[ 1 - \left(\frac{T_c}{T}\right)^{3/2} \right]^2. \]  
(54)

This shows that \( \mu \to -0 \) as \( T \to T_c + 0 \).
The grand potential $\Omega = -PV$ defines the pressure
\[ P = -T \int \ln(1 - e^{-\beta a}) \frac{dk}{(2\pi)^3} = T \frac{\rho_0}{\lambda_T^3} g_{1/2}(z). \]  \hfill (55)

For high temperatures, we find the virial expansion,
\[ P = \rho T \sum_{n=0}^{\infty} a_n (\rho \lambda_T^3)^n \]  \hfill (56)

that is useful for $\rho \lambda_T^3 \ll 1$. The low virial coefficients are
\[ a_0 = 1, \quad a_1 = -\frac{1}{4\sqrt{2}}, \quad a_2 = -\left(\frac{2}{9\sqrt{3}} - \frac{1}{8}\right). \]

At very high temperatures ($T \gg T_c$) one has $P \approx \rho T$.

It is straightforward to derive other thermodynamic quantities above $T_c$, such as energy $E$, entropy $S$, and specific heat $C_V$, for which we find
\[ \frac{E}{N} = \frac{3T}{2\rho \lambda_T^3} g_{1/2}(z), \quad \frac{S}{N} = \frac{5}{2\rho \lambda_T^3} g_{1/2}(z) - \ln z, \]
\[ PV = \frac{2}{3} E, \quad C_V = \frac{15}{4\rho \lambda_T^3} g_{1/2}(z) - \frac{9\rho \lambda_T^3}{4g_{1/2}(z)}. \]  \hfill (57)

At $T = T_c$, when $z = 1$, then $g_{1/2}(1)$ diverges and the specific heat becomes
\[ C_V(T_c) = \frac{15(5/2)}{4\zeta(3/2)} \approx 1.925. \]

For all temperatures $T \geq T_c$, a good approximation for the specific heat, following from the expansion of $g_{1/2}(e^{-\alpha})$ and using $\alpha$ above $T_c$, is
\[ C_V \approx 1.496 + 0.341 \left(\frac{T_c}{T}\right)^{3/2} + 0.089 \left(\frac{T_c}{T}\right)^{5/2}. \]  \hfill (58)

This expression is exact at $T_c$ and is accurate within an error of 1% for all $T \geq T_c$, with the limit $\lim_{T \to \infty} C_V = 3/2$.

The isothermal compressibility is
\[ \kappa_T = \frac{1}{\rho N} \left(\frac{\partial N}{\partial \mu}\right)_{TV} = \frac{1}{\rho} \left(\frac{\partial^2 P}{\partial \mu^2}\right)_{TV} = \frac{\beta}{\rho^2 \lambda_T^3} g_{1/2}(z). \]  \hfill (59)

At high temperature $T \gg T_c$, when $z \ll 1$,
\[ \kappa_T \approx \frac{1}{\rho T} \quad (T \gg T_c). \]  \hfill (60)

While in the vicinity of the condensation point, where $z \sim 1$ and $g_{1/2}(e^{-\alpha}) \approx \sqrt{\pi} \alpha^{-1/2}$, the compressibility is
\[ \kappa_T \approx 0.921 \frac{\rho T}{\lambda_T^3} \left[1 - \left(\frac{T_c}{T}\right)^{3/2}\right]^{-1}, \]  \hfill (61)

which diverges at $T_c$.

We should not expect that the normal gas above the condensation temperature could exhibit superfluidity. But it is instructive to demonstrate this explicitly. To this end, we need to find $\langle \hat{P}^2 \rangle$. Applying to the average
\[ \langle \hat{n}_i \hat{n}_p \rangle = \langle \alpha_i^\dagger \alpha_p^\dagger \alpha_q \alpha_p \rangle + \delta_{qp}(\alpha_i \alpha_k) \]

the Wick theorem gives
\[ \langle \hat{n}_i \hat{n}_p \rangle = \delta_{qp} \rho \rho (1 + \rho) + \rho \rho^2. \]

In equilibrium,
\[ \langle \hat{P} \rangle = \sum_k k n_k = 0. \]

And we obtain
\[ \langle \hat{P}^2 \rangle = \sum_k k^2 n_k (1 + n_k) = \frac{8\sqrt{\pi}}{\lambda_T^3} \nu \int_0^\infty \frac{z d^{1/2} e^u}{(e^u - z)^2} du. \]

Then we use the integrals
\[ \int_0^\infty \frac{u^{1/2} e^u}{(e^{u} - z)^2} du = -\lim_{\lambda \to 1} \frac{d}{d\lambda} \int_0^\infty \sqrt{\lambda} \frac{du}{e^u - z}, \]
\[ \int_0^\infty \frac{u^{1/2} e^u}{e^u - z} du = \frac{1}{\lambda^{3/2}} \int_0^\infty \frac{du}{e^u - z}, \]
\[ \int_0^\infty \frac{u^{1/2} e^u}{(e^u - z)^2} du = \frac{3}{2} \int_0^\infty \frac{du}{e^u - z}. \]

As a result, we come to the value
\[ \langle \hat{P}^2 \rangle = \frac{6\pi}{\lambda_T^3} g_{1/2}(z) V = 3mTN. \]

Therefore
\[ n_s = 1 - \frac{\langle \hat{P}^2 \rangle}{3mTN} = 0, \]

which means that there is no superfluidity above $T_c$.

### 2.6. Condensed gas

Below the condensation temperature, the chemical potential of the ideal Bose gas $\mu \to -0$ and the fugacity $z \to 1$. The total number of atoms is the sum $N = N_0 + N_1$ of the number of condensed atoms
\[ N_0 = (e^{-\beta_0} - 1)^{-1} = \frac{z}{1 - z} \quad (\mu \to -0) \]

and the number of uncondensed atoms
\[ N_1 = \frac{V}{\lambda_T^3} g_{1/2}(1). \]

The chemical potential, for large $N_0$, tends to zero as
\[ \mu \to -T \ln \left(1 + \frac{1}{N_0}\right) \to -0. \]

The fractions of condensed and uncondensed atoms, respectively, are
\[ n_0 = 1 - \left( \frac{T}{T_c} \right)^{3/2}, \quad n_1 = \left( \frac{T}{T_c} \right)^{3/2}. \] (62)

Taking into account that \( g_r(1) = \zeta(n) \) for \( n > 1 \), we have
\[ \rho \lambda^3 T = \left( \frac{3}{2} \right) \left( \frac{T_c}{T} \right)^{3/2}. \] (63)

For the pressure, energy, entropy, and specific heat, we find
\[ P = \frac{\zeta(5/2)}{\zeta(3/2)} \rho T_c \left( \frac{T}{T_c} \right)^{5/2}, \quad E = \frac{3\zeta(5/2)}{2\zeta(3/2)} \rho T_c \left( \frac{T}{T_c} \right)^{5/2}, \]
\[ S/N = \frac{5\zeta(5/2)}{2\zeta(3/2)} \left( \frac{T}{T_c} \right)^{3/2}, \quad C_V = 15\zeta(5/2) \left( \frac{T}{T_c} \right)^{3/2}. \] (64)

At the critical temperature, the specific heat displays the jump in the value,
\[ C_V(T_c - 0) - C_V(T_c + 0) = 1.925, \]
and in the derivative,
\[ \left( \frac{\partial C_V}{\partial T} \right)_{T_c - 0} - \left( \frac{\partial C_V}{\partial T} \right)_{T_c + 0} = \frac{27\zeta^2(3/2)}{16\pi T_c} = 3.666. \]

To find the superfluid fraction, we need to calculate \( \langle \hat{p}^2 \rangle = 3mT N_0 \). As a result, we obtain
\[ n_s = 1 - n_1 = 1 - \left( \frac{T}{T_c} \right)^{3/2}. \] (65)

It turns out that for an ideal Bose gas, \( n_s = n_0 \). That is, the Bose–Einstein condensate of an ideal gas is totally superfluid. However, the Landau criterion of superfluidity does not hold, since
\[ \min \frac{\omega_k}{k} = 0, \]
while this limit should be positive.

Moreover, the compressibility exhibits anomalous behaviour. For the latter, we have
\[ \kappa_T = \frac{1}{\rho N} \frac{\partial N}{\partial \mu} = \frac{1}{\rho N} \left( \frac{\partial N_0}{\partial \mu} + \frac{\partial N_1}{\partial \mu} \right) \]
with the relations
\[ \text{var}(\hat{N}_0) = T \frac{\partial N_0}{\partial \mu}, \quad \text{var}(\hat{N}_1) = T \frac{\partial N_1}{\partial \mu}. \]

Therefore the compressibility can be written as
\[ \kappa_T = \frac{1}{\rho T N} \left[ \text{var}(\hat{N}_0) + \text{var}(\hat{N}_1) \right]. \]

For the derivatives of the numbers of particles, we have
\[ \frac{\partial N_0}{\partial \mu} = \beta N_0 (1 + N_0), \quad \frac{\partial N_1}{\partial \mu} = \frac{\beta N_1}{\rho \lambda_T} g_{1/2}(z) \quad (z \rightarrow 1). \]

Here we confront the problem, since the value \( g_{1/2}(1) \) diverges. Strictly speaking, this divergence is caused by thermodynamic limit. In order to avoid the divergence, we have to consider a finite system possessing a minimal energy \( k_{\text{min}}^2 / 2m \).

For a system in a box, it is admissible to take the minimal wave vector
\[ k_{\text{min}} = \frac{\pi}{L}, \quad (L^3 = V). \] (66)

Then we can define [17] the modified Bose–Einstein functions, where the integration starts not from zero, but from a minimal value
\[ \mu_{\text{min}} = \frac{\beta k_{\text{min}}^2}{2m} = \frac{\pi^2 \beta}{4L^2}. \] (67)

In particular, the modified function \( g_{1/2}(1) \) becomes
\[ g_{1/2}(1) = \frac{1}{\sqrt{\pi}} \int_{\mu_{\text{min}}}^{\infty} \frac{u^{-1/2}}{e^u - 1} \, du. \]

This yields
\[ \hat{g}_{1/2}(1) = \frac{1}{\sqrt{\pi}} \int_{\mu_{\text{min}}}^{\infty} \frac{du}{u^{3/2}} = \frac{2}{\sqrt{\pi} \mu_{\text{min}}}. \]

In view of the minimal value (67), one has
\[ \hat{g}_{1/2}(1) = \frac{4L}{\pi \lambda_T}. \]

Taking into account
\[ \frac{\partial \hat{N}_1}{\partial \mu} = \frac{m^2 T}{\pi^3} V^{4/3}, \]
we get
\[ \text{var}(\hat{N}_1) = m^2 T^2 / \pi^3 V^{1/3}. \]

In this way, the compressibility is
\[ \kappa_T = \frac{\text{var}(\hat{N}_1)}{\rho T N} = \frac{m^2 T^2}{\pi^5} V^{1/3}. \] (68)

If one assumes the occurrence of Bose condensation, so that \( N_0 \propto N \), but without gauge symmetry breaking, then \( \text{var}(\hat{N}_0) \propto N^2 \). These fluctuations are, of course, thermodynamically anomalous, and such a system cannot be stable [1], since \( \kappa_T \propto N \). This is what one names the ‘grand canonical catastrophe’. However, here there is no any catastrophe, but there is just a simple mistake of describing a Bose-condensed system without gauge symmetry breaking. Breaking the latter makes the condensate fluctuations effectively zero. Using the Bogolubov shift implies that \( \text{var}(\hat{N}_0) = 0 \).

Nevertheless, even breaking gauge symmetry, one has \( \text{var}(\hat{N}_1) \propto N^{1/3} \), which means thermodynamically anomalous fluctuations, as far as the compressibility \( \kappa_T \propto \text{var}(\hat{N}_1) / N \) diverges as \( \kappa_T \propto N^{1/3} \). This tells us that the condensed ideal Bose gas is a pathological object that cannot exist in nature.

It is worth emphasizing that it is not the grand canonical ensemble that is guilty for the divergence of \( \text{var}(\hat{N}_1) \), but the same happens in the canonical ensemble, where also \( \text{var}(\hat{N}_1) \propto N^{1/3} \). On the other hand, making the formal analytic continuation \( g_{1/2}(1) \rightarrow \zeta(1/2) \), with \( \zeta(1/2) = -1.46035 \), leads to a negative \( \kappa_T \), that is, again to instability.
In this way, the sole conclusion is that the ideal uniform Bose-condensed gas is an unstable object. Fortunately, any real gas possesses atomic interactions, although they can be weak, but not exactly zero. And, as will be shown in the following sections, atomic interactions can stabilize the Bose-condensed gas.

2.7. Superfluidity and condensation

As we have seen above, in the ideal Bose gas, the condensate and superfluid fractions are identical. Generally, this does not need to be always so. Moreover, the phenomena of condensation and superfluidity can exist separately from each other. To illustrate this, let us consider a simple case, where the particle distribution has the form \( n_k = (e^{\omega_k} - 1)^{-1} \), with an effective spectrum

\[
\omega_k = Ak^n - \mu. \tag{69}
\]

A \( d \)-dimensional space is assumed. The spectrum can differ from \( k^2/2m \) because of interactions or external fields. The superfluid fraction in a \( d \)-dimensional space is given by the formula

\[
n_s = 1 - \frac{\langle \hat{P}^2 \rangle}{mTNd}. \tag{70}
\]

For any \( \omega_k \), we have

\[
\frac{\partial n_k}{\partial \omega_k} = -\beta n_k (1 + n_k), \quad \langle \hat{P}^2 \rangle = -TV \int k^{d-1} \frac{\partial \omega_k}{\partial \omega_k} \frac{dk}{(2\pi)^d}.
\]

When the system is uniform and isotropic, the replacement

\[
\frac{dk}{(2\pi)^d} \rightarrow \frac{2k^{d-1}dk}{(4\pi)^{d/2}\Gamma(d/2)}
\]

is valid, which gives

\[
\langle \hat{P}^2 \rangle = TV \int n_k \frac{\partial \omega_k}{\partial \omega_k} \frac{k^{d+1}}{(2\pi)^d},
\]

where \( \omega_k \equiv \partial \omega_k/\partial k \).

Under the effective spectrum (69),

\[
\frac{\langle \hat{P}^2 \rangle}{V} = \frac{d+2-n}{nA} \int n_k k^{2-n} \frac{dk}{(2\pi)^d}.
\]

For any \( d \), if \( n \rightarrow 2 \) and \( A \rightarrow 1/2m \), then \( \langle \hat{P}^2 \rangle \rightarrow mTNd \), and \( n_s \rightarrow 0 \).

But generally, for the given effective spectrum, we have

\[
\frac{\langle \hat{P}^2 \rangle}{V} = \frac{2(d+2-n)\Gamma(d+2-n)/n}{(4\pi)^{d/2}\Gamma(d/2)n^2(A/\beta)^{d+2/n}} g_{d+2-n}(z),
\]

with the fugacity \( z \) and, respectively, the chemical potential \( \mu = \mu(T) \) defined by the equation

\[
\rho = \frac{2\Gamma(d/n)g_{d,0}(z)}{(4\pi)^{d/2}\Gamma(d/2)n(\beta A)^{d/n}}.
\]

Bose–Einstein condensation can happen at the temperature

\[
T_c = A \left[ \frac{(4\pi)^{d/2}\Gamma(d/2)n\rho}{2\Gamma(d/n)\zeta(d/n)} \right]^{1/d}. \tag{71}
\]

Since \( \Gamma(x) > 0 \) for \( x > 0 \), the condensation temperature \( T_c \) does not exist for \( d < n \). It is zero, \( T_c = 0 \), for \( d = n \), and \( T_c > 0 \) when \( d > n \). The condensate fraction is

\[
n_0 = 1 - \left( \frac{T}{T_c} \right)^{dn} \quad (T \leq T_c). \tag{72}
\]

In the presence of the condensate, the superfluid fraction reads as

\[
n_s = 1 - Bg_s \left( \frac{d+2-n}{n} \right)^{T(d+2-n)/n}, \tag{73}
\]

where

\[
B = \frac{2(d+2-n)\Gamma(d+2-n)/n}{(4\pi)^{d/2}\Gamma(d/2)n^2(\beta A)^{d+2/n}d^d}.
\]

As is seen, in general, \( n_s \) does not coincide with \( n_0 \). The superfluid fraction \( n_s \) coincides with the condensate fraction \( n_0 \) only for \( n = 2 \) and \( A = 1/2m \).

But, in principle, superfluidity can exist without condensation. Then the superfluid fraction is given by the expression

\[
n_s = 1 - Bg_{d+2-n}(z)^{T(d+2-n)/n}. \tag{74}
\]

Thus, Bose–Einstein condensation can exist without superfluidity. And superfluidity can occur without Bose–Einstein condensation. The possibility for the occurrence of superfluidity without Bose condensation and vice versa can be understood remembering that these phenomena are due to different causes. Bose–Einstein condensation happens if and only if global gauge symmetry is broken. While superfluidity does not require broken gauge symmetry, while requires the existence of strong pair correlations. Strictly speaking, Bose–Einstein condensation is neither a necessary nor sufficient condition for superfluidity.

Treating the condensate, \( n_0 \), and superfluid, \( n_s \), fractions as order parameters, generally, it is admissible to have four possibilities corresponding to four different phases:

(i) uncondensed non-superfluid phase,

\[
n_0 = 0, \quad n_s = 0,
\]

(ii) Bose-condensed non-superfluid phase,

\[
n_0 > 0, \quad n_s = 0,
\]

(iii) uncondensed superfluid,

\[
n_0 = 0, \quad n_s > 0,
\]

(iv) Bose-condensed superfluid,

\[
n_0 > 0, \quad n_s > 0.
\]

2.8. Bogolubov shift

It has been mentioned above that Bose–Einstein condensation implies global gauge symmetry breaking that can be realized by means of the Bogolubov shift for the field operator. In the
in the present section, the physical meaning of this shift is explained in more details.

For the beginning, let us keep in mind a uniform system, as has been done by Bogolubov \[8, 9, 18, 19\]. For a uniform system, the field operator can be expanded over the plane waves,

\[ \varphi_0(r) = \frac{1}{\sqrt{V}} \]

The operators in the momentum representation satisfy the commutation relations

\[ [a_k, a_p^\dagger] = 0, \quad [a_k, a_p] = \delta_{kp}. \]

In the field-operator expansion, it is possible to separate out the zero-momentum term, getting

\[ \psi(r) = \psi_0 + \psi_1(r), \quad (75) \]

where

\[ \psi_0 \equiv \frac{a_0}{\sqrt{V}}, \quad \psi_1(r) \equiv \sum_{k=0} a_k \varphi_k(r). \]

The zero-momentum term is assumed to correspond to Bose-condensed atoms, while the second term, to uncondensed atoms.

The number-of-particle operators of condensed and uncondensed atoms, respectively, are

\[ \hat{N}_0 = \int \psi_0^\dagger(r) \psi_0(r) dr = \sum_{k=0} a_k^\dagger a_k, \quad \hat{N}_1 = \int \psi_1^\dagger(r) \psi_1(r) dr = \sum_{k=0} a_k^\dagger a_k, \quad (76) \]

The field operators of condensed and uncondensed atoms are orthogonal to each other,

\[ \int \psi_0^\dagger(r) \psi_1(r) dr = 0, \]

since

\[ \sum_{k=0} a_k \int \varphi_0^\dagger(r) \varphi_k(r) dr = \sum_{k=0} a_k \delta_{k0} = 0. \]

Therefore the total number-of-particle operator is the sum

\[ \hat{N} = \hat{N}_0 + \hat{N}_1. \]

For the operators of condensed atoms, we have the commutation relations

\[ [a_0, a_0^\dagger] = 1, \quad \langle \psi_0, \psi_0^\dagger \rangle = \frac{1}{V}. \]

Bose–Einstein condensation implies a microscopic occupation of the lowest single-particle state, \( N_0 = \langle a_0^\dagger a_0 \rangle \sim N \). Therefore

\[ \frac{[a_0, a_0^\dagger]}{\langle a_0^\dagger a_0 \rangle} = \frac{1}{N_0} \ll 1. \]

This shows that the commutator \([a_0, a_0^\dagger] = 1\) is negligible as compared to the number of atoms \( N \). On the contrary \( n_k = \langle a_k^\dagger a_k \rangle \sim 1 \), or even much smaller, \( n_k \ll 1 \). Because of this the expression

\[ \frac{[a_k, a_k^\dagger]}{\langle a_k^\dagger a_k \rangle} = \frac{1}{N_0} \ll 1. \]

is of order 1 or even much larger than 1.

The commutator of uncondensed atoms

\[ \langle \psi_0, \psi_0^\dagger \rangle = \sum_{k=0} \varphi_k^\dagger(r) \varphi_k(r), \]

in thermodynamic limit, is close to the commutator

\[ \langle \psi_0, \psi_0^\dagger \rangle = \langle \psi^\dagger_1, \psi_1 \rangle = \frac{1}{V} + \sum_{k=0} \varphi_k^\dagger(r) \varphi_k(r) = \delta(r - r'). \]

The above properties demonstrate that, in thermodynamic limit, the operator \( a_0 \) can be treated as a number, together with the operator \( \psi_0 \). Thus, in thermodynamic limit, the following replacements are admissible: \( \psi_0 \rightarrow \eta \) and \( |\eta|^2 = \rho_0 \), with \( a_0 \rightarrow \sqrt{N_0} \). Summarizing, for the field operator \( \psi(r) \), one can use the Bogolubov shift

\[ \psi(r) \rightarrow \eta(r) + \psi(r), \quad (77) \]

The first term is called the \textit{condensate wave function}. And the second term corresponds to the field operator of uncondensed atoms. This shift is valid for non-uniform systems as well. In the case of a uniform system, \( \eta(r) \) becomes a constant \( \eta \).

The Bogolubov shift breaks global gauge symmetry. Another method of gauge symmetry breaking is by introducing infinitesimal sources \[1\]. The method of gauge symmetry breaking by means of infinitesimal sources is equivalent to the Bogolubov shift. This is illustrated below by a simple model with the Hamiltonian

\[ H = \sum_k \omega_k a_k^\dagger a_k, \]

in which \( \omega_k \geq 0 \) is arbitrary, and \( k \) is a multi-index labelling quantum microstates. It is easy to see that

\[ \langle a_k^\dagger a_k \rangle = (e^{i\omega_k} - 1)^{-1}, \quad \langle a_k^\dagger a_0 \rangle = (e^{i\omega_0} - 1)^{-1}, \]

where \( \omega_0 \equiv \inf \omega_k \). The criterion for the condensate existence is

\[ \lim_{N \to \infty} \frac{\langle a_k^\dagger a_0 \rangle}{N} > 0. \]

This means that \( \omega_0 \rightarrow 0 \) as \( N \rightarrow \infty \). Therefore

\[ \langle a_k^\dagger a_0 \rangle \simeq \frac{T}{\omega_0} (\omega_0 \rightarrow 0). \]

To break the gauge symmetry by an infinitesimal source, one adds to the system Hamiltonian a small term, thus defining

\[ H_\varepsilon \equiv H - \varepsilon \sqrt{N_0} (a_0^\dagger + a_0). \]

The latter Hamiltonian is not gauge-invariant with respect to \( a_0 \). It can be diagonalized by the canonical transformation

\[ a_0 = b_0 + \frac{\varepsilon}{\omega_0} \sqrt{N_0}. \]
In terms of the new field operators, the Hamiltonian is diagonal,

\[ H = \omega_0 b_0^\dagger b_0 + \sum_{k=0} \omega_k a_k^\dagger a_k = \frac{\epsilon^2}{\omega_0} N_0. \]

This new Hamiltonian is gauge-invariant with respect to \( b_0 \) and \( a_k \), where \( k \neq 0 \).

Denoting by \( \langle \ldots \rangle \) the statistical averages with respect to \( H \), we find

\[ \langle b_0^\dagger b_0 \rangle = \langle b_0^0 b_0 \rangle = 0, \quad \langle b_0^1 b_0 \rangle = (e^{i\omega_0} - 1)^{-1}, \]

\[ \langle a_0^\dagger a_0 \rangle = \langle a_0^0 a_0 \rangle. \]

and

\[ \langle a_k \rangle = 0 \quad (k \neq 0), \quad \langle a_0 \rangle = \frac{\epsilon}{\omega_0} \sqrt{N_0}, \]

\[ \langle a_0^\dagger a_0 \rangle = \langle a_0^1 a_0 \rangle = \frac{\epsilon^2}{\omega_0^2} N_0. \]

Using these equations gives the inequalities

\[ \langle b_0^\dagger b_0 \rangle \leq \langle a_0^\dagger a_0 \rangle, \quad \langle a_0 \rangle \leq \langle a_0^\dagger a_0 \rangle. \]

The latter yield the inequality

\[ \lim_{N \to \infty} \frac{\langle a_0^\dagger a_0 \rangle}{N} \leq \lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0^\dagger a_0 \rangle}{N}. \]

By definition, \( \langle a_0^\dagger a_0 \rangle = N_0 \). From the above equations, we have

\[ N_0 \approx \frac{T}{\omega_0} + \frac{\epsilon^2}{\omega_0^2} N_0, \]

which results in the expression

\[ \omega_0 \approx \frac{T}{2N_0} \left[ 1 + \sqrt{1 + (2\epsilon/kN_0)^2} \right]. \]

Under \( \epsilon = 0 \) and large \( N_0 \), we get \( \omega_0 \approx \epsilon \). In this way, we come to the equation \( a_0 \approx b_0 + \sqrt{N_0} \), which is a particular kind of the Bogolubov shift.

In addition, we have

\[ \langle a_0 \rangle \approx \sqrt{N_0}, \quad \langle a_0^\dagger a_0 \rangle \approx \langle a_0 \rangle^2. \]

Summarizing, we obtain the equation

\[ \lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0^\dagger a_0 \rangle}{N} = \lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0 \rangle^2}{N}. \]

The left-hand side of this equation defines the fraction of condensed atoms, while the right-hand side demonstrates gauge symmetry breaking. Therefore gauge symmetry breaking is a sufficient condition for the existence of Bose–Einstein condensation.

Also we have the inequality

\[ \lim_{N \to \infty} \frac{\langle a_0^\dagger a_0 \rangle}{N} \leq \lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0 \rangle^2}{N}. \]

which tells us that Bose–Einstein condensation necessarily implies spontaneous gauge symmetry breaking.

These findings can be formulated in the statement: spontaneous gauge symmetry breaking is the necessary and sufficient condition for Bose–Einstein condensation. General theorems confirming this statement have been proven by Bogolubov [18, 19], Ginibre [20], Roepstorff [21], and Lieb et al [22]. A detailed discussion can be found in review articles [10, 23, 24].

The Bogolubov shift of the field operator, in general, is applicable to arbitrary Bose systems, whether uniform or nonuniform, equilibrium or not. In the general case, the Bogolubov shift is

\[ \psi(r, t) \to \eta(r, t) + \psi_1(r, t). \]

The orthogonality condition remains:

\[ \int \eta^*(r, t) \psi_1(r, t) \, dr = 0. \]

And the quantum-number conservation condition is also valid:

\[ \langle \psi_1(r, t) \rangle = 0. \]

More mathematical details, related to the Bogolubov shift, will be considered in the following sections.

2.9. Bogolubov approximation

The first microscopic approach to the description of weakly interacting Bose-condensed gas was developed by Bogolubov [8, 9, 18, 19]. This is what is now named the Bogolubov approximation.

The main assumption of this approximation is that the system is almost completely Bose-condensed, so that the number of condensed atoms is very close to the total number of atoms in the system,

\[ \frac{N - N_0}{N} \ll 1. \]

Physically this can happen when atomic interactions are very weak and the system temperature is very low, which can be represented in the form of the inequalities

\[ \rho |a_i|^2 \ll 1, \quad T \ll T_c, \]

where \( a_i \) is scattering length and \( T_c \) critical temperature.

The condition of weak interactions can also be written in another way, noticing that the potential energy per particle is \( \rho \Phi_0/2 \), where

\[ \Phi_0 \equiv \int \Phi(r) \, dr, \]

while the kinetic energy per particle is \( \rho^{2/3} 2m \). The condition of weak interactions can be understood as the smallness of the potential energy as compared to the kinetic energy, which gives

\[ |m \Phi_0 \rho^{1/3}| \ll 1. \]

A system of spinless Bose atoms is characterized by the Hamiltonian
Here $U = U(r)$ is an external potential and the pair interaction potential is symmetric, so that $\Phi(-r) = \Phi(r)$.

For a uniform system, $U(r) = 0$. The interaction potential is assumed to possess the Fourier transform,

$\Phi(r) = \frac{1}{V} \sum_k \Phi_k e^{ik \cdot r}, \quad \Phi_k = \int \Phi(r) e^{-ik \cdot r} dr. \tag{85}$

The transform $\Phi_k$ is symmetric, such that $\Phi_{-k} = \Phi_k$, since $\Phi(-r) = \Phi(r)$.

Expanding the field operator over the plane waves,

$\psi(r) = \sum_k a_k \varphi_k(r), \quad a_k = \int \varphi_k^*(r) \psi(r) dr,$

one separates out the condensate term:

$\psi(r) = \frac{a_0}{\sqrt{V}} + \psi_1(r).$

The form $a_0^\dagger a_0 = \hat{N}_0$ is the number-operator of condensed atoms. Generally, $a_0^\dagger a_0 = \hat{N}_0 e^{\mu \rho}$, with $\mu$ being a real number. It is always possible to choose $\mu = 0$ by means of a gradient transformation.

Substituting the above field operator into the initial Hamiltonian yields the Hamiltonian

$H = \sum_{n=0}^4 H^{(n)}, \tag{86}$

containing five terms classified according to the number of the field operators $\psi_1(r)$ in the products. The zero-order term is

$H^{(0)} = \frac{\hat{N}_0^2}{2V} \Phi_0 - \mu \hat{N}_0.$

The first-order term $H^{(1)} = 0$, since $\int \psi_1(r) dr = 0$. The second-order term leads to

$H^{(2)} = \sum_{k=0} \left[ \frac{k^2}{2m} + \frac{\hat{N}_0}{V} (\Phi_0 + \Phi_k) - \mu \right] a_k^\dagger a_k$

$+ \frac{\hat{N}_0}{2V} \sum_{k=0} \Phi_k (a_k^\dagger a_{-k} + a_{-k}^\dagger a_k).$

And the third-order term yields

$H^{(3)} = \frac{1}{V} \sum_{k,p} \Phi_k (a_k^\dagger a_p^\dagger a_{k+p} a_{-k-p} + a_{-k}^\dagger a_{k+p}^\dagger a_k a_0).$

Here the prime means $k \neq 0$, $p \neq 0$, and $k + p \neq 0$. The fourth-order term gives

$H^{(4)} = \frac{1}{2V} \sum_{k,p} \Phi_k (a_k^\dagger a_p^\dagger a_{k+p} a_{-k-p} + a_{-k}^\dagger a_{k+p}^\dagger a_k a_0).$

with $p \neq 0$, $q \neq 0$, $k + p \neq 0$, and $k - q \neq 0$. In the expressions above, the symmetry $\Phi_{-k} = \Phi_k$ is used.

The main steps of the Bogolubov approximation are as follows. First, in view of the assumption that almost all atoms are Bose-condensed, the terms $H^{(3)}$ and $H^{(4)}$ in the Hamiltonian are considered as small perturbations and are omitted. This gives

$H = \frac{\hat{N}_0^2}{2V} \Phi_0 - \mu \hat{N}_0 + \sum_{k=0} \left[ \frac{k^2}{2m} + \frac{\hat{N}_0}{V} (\Phi_0 + \Phi_k) - \mu \right] a_k^\dagger a_k$

$+ \frac{\hat{N}_0}{2V} \sum_{k=0} \Phi_k (a_k^\dagger a_{-k} + a_{-k}^\dagger a_k).$

At the second step, one replaces in the Hamiltonian the operator $\hat{N}_0$ by the number $\hat{N}_0$, keeping in mind that $a_0$ becomes a number in thermodynamic limit. Then

$H = \frac{N_0^2}{2V} \Phi_0 - \mu N_0 + \sum_{k=0} \omega_k a_k^\dagger a_k + \frac{N_0}{2} \sum_{k=0} \Phi_k (a_k^\dagger a_{-k} + a_{-k}^\dagger a_k), \tag{87}$

where

$\omega_k = \frac{k^2}{2m} + \frac{N_0}{V} (\Phi_0 + \Phi_k) - \mu.$

At the third step, according to assumption (81), one replaces $N_0$ by $N$, getting the Hamiltonian

$H = \frac{N^2}{2V} \Phi_0 + \sum_{k=0} \omega_k a_k^\dagger a_k - \mu N + \frac{1}{2} \sum_{k=0} \Delta_k (a_k^\dagger a_{-k} + a_{-k}^\dagger a_k), \tag{87}$

with the notation

$\Delta_k \equiv \rho \Phi_k, \quad \omega_k = \frac{k^2}{2m} + \rho (\Phi_0 + \Phi_k) - \mu. \tag{88}$

It is important to pay attention to the condition that the studied system be stable, since we remember that the ideal Bose-condensed gas is unstable. To this end, we consider the compressibility

$\kappa_T = - \frac{1}{V} \left( \frac{\partial P}{\partial V} \right)^{-1}_{TN} = \frac{1}{V} \left( \frac{\partial^2 F}{\partial V^2} \right)^{-1}_{TN}.$

At low temperature $T \to 0$, we have $F \to E$. Then, under very weak interactions, we find

$E \simeq \frac{N^2}{2V} \Phi_0, \quad \kappa_T \simeq \frac{1}{\rho \Phi_0}. \tag{89}$

This tells us that the system is stable when

$\Phi_0 > 0 \quad (0 \leq \kappa_T < \infty). \tag{89}$

By the way, from here it is clear why the ideal Bose-condensed gas becomes unstable, since for the latter $\Phi_0 \to 0$, hence $\kappa_T \to \infty$. But interactions can stabilize the Bose-condensed gas, provided the stability condition (89) holds true.

Hamiltonian (87) can be diagonalized by means of the Bogolubov canonical transformation
\begin{align}
  a_k &= u_k b_k + v_k^* b_k^\dagger, \quad a_k^\dagger = u_k^* b_k^\dagger + v_k b_{-k}, \\
  b_k &= u_k^* a_{-k} - v_k^* a_{-k}^\dagger, \quad b_k^\dagger = u_k a_k - v_k a_{-k}, \tag{90}
\end{align}

where the quantities \( u_k \) and \( v_k \) are called the Bogolubov coefficient functions and the operators \( b_k \) correspond to collective excitations, called bogolons.

The new operators \( b_k \) obey the Bose–Einstein statistics, with the commutation relations \([b_k, b_{k'}] = 0 \) and \([b_k, b_{k'}^\dagger] = \delta_{k k'}\). The commutator \([a_k, a_{k'}]\) gives \( u_k v_k^* - v_k^* u_k^* = 0 \). The commutator \([a_k, a_{k'}^\dagger]\) gives \(|u_k|^2 - |v_{-k}|^2 = 1\). We also use the interaction-potential symmetry \( \Phi_k = \Phi_k^\dagger \), which results in the properties \( \omega_{-k} = \omega_k = \omega_k \). By the gradient transformations for the operators \( a_k \) and \( b_k \), it is admissible to take the Bogolubov coefficient functions to be symmetric and real, such that \( u_k^* = u_{-k} = u_k \) and \( v_k^* = v_{-k} = v_k \).

The diagonalization yields the equations

\begin{equation*}
  2\omega_k u_k v_k + (u_k^2 + v_k^2)\Delta_k = 0,
\end{equation*}

\begin{equation*}
  u_k^2 = \frac{\sqrt{\omega_k^2 + \Delta_k^2 + \varepsilon_k}}{2\varepsilon_k}, \quad v_k^2 = \frac{\sqrt{\omega_k^2 + \Delta_k^2} - \varepsilon_k}{2\varepsilon_k}.
\end{equation*}

Here \( \varepsilon_k \) is the Bogolubov spectrum

\begin{equation*}
  \varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2}. \tag{91}
\end{equation*}

The equations for the coefficient functions can be represented as

\begin{equation*}
  u_k^2 - v_k^2 = 1, \quad u_k v_k = -\frac{\Delta_k}{2\varepsilon_k}, \quad u_k^2 + v_k^2 = \frac{\sqrt{\omega_k^2 + \Delta_k^2}}{\varepsilon_k}.
\end{equation*}

Keeping in mind the spectrum (91) gives

\begin{equation*}
  \Delta_k^2 = \omega_k^2 - \varepsilon_k^2, \quad u_k^2 = \frac{|\omega_k| + \varepsilon_k}{2\varepsilon_k}, \quad v_k^2 = \frac{|\omega_k| - \varepsilon_k}{2\varepsilon_k}.
\end{equation*}

Finally, we obtain the diagonal Bogolubov Hamiltonian

\begin{equation*}
  H_0 = E_0 + \sum_{k=0} N \varepsilon_k b_k^\dagger b_k - \mu N, \tag{92}
\end{equation*}

in which the first term plays the role of the ground-state energy

\begin{equation*}
  E_0 = \frac{1}{2} N \rho \Phi_0 - \sum_{k=0} \varepsilon_k v_k^2.
\end{equation*}

The latter can also be written as

\begin{equation*}
  E_0 = \frac{1}{2} N \rho \Phi_0 - \frac{1}{2} \sum_{k=0} |\omega_k| - \varepsilon_k. \tag{93}
\end{equation*}

The reason of separating the terms with \( k = 0 \) is the existence of Bose condensate. Otherwise, these terms would be absent. And the existence of the condensate requires the validity of the condition for condensate existence:

\begin{equation*}
  \lim_{k \to 0} \varepsilon_k = 0, \quad \varepsilon_k \geq 0. \tag{94}
\end{equation*}

In the limit of zero momentum,

\begin{equation*}
  \lim_{k \to 0} (\omega_k^2 - \Delta_k^2) = 0, \quad \lim_{k \to 0} \omega_k = 2\rho \Phi_0 - \mu, \quad \lim_{k \to 0} \Delta_k = \rho \Phi_0.
\end{equation*}

Then from condition (94) we find the chemical potential

\begin{equation*}
  \mu = \rho \Phi_0. \tag{95}
\end{equation*}

With

\begin{equation*}
  \omega_k = \frac{k^2}{2m} + \rho \Phi_k,
\end{equation*}

we get the Bogolubov spectrum

\begin{equation*}
  \varepsilon_k = \sqrt{\frac{\Delta_k}{m} k^2 + \frac{k^2}{2m}}. \tag{96}
\end{equation*}

In the long-wave limit, the spectrum is of phonon type, \( \varepsilon \simeq ck \), with the sound velocity

\begin{equation*}
  c = \lim_{k \to 0} \frac{\Delta_k}{\sqrt{m}} = \frac{\rho}{\sqrt{m}} \Phi_0, \tag{97}
\end{equation*}

where \( \Phi_0 = \int \Phi(\mathbf{r}) \, d\mathbf{r} > 0 \).

The terms under the square root of \( \varepsilon_k \) are approximately equal at \( k_0 = 2mc \). For long waves, when \( k \ll k_0 \), the spectrum is

\begin{equation*}
  \varepsilon_k \simeq ck \left[ \frac{\Phi_k}{\sqrt{\Phi_0}} + \frac{1}{2} \left( \frac{k}{k_0} \right)^2 - \frac{1}{8} \left( \frac{k}{k_0} \right)^4 \right],
\end{equation*}

restoring the phonon form \( \varepsilon_k \simeq ck \) as \( k \to 0 \).

For short waves, when \( k \gg k_0 \), one has

\begin{equation*}
  \varepsilon_k \simeq \frac{k^2}{2m} + \Delta_k - \frac{m \Delta_k^2}{k^2}.
\end{equation*}

And the spectrum is of the single-particle type

\begin{equation*}
  \varepsilon_k \simeq \frac{k^2}{2m} (k \to \infty).
\end{equation*}

Important quantities, defining thermodynamic characteristics, are the normal average

\begin{equation*}
  n_k = \langle a_k^\dagger a_k \rangle, \tag{98}
\end{equation*}

which is the momentum distribution of atoms, and the anomalous average

\begin{equation*}
  \sigma_k = \langle a_k a_{-k} \rangle, \tag{99}
\end{equation*}

for which \( |\sigma_k| \) describes the distribution of pair-correlated atoms.

Averaging with the Bogolubov Hamiltonian \( H_0 \), we have

\begin{equation*}
  n_k = (u_k^2 + v_k^2) m + v_k^2, \quad \sigma_k = u_k v_k (1 + 2m),
\end{equation*}
with the bogolon distribution

$$n_k \equiv \langle b_k^\dagger b_k \rangle = (e^{\beta \varepsilon_k} - 1)^{-1}.$$  

Invoking the coefficient functions $u_k$ and $v_k$ yields the normal and anomalous averages

$$n_k = \frac{\omega_k}{2\varepsilon_k}(1 + 2\pi_k) - \frac{1}{2}, \quad \alpha_k = -\frac{\Delta_k}{2\varepsilon_k}(1 + 2\pi_k).$$  

Here we can use the equality

$$1 + 2\pi_k = \coth\left(\frac{\varepsilon_k}{2T}\right).$$

Recall that, according to the main assumption of the Bogolubov approximation, it is applicable when the system is almost completely Bose-condensed. This implies very low temperatures, close to zero, and asymptotically weak interactions, when the condensate depletion is very small. Under these conditions, we can expect that the influence of uncondensed atoms is weak, because of which in some estimates it is admissible to replace the condensate density $\rho_0$ by the average density $\rho$.

2.10. Dilute gas

A system is dilute, when atomic interactions are short-range, such that the effective interaction radius $r_0$ is much shorter than the mean interatomic distance, which can be expressed as

$$\rho r_0^3 \ll 1.$$  

Then it is possible to assume that the physical processes are mostly influenced by small momenta, where kinetic energy is much less than potential energy, $k^2/2m \ll \rho_0 \Phi_0/2$, hence where $k < \sqrt{\rho_0 \Phi_0}$. In other words, when $k \ll k_0$, where $k_0 \equiv 2mc = 2\sqrt{\rho_0 \Phi_0}$.

For a dilute system, the exact form of the interaction potential $\Phi(r)$ is not of great importance, and it is admissible to use the local effective potential.

$$\Phi(r) = \Phi_0 \delta(r), \quad \Phi_0 = 4\pi a_u/m.$$  

With this potential, $\Phi_0 = \Phi_0$ and, resorting to the Bogolubov approximation of the previous section, we have

$$\Delta_k = \rho \Phi_0, \quad \mu = \rho \Phi_0, \quad \omega_k = \frac{k^2}{2m} + \rho \Phi_0.$$  

The Bogolubov sound velocity is

$$c \equiv \sqrt{\frac{\rho \Phi_0}{m}} = \sqrt{\frac{4\pi \rho a_u}{m}}.$$  

And the Bogolubov spectrum takes the form

$$\varepsilon_k = \sqrt{\omega_k^2 - m^2c^2} = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2}.$$  

The wave vector, where $ck$ equals $k^2/2m$, is $k_0 = 2mc$.

Thus, in the Bogolubov approximation, one has

$$\Delta_k = \mu = mc^2, \quad \omega_k = \frac{k^2}{2m} + mc^2, \quad \omega_k^2 = \varepsilon_k^2 + m^2c^4.$$  

The normal and anomalous averages become

$$n_k = \frac{\sqrt{\varepsilon_k^2 + m^2c^4}}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2}, \quad \alpha_k = -\frac{\sqrt{mc^2}}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right).$$  

Note that under the asymptotically weak interactions, when $\Phi_0 \to 0$, hence $c \to 0$, the anomalous average tends to zero, $\alpha_k \to 0$. Because of this, in the Bogolubov approximation, that itself is valid only for weak interactions, it is tempting to omit the anomalous averages. This, however, is not quite correct, as is shown below.

Let us consider expressions (105) in the region of small excitation energies

$$\varepsilon_k \ll mc^2, \quad \varepsilon_k \ll T.$$  

In this region, the bogolon distribution is

$$n_k \simeq \frac{T}{\varepsilon_k} - \frac{1}{2} + \frac{\varepsilon_k}{12T} - \frac{\varepsilon_k^3}{720T^3}.$$  

And we find the expansions for the normal average

$$n_k \simeq \frac{Tmc^2}{\varepsilon_k^2} + \frac{mc^2}{12T} + \frac{T}{2mc^2} - \frac{1}{2} + \frac{mc^2}{3T} - \frac{T}{mc^2} - \frac{m^3c^6}{90T^3} \varepsilon_k^2$$

and for the anomalous average

$$\alpha_k \simeq -\frac{Tmc^2}{\varepsilon_k^2} + \frac{mc^2}{12T} + \frac{mc^2}{720T^3}.$$  

From these expressions, it is evident that these averages are of the same order of magnitude. In particular,

$$\lim_{k \to 0}(\alpha_k | - n_k|) = \frac{1}{2}\left(1 - \frac{T}{mc^2}\right).$$  

Under large excitation energies, when

$$\varepsilon_k \gg mc^2, \quad \varepsilon_k \gg T,$$

we get the normal average

$$n_k \simeq \frac{mc^2}{2\varepsilon_k} - \left(\frac{mc^2}{2\varepsilon_k}\right)^4 + e^{-\beta \varepsilon_k}$$

and the anomalous average

$$\alpha_k \simeq -\frac{mc^2}{2\varepsilon_k}(1 + 2e^{-\beta \varepsilon_k}).$$  

Here $|\alpha_k|$ is much larger than $n_k \ll |\alpha_k|$.

In this way, at low temperatures $T \ll T_c$, where the Bogolubov approximation is assumed to be valid, the
anomalous average is as important as the normal one. And omitting $\sigma_t$ is not admissible.

The relation between the normal and anomalous averages can be derived from the Bogolubov inequality (see [1])

$$\langle \hat{A} \hat{B} \rangle \leq \langle \hat{A} \hat{A}^\dagger \rangle \langle \hat{B} \hat{B}^\dagger \rangle,$$

which gives

$$\langle a_i a_j \rangle \leq \langle (a_i a_i^\dagger) (a_j^\dagger a_j) \rangle.$$  

Taking into account that $n_k = n_{-k}$ and $\sigma_i^2 = \sigma_k$, we get

$$\sigma_i^2 \leq n_k(1 + n_k).$$

Instead of this inequality, by invoking expressions (105), we can get the equality

$$n_k(1 + n_k) = \sigma_i^2 = \left[ 2 \sinh \left( \frac{\rho_k}{27} \right) \right]^{-2}.$$  

Formally setting here $T = 0$ gives $\sigma_i^2 = n_k(1 + n_k)$. This again shows that the normal and anomalous averages are closely related and the latter is not negligible as compared to the former.

The normal average defines the density of normal, uncondensed, atoms

$$\rho_n = \frac{N_l}{V} = \int n_k \frac{d\mathbf{k}}{(2\pi)^3}.$$  

(106)

With the replacement $x = \varepsilon_k / mc^2$, this yields

$$\rho_1 = \frac{(mc)^3}{(2\pi)^3} \int_0^\infty \left( \sqrt{1 + x^2} - 1 \right)^{1/2} \times \left[ \coth \left( \frac{mc^2}{2T} \right) - \frac{x}{\sqrt{1 + x^2}} \right] dx.$$  

Adding and subtracting 1 in the square brackets and using the integral

$$\int_0^\infty \left( \sqrt{1 + x^2} - 1 \right)^{1/2} \left( 1 - \frac{x}{\sqrt{1 + x^2}} \right) dx = \frac{2\sqrt{2}}{3}$$

results in the expression

$$\rho_1 = \frac{(mc)^3}{3\pi^2} \times \left\{ 1 + \frac{3\sqrt{2}}{4} \int_0^\infty \left( \sqrt{1 + x^2} - 1 \right)^{1/2} \left[ \coth \left( \frac{mc^2}{2T} \right) - 1 \right] dx \right\}.$$  

(107)

To analyze the behaviour of the normal density at low temperatures, when

$$\frac{T}{mc^2} \ll 1,$$

we accomplish the following steps. Employing the expansion

$$\sqrt{2} \left( \sqrt{1 + x^2} - 1 \right)^{1/2} \simeq x - \frac{1}{8} x^3 + \frac{7}{128} x^5 - \frac{33}{1024} x^7,$$

we calculate the integral

$$\int_0^\infty x^n \left[ \coth(px) - 1 \right] dx = \frac{\Gamma(n)\zeta(n)}{2^n \pi^n},$$

in which Re $n > 1$ and the zeta function of the even argument

$$\zeta(2n) = \frac{(2\pi)^{2n}}{2(2n)!} |B_{2n}|$$

is expressed through the Bernoulli numbers $B_n$. These are defined as

$$B_{2n+1} = 0 \quad (n = 1, 2, \ldots), \quad B_0 = 1,$$

$$B_1 = -\frac{1}{2} \quad B_2 = \frac{1}{6},$$

$$B_4 = -\frac{1}{30} \quad B_6 = \frac{1}{42} \quad B_8 = -\frac{1}{30} \quad B_{10} = \frac{5}{66},$$

and so on. Then we have the integral

$$\int_0^\infty x^{2n-1} \left[ \coth(px) - 1 \right] dx = \frac{\pi^{2n} |B_{2n}|}{2n \pi^{2n}}.$$  

Thus, we find the low-temperature behaviour of the normal density

$$\rho_1 \approx \frac{(mc)^3}{3\pi^2} \left[ 1 + \frac{\pi^2}{4} \left( \frac{T}{mc^2} \right)^2 - \frac{\pi^4}{80} \left( \frac{T}{mc^2} \right)^4 + \frac{\pi^6}{96} \left( \frac{T}{mc^2} \right)^6 \right] - \frac{33\pi^8}{1280} \left( \frac{T}{mc^2} \right)^8.$$  

For the normal fraction $n_1 = \rho_1/\rho$, we obtain

$$n_1 \approx \frac{8}{3\sqrt{\pi}} \sqrt{\rho a_s^3} \left[ 1 + \frac{\pi^2}{4} \left( \frac{mT}{4\pi\rho a_s} \right)^2 \right].$$  

(108)

Therefore the fraction of condensed atoms $n_0 = 1 - n_1$ becomes

$$n_0 = 1 - \frac{8}{3\sqrt{\pi}} \sqrt{\rho a_s^3} \left[ 1 + \frac{\pi^2}{4} \left( \frac{T}{mc^2} \right)^2 \right].$$  

(109)

The existence of atomic interactions and temperature depletes the condensate.

In the opposite limit of weak interactions, but finite temperature, when

$$\frac{mc^2}{T_c} \ll 1 \quad T_c \equiv \frac{2\pi}{m \zeta(3/2)} \left( \frac{\rho}{\sigma} \right)^{2/3},$$

the normal density (107) reduces to

$$\rho_1 \approx \rho \left( \frac{T}{T_c} \right)^{3/2} + \frac{(mc)^3}{3\pi^2}.$$  

This gives the condensate fraction

$$n_0 \approx 1 - \left( \frac{T}{T_c} \right)^{3/2} - \frac{(mc)^3}{3\pi^2 \rho}.$$  

(110)
Recall that the limit $c \to 0$ is not well defined, since the ideal gas is unstable everywhere for $T \leq T_c$, as has been explained above. This instability is easy to understand calculating the compressibility that, in the Bogolubov approximation, is 

$$\kappa_T = \frac{1}{\rho mc^2}.$$ 

As is evident, the compressibility diverges when $c \to 0$, which means instability.

Let us stress again the importance of the anomalous average. Sometimes, appealing to the fact that the anomalous average tends to zero in the limit of asymptotically weak interactions, one assumes that it can be neglected, while retaining the normal average. In doing this, one mentions Popov who allegedly advocated such an omission. This, however, is wrong, since Popov, as can be easily inferred from his book [25], has never suggested such an incorrect trick. As is shown in the present section, the anomalous average can be important even under weak interactions. Moreover, the omission of the anomalous average results in the divergence of the compressibility, thus, implying instability of the system (see details in [26]). However, those quantities that do not require the use of the anomalous averages can be estimated in the Bogolubov approximation, providing reasonable evaluations for asymptotically weak interactions and low temperatures. But, strictly speaking, the omission of the anomalous average is justified only under the simultaneous omission of the normal average defining the density $\rho_0$ of uncondensed atoms. That is, under the Bogolubov approximation, both the normal as well as the anomalous averages are assumed to be negligible as compared to the condensate fraction.

### 2.11. Particle energy

In the Bogolubov approximation, it is straightforward to define the energy and the related characteristics of the dilute system. Thus the internal energy $E = \langle H_0 \rangle + \mu N$ yields

$$E = E_0 + V \int \frac{\varepsilon_k n_k}{(2\pi)^3} dk,$$

with the ground-state energy

$$\frac{E_0}{N} = \frac{1}{2} \rho \Phi_0 + \frac{1}{2\rho} \int (\varepsilon_k - \omega_k) \frac{dk}{(2\pi)^3}. \quad (111)$$

Using the integral

$$\int \frac{\varepsilon_k n_k}{(2\pi)^3} \frac{dk}{(2\pi)^3} = \frac{1}{(2\pi)^3} \int_0^\infty \frac{\varepsilon_k}{(2\pi)} \left[ \coth \left( \frac{\varepsilon_k}{2T} \right) - 1 \right] k^2 dk,$$

the internal energy can be written as

$$\frac{E}{N} = \frac{E_0}{N} + \frac{\sqrt{2}(mc^3)^5}{(2\pi)^4 m \rho} \int_0^\infty \frac{\left( \frac{mc^2}{2T} x \right)^{(n+1)}}{(2\pi)^3} \left[ \coth \left( \frac{mc^2}{2T} x \right) - 1 \right] dx. \quad (112)$$

The grand potential $\Omega = -T \ln \operatorname{Tr} e^{-\beta H}$ takes the form

$$\Omega = E_0 - \mu N + TV \int \ln(1 - e^{-\beta \varepsilon_k}) \frac{dk}{(2\pi)^3}. \quad (113)$$

The free energy $F = \Omega + \mu N$ becomes

$$F = E_0 + \frac{\sqrt{2}(mc^3)^5}{(2\pi)^4 \rho} N \int_0^\infty x \left( \frac{1 + x^2}{\sqrt{1 + x^2}} - 1 \right)^{1/2} \times \ln(1 - e^{-\beta mc^2 x}) dx. \quad (114)$$

The same expression for $F$ can also be found from the relation between $F$ and $E$.

The average kinetic energy per particle, defined as

$$\bar{K} = \frac{1}{\rho} \int \frac{k^2 n_k}{(2\pi)^3} \frac{dk}{(2\pi)^3}, \quad (115)$$

takes the form

$$\bar{K} = K_0 + \frac{1}{4m \rho} \int k^2 \frac{\omega_k}{\varepsilon_k} \left[ \coth \left( \frac{\varepsilon_k}{2T} \right) - 1 \right] \frac{dk}{(2\pi)^3} \quad (116)$$

where

$$K_0 = \frac{1}{4m \rho} \int k^2 \left( \frac{\omega_k}{\varepsilon_k} - 1 \right) \frac{dk}{(2\pi)^3}. \quad (117)$$

Considering the internal energy, free energy, and kinetic energy at low temperatures, where $T/mc^2 \ll 1$, we use the integral

$$\int_0^\infty \frac{x^n}{(2\pi)^3} \ln(1 - e^{-ax}) dx = -\left( \frac{2}{a} \right)^{n+1} \frac{\pi^{n+2} \Gamma(n+2)}{(n+1)(n+2)}. \quad (118)$$

As a result, we obtain the low-temperature expressions

$$\frac{E}{N} \approx \frac{E_0}{N} + \frac{\pi^2(mc^3)^5}{30m \rho} \left( \frac{T}{mc^2} \right)^4, \quad (119)$$

$$\frac{F}{N} \approx \frac{E_0}{N} + \frac{\pi^2(mc^3)^5}{90m \rho} \left( \frac{T}{mc^2} \right)^4, \quad (120)$$

$$\bar{K} \approx K_0 + \frac{\pi^2(mc^3)^5}{60m \rho} \left( \frac{T}{mc^2} \right)^4. \quad (121)$$

In the opposite limit of weak interactions, such that $mc^2/T_c \ll 1$, where $T_c$ is the ideal-gas critical temperature, we find

$$\frac{E}{N} \approx \frac{E_0}{N} + \frac{3\zeta(5/2)}{2\zeta(3/2)} \frac{T_{c}^{5/2}}{T_c} - \frac{1}{2} mc^2 \left( \frac{T}{T_c} \right)^{3/2}, \quad (122)$$

$$\frac{F}{N} \approx \frac{E_0}{N} - \frac{\zeta(5/2)}{\zeta(3/2)} \frac{T_{c}^{5/2}}{T_c} + mc^2 \left( \frac{T}{T_c} \right)^{3/2}, \quad (123)$$

18
\[ \mathcal{K} \approx K_0 + \frac{3\zeta(5/2)}{2\zeta(3/2)} \left( \frac{T}{T_f} \right)^{5/2} - \frac{3mc^2}{2} \left( \frac{T}{T_f} \right)^{3/2}. \] (119)

In the limit \( c \to 0 \), we return to the expressions for the ideal gas. However, since this limit is not well defined, the following corrections, proportional to \( c^2 \), should be considered only as approximate estimates.

### 2.12. Regularization procedure

Accomplishing the calculations of the previous section, we meet divergences in the expressions for \( E_0 \) and \( K_0 \). Physically, this is connected with the used assumption of the dilute gas, when the exact interaction potential is replaced by its local form (102). There are several ways to avoid this divergence by regularizing the divergent integrals.

First of all, it is possible to take not the local, but a more realistic interaction potential leading to the momentum dependence of the Fourier transform \( \Phi_k \). Then all equations become essentially more complicated.

The second way could be by means of the cutoff regularization, when the upper limit in the divergent integrals is cut by a cutoff momentum. For example, one can take as such a limit \( k_0 = 2mc \). But the disadvantage of this method is the arising cutoff dependence.

The other way is to resort to an analytic continuation with respect to some parameters, extending the divergent integrals. This gives

\[ \int f_k \, dk \to \lim_{d \to 3} \int f_k \, dk. \]

(120)

When the function \( f_k \) depends only on \( k \parallel |k| \), then

\[ dk \to \frac{2\pi^{d/2}}{\Gamma(d/2)} k^{d-1}dk. \]

And the \( d \)-dimensional integral reads as

\[ \int f_k \, dk = \frac{2}{(2\pi)^d} \frac{2}{\Gamma(d/2)} \int_0^{\infty} f_k k^{d-1} \, dk. \]

In this case, the dimensional regularization (120) becomes

\[ \int f_k \, dk = \frac{1}{2\pi^2} \left( \frac{2\pi^d}{\Gamma(d/2)} \right)^{1/2} \int_0^{\infty} f_k k^{d-1} \, dk. \]

In the process of the regularization, one often meets the integrals, that are divergent in the \( d \)-dimensional space, but are expressed through the Euler beta functions in the \( d \)-dimensional space. The often met such integrals are of the type

\[ I_d(m, n) \equiv \int_0^{\infty} \frac{x^{\mu-1}}{(1+x)^{n+d}} \, dx, \]

where the Euler beta function is

\[ B(\mu, \nu) \equiv \int_0^{\infty} \frac{x^{\mu-1}}{(1+x)^{n+d}} \, dx, \]

with

\[ \mu = \frac{m+d-n}{2}, \quad \nu = \frac{2n-m-d}{2}. \]

The integral for \( B(\mu, \nu) \) converges for \( \mu > 0, \nu > 0 \). Therefore, the integral for \( I_d(n, m) \) converges for

\[ n < m + d < 2n, \quad n - m < d < 2n - m. \]

The Euler beta function is represented through the gamma functions as

\[ B(\mu, \nu) = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu + \nu)} = B(\nu, \mu). \]

And the gamma function \( \Gamma(z) \) can be analytically continued to the whole plane of complex \( z \). Thus we come to the integral

\[ I_d(n, m) = \frac{\Gamma\left( \frac{m+d-n}{2} \right) \Gamma\left( \frac{2n-m-d}{2} \right)}{2\Gamma(n/2)}, \]

where \( m, n, \) and \( d \) are any complex numbers.

In many cases, the relations

\[ \Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}, \quad \Gamma(-z)\Gamma(z) = \frac{\pi}{z \sin(\pi z)} \]

are useful.

For example, let us calculate the ground-state energy (111), in which we meet a divergent integral. This integral, in \( d \) dimensions, has the form

\[ \int \frac{\omega^2 - \omega_k^2}{2\rho} \, dk = \frac{(mc)^{d+2}}{\pi^{d-2}} \frac{\Gamma(d/2)m\rho}{\Gamma(1-\frac{d}{2})} \int_0^{\infty} \left( 2x\sqrt{1 + x^2} - 1 - 2x^2 \right) x^{d-1} \, dx. \]

Employing the dimensional regularization, we analytically continue the result of the integration to \( d = 3 \), using the values

\[ \Gamma\left( \frac{1}{2} \right) = -2\sqrt{\pi}, \quad \Gamma\left( -\frac{3}{2} \right) = \frac{4\sqrt{\pi}}{3} \]

\[ \Gamma\left( -\frac{5}{2} \right) = -8\sqrt{\pi}, \quad I_d(0, -1) = \frac{2}{15}. \]

This gives

\[ \int \frac{\omega^2 - \omega_k^2}{2\rho} \, dk = \frac{8(mc)^5}{15\pi^2 m\rho}. \]

And we get the ground-state energy

\[ \frac{E_0}{N} \approx \frac{\rho B_0}{2} + \frac{8(mc)^5}{15\pi^2 m\rho}. \]

Taking into account that in the Bogolubov approximation for a dilute gas, one has

\[ \Delta = mc^2 = \rho B_0, \quad mc = \sqrt{m\rho B_0} = 2\sqrt{\pi\rho a}, \]

we obtain

19
\[ E_0 = \frac{2}{N} \frac{\rho a_s}{m} \left( 1 + \frac{128}{15 \sqrt{\pi}} \sqrt{\rho a_s^2} \right) \]  

(121)

If \( \int f_k \, dk \), by its physical definition, is strictly sign-defined, say positive (non-negative), then the dimensional regularization for \( \int f_k \, dk \) can be understood as the limiting procedure

\[ \int f_k \, dk = \lim_{\delta \to 0} \int f_k \, dk / (2\pi)^d. \]

(122)

As an example, let us consider the kinetic energy at zero temperature, \( K_0 \geq 0 \). This can be written as

\[ K_0 = \lim_{\delta \to 0} \left| \int \frac{k^2}{4m\rho} \left( \frac{\omega_k}{\varepsilon_k} - 1 \right) \frac{dk}{(2\pi)^d} \right|. \]

Calculating the integral

\[ \int \frac{k^2}{4m\rho} \left( \frac{\omega_k}{\varepsilon_k} - 1 \right) \frac{dk}{(2\pi)^d} = \frac{2(mc)^2}{\pi^{d/2} 1 / (d/2) \rho} \times \int_0^\infty \frac{1 + 2x^2}{2x^2} \frac{dx}{2x} \]

and using the values

\[ I_3(2, 1) = \frac{2}{3}, \quad I_3(4, 1) = -\frac{8}{15}, \]

we come to the expression

\[ K_0 = \frac{4(mc)^2}{5\pi^2 \rho m} = \frac{128\sqrt{\pi} \rho a_s}{5m} \sqrt{\rho a_s^3}. \]

(123)

As is mentioned above, it would be possible to use the cutoff regularization. However this would lead to the cutoff dependence, so that choosing a particular cutoff would give an expression that could be different from (123). Thus, if we cut the integral for the average kinetic energy by a finite value \( k_0 = 2mc \), we get the value of \( K_0 \) that is eight times smaller than (123). Therefore the dimensional regularization, containing no free parameters, seems to be preferable.

### 2.13. Particle fluctuations

The system properties essentially depend on particle fluctuations that influence many observable quantities [1]. First of all, these fluctuations show whether the considered system is stable.

Investigating particle fluctuations, it is necessary to use correct calculations, otherwise it is easy to come to wrong unphysical conclusions. Unfortunately, there exist numerous publications claiming that particle fluctuations in Bose-condensed systems are thermodynamically anomalous. This is certainly principally wrong, since thermodynamically anomalous particle fluctuations are connected with a divergent compressibility, which makes the system unstable [1]. If particle fluctuations in Bose-condensed systems would be thermodynamically anomalous, there could exist neither equilibrium Bose-condensed systems, nor equilibrium superfluid helium. In the present section, we explain the standard mistake made by those who claim the occurrence of thermodynamically anomalous fluctuations and we show the correct way of calculating these fluctuations. The correct calculations yield thermodynamically normal fluctuations, as it has to be [29, 30].

Particle fluctuations are quantified by the variance of the particle-number operator,

\[ \text{var}(\hat{N}) = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2. \]

(124)

In the presence of Bose–Einstein condensate, the particle-number operator is \( \hat{N} = \hat{N}_0 + \hat{N}_1 \). Therefore the variance reads as

\[ \text{var}(\hat{N}) = \text{var}(\hat{N}_0) + \text{var}(\hat{N}_1) + 2\text{cov}(\hat{N}_0, \hat{N}_1), \]

with the covariance

\[ \text{cov}(\hat{N}_0, \hat{N}_1) \equiv \frac{1}{2} \langle \hat{N}_0 \hat{N}_1 + \hat{N}_1 \hat{N}_0 \rangle - \langle \hat{N}_0 \rangle \langle \hat{N}_1 \rangle. \]

By their definition, \( \langle N_0, N_1 \rangle = 0 \), hence the covariance

\[ \text{cov}(\hat{N}_0, \hat{N}_1) \equiv \langle \hat{N}_0 \hat{N}_1 \rangle - \langle \hat{N}_0 \rangle \langle \hat{N}_1 \rangle \]

acquires the form of a correlation function. In the Bogolubov theory, \( \langle \hat{N}_0 \hat{N}_1 \rangle = \langle \hat{N}_0 \rangle \langle \hat{N}_1 \rangle \), because of which \( \text{cov}(\hat{N}_0, \hat{N}_1) = 0 \). Thus variance (124) takes the form

\[ \text{var}(\hat{N}) = \text{var}(\hat{N}_0) + \text{var}(\hat{N}_1). \]

(125)

According to the Bogolubov approximation, the operator \( \hat{N}_0 \) is replaced by the number \( N_0 \). Hence \( \langle \hat{N}_0^2 \rangle = \langle \hat{N}_0 \rangle^2 \). Consequently, \( \text{var}(\hat{N}_0) = \langle \hat{N}_0^2 \rangle - \langle \hat{N}_0 \rangle^2 = 0 \). In this way,

\[ \text{var}(\hat{N}) = \text{var}(\hat{N}_1) = \langle \hat{N}_1^2 \rangle - \langle \hat{N}_1 \rangle^2. \]

The variance of the particle-number operator of uncondensed atoms can be written as

\[ \langle \hat{N}_1^2 \rangle = \sum_{k,p=0} a_k a_k^\dagger a_p a_p^\dagger. \]

Here, one substitutes the Bogolubov transformation \( a_k = u_k b_k + v_k b_k^\dagger \). As a result, one comes to the four-operator terms containing the products of four operators \( b_k \equiv b_k \). By employing the Bogolubov Hamiltonian \( H_B \), one has

\[ \langle b_k^\dagger b_k b_k^\dagger b_k \rangle = \langle b_k^\dagger b_k \rangle = 0, \]

and also

\[ \langle b_k^\dagger b_k b_k^\dagger b_k \rangle = \langle b_k^\dagger b_k \rangle = \langle b_k^\dagger b_k \rangle = \langle b_k^\dagger b_k \rangle = \langle b_k^\dagger b_k \rangle, \]

with

\[ \langle b_k b_p \rangle = \delta_{kp} \langle b_k^0 \rangle. \]

In that way, one gets

\[ \text{var}(\hat{N}_1) = \sum_{k=0} \left[ (u_k^2 + v_k^2)^2 + 4u_k^2 v_k^2 \right] n_k (1 + n_k) + 2u_k^2 v_k^2. \]

Here, one substitutes the expressions corresponding to the dilute gas,

\[ u_k^2 = \frac{\sqrt{\varepsilon_k^2 + m^2 c^4} + \varepsilon_k}{2\varepsilon_k}, \quad v_k^2 = \frac{\sqrt{\varepsilon_k^2 + m^2 c^4} - \varepsilon_k}{2\varepsilon_k}, \]
\[ u_k^2 - v_k^2 = 1, \quad u_k v_k = \frac{mc^2}{2\epsilon_k}, \quad u_k^2 + v_k^2 = \frac{\sqrt{\epsilon_k^2 + m^2c^4}}{\epsilon_k}, \]

where \( \epsilon_k \) is the Bogolubov spectrum (104). This gives

\[ \text{var}(\hat{N}) = \frac{N}{\rho} \int \left( \frac{m^2c^4}{2\epsilon_k^2} + 2\frac{m^2c^4}{\epsilon_k^2} \right) \pi(1 + \pi_k) \frac{dk}{(2\pi)^3}. \]

The main contribution to the above integral comes from the infrared region, where \( k \to 0, \epsilon_k \approx ck, \) and \( \pi_k \approx T/\epsilon_k. \) As a result, there occurs the infrared divergence

\[ \int \frac{\pi_k c^2}{\epsilon_k} \frac{dk}{\epsilon_k} \propto \ln k_{\text{min}}, \quad \int \frac{\pi_k c^2}{\epsilon_k} \frac{dk}{\epsilon_k} \propto \frac{1}{k_{\text{min}}} \]

where \( k_{\text{min}} \sim \pi/L \propto 1/N^{1/3}. \) Then the anomalous behaviour of the variance \( \text{var}(\hat{N}) \propto N^{4/3} \) leads to the divergent compressibility \( \kappa_T \propto \text{var}(\hat{N})/N \propto 1/N^{1/3}, \) which implies instability.

The arising instability, caused by thermodynamically anomalous particle fluctuations, has nothing to do with physics, but is the result of incorrect calculations. The mistake is in considering the fourth-order operator terms \( (\alpha_i^\dagger \alpha_i^\dagger \alpha_i \alpha_i) \) invoking the Bogolubov approximation that is a second-order approximation with respect to such operator products. Going outside of the region of applicability of the approximation leads to wrong results.

To correctly calculate particle fluctuations, it is necessary to be able to separate out the terms appropriate for the chosen approximation and to omit the terms of higher orders, which have been also omitted in the used approximation.

The correct way of studying particle fluctuations is as follows. It is possible to present the number-operator variance as

\[ \text{var}(\hat{N}) = N \left\{ 1 + \rho \int [g(\mathbf{r}) - 1] d\mathbf{r} \right\}, \]

involving the pair correlation function

\[ g(\mathbf{r}_2) = \frac{1}{\rho^2} \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \right\rangle, \]

with \( \mathbf{r}_2 \equiv \mathbf{r}_1 - \mathbf{r}_2. \)

We substitute here the Bogolubov shift \( \psi(\mathbf{r}) \to \eta \psi(\mathbf{r}). \) And we use the following property: if a set of operators satisfies the Wick theorem, then their linear combinations also satisfy this theorem. In our case the operators \( b_k \) do satisfy the Wick theorem because of the structure of the Bogolubov Hamiltonian \( H_B. \) Hence the operators \( a_k, \) as well as \( \psi(\mathbf{r}), \) also satisfy this theorem. This gives

\[ \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \right\rangle = \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \right\rangle \]

\[ + \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \right\rangle + \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \right\rangle = 0, \]

since \( \psi(\mathbf{r}_1) = 0 \) and \( \langle a_k \rangle = 0 \) for \( k \neq 0. \)

In the real space, the normal average is the first-order density matrix

\[ \rho_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \left\langle \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \right\rangle, \]

and the anomalous average is

\[ \sigma(\mathbf{r}_1, \mathbf{r}_2) \equiv \left\langle \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \right\rangle \].

Using this gives

\[ \left\langle \psi(\mathbf{r}_1) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_2) \right\rangle = \rho_0^2 + |\rho(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\sigma(\mathbf{r}_1, \mathbf{r}_2)|^2. \]

Thus, we obtain the pair correlation function (127) in the form

\[ g(\mathbf{r}_2) = 1 + \frac{2\rho_0}{\rho^2} \text{Re} \left[ \rho(\mathbf{r}_1, \mathbf{r}_2) + \sigma(\mathbf{r}_1, \mathbf{r}_2) \right] \]

\[ + \frac{1}{\rho^2} \left[ |\rho(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\sigma(\mathbf{r}_1, \mathbf{r}_2)|^2 \right]. \]

Fourier transforming averages (128) and (129), we have

\[ \rho(\mathbf{r}_1, \mathbf{r}_2) = \int n_k e^{ik \cdot \mathbf{r}_2} \frac{dk}{(2\pi)^3}, \quad \sigma(\mathbf{r}_1, \mathbf{r}_2) = \int \sigma_k e^{ik \cdot \mathbf{r}_2} \frac{dk}{(2\pi)^3}, \]

Noticing that \( \rho(\mathbf{r}_1, \mathbf{r}_2) \) and \( \sigma(\mathbf{r}_1, \mathbf{r}_2) \) are real due to the symmetry properties of \( n_k \) and \( \sigma_k. \) Using the equality

\[ \int [g(\mathbf{r}) - 1] d\mathbf{r} = \frac{2\rho_0}{\rho^2} \lim_{k \to 0} (n_k + \sigma_k) + \frac{1}{\rho^2} \int (n_k^2 + \sigma_k^2) \frac{dk}{(2\pi)^3}, \]

we find

\[ \int [g(\mathbf{r}) - 1] d\mathbf{r} = \frac{2\rho_0}{\rho^2} \lim_{k \to 0} (n_k + \sigma_k) + \frac{1}{\rho^2} \int (n_k^2 + \sigma_k^2) \frac{dk}{(2\pi)^3}. \]

Now let us remember that in the Bogolubov approximation, in addition to the replacement \( \rho_0 \to \rho, \) the operator terms have been neglected having the order higher then two with respect to the operators \( a_k. \) Here, the term, containing \( n_k^2 + \sigma_k^2, \) is of fourth order with respect to these operators \( a_k. \) Hence, there is no any reason of taking account of such terms that, in the Bogolubov second-order approximation have to be neglected. Thus we come to the variance

\[ \text{var}(\hat{N}) = N \left[ 1 + 2 \lim_{k \to 0} (n_k + \sigma_k) \right]. \]

Employing the expressions of \( n_k \) and \( \sigma_k \) gives

\[ \lim_{k \to 0} (n_k + \sigma_k) = \frac{1}{2} \left( \frac{T}{mc^2} - 1 \right). \]

Therefore we obtain the variance

\[ \text{var}(\hat{N}) = \frac{TN}{mc^2}, \]

corresponding to thermodynamically normal fluctuations. Respectively, the compressibility

\[ \kappa_T = \frac{\text{var}(\hat{N})}{\rho TN} = \frac{1}{\rho mc^2} \]

does not diverge, as it has to be for an equilibrium stable system.

From here, we again see that in the case of the ideal gas, when \( \Phi_0 \to 0 \) and \( c \to 0, \) the compressibility diverges, \( \kappa_T \to \infty, \) signifying the instability of the ideal Bose-condensed gas. But interactions do stabilize the system.
Also, let us recall the general exact relations (see [1]) for the central structural factor \( S(0) \) at \( k = 0 \),

\[
S(0) = \frac{\text{var}(\hat{N})}{N} = \rho T \kappa_T,
\]

the sound velocity \( s \),

\[
s^2 = \frac{1}{m} \left( \frac{\partial P}{\partial \rho} \right)_T = \frac{1}{m \rho \kappa_T^2},
\]

and the isothermal compressibility,

\[
\kappa_T = \frac{S(0)}{\rho T} = \frac{1}{m \rho \kappa_T^2}.
\]

These relations clearly demonstrate that in an unstable system, with a divergent compressibility, there would occur senseless values of an infinite structure factor and zero sound velocity.

### 2.14. Superfluid fraction

The general formula for the superfluid fraction in a three-dimensional space is

\[
n_s = 1 - \frac{\beta}{3mN} \text{var}(\hat{\mathbf{P}}).
\]

(133)

In equilibrium, \( \langle \hat{\mathbf{P}} \rangle = 0 \), hence \( \text{var}(\hat{\mathbf{P}}) = \langle \hat{\mathbf{P}}^2 \rangle \).

The Bogolubov shift for a uniform system reads as

\[
\psi(r) \rightarrow \hat{\psi}(r) = \eta \psi(r), \quad \rho_0 = \eta^2.
\]

Using this, we have

\[
\langle \psi^\dagger(r_2) \hat{\psi}(r_1) \rangle = \rho_0 + \rho_1(r_1, r_2),
\]

where

\[
\rho_1(r_1, r_2) = \langle \psi^\dagger(r_2) \psi(r_1) \rangle = \int n_k e^{i k \cdot r_2} \frac{d \mathbf{k}}{(2\pi)^3}.
\]

Therefore

\[
\int \lim_{r_3 = r_1} \nabla_3 \cdot \nabla_3 \rho_1(r_1, r_2) d r_3 = V \int k^2 n_k \frac{d \mathbf{k}}{(2\pi)^3}.
\]

In the Bogolubov approximation, the Wick theorem is valid for the operators \( \psi(r) \). This makes it possible to represent the second-order density matrix as

\[
\rho_2(r_3, r_4, r_2, r_1) = \langle \psi^\dagger(r_3) \psi^\dagger(r_2) \psi(r_1) \psi(r_4) \rangle
\]

\[
= \rho_0^2 + \rho_0 \left[ \rho_1(r_3, r_1) + \rho_1(r_4, r_1) + \rho_1(r_3, r_2) + \rho_1(r_4, r_2) + \rho_1(r_3, r_4) + \rho_1(r_1, r_4) \right]
\]

\[
+ \rho_2(r_3, r_2) + \sigma_1(r_3, r_4) + \sigma_1(r_1, r_2)
\]

\[
+ \rho_1(r_1, r_2) \rho_1(r_3, r_4) + \rho_1(r_1, r_4) \rho_1(r_3, r_2) + \rho_1(r_1, r_2) \rho_1(r_3, r_4) + \rho_1(r_1, r_4) \rho_1(r_3, r_2) + \sigma_1^2(r_3, r_2) \sigma_1(r_1, r_2).
\]

For the anomalous average

\[
\sigma_1(r_3, r_2) = \langle \psi_1(r_2) \psi_1(r_1) \rangle
\]

\[
= \int n_k e^{i k \cdot r_2} \frac{d \mathbf{k}}{(2\pi)^3},
\]

we meet the integrals of the type

\[
\int \delta(k) f(k) \sigma_k \frac{d \mathbf{k}}{(2\pi)^3} \equiv f(0) \lim_{k \to 0} \sigma_k,
\]

\[
\int \delta(k) k^2 \sigma_k \frac{d \mathbf{k}}{(2\pi)^3} = 0.
\]

Using the above expressions, we have

\[
\int \lim_{r_3 = r_1} \nabla_3 \cdot \nabla_3 \rho_1(r_1, r_2) d r_3 = -V \int k^2 (n_k^2 - \sigma_k^2) \frac{d \mathbf{k}}{(2\pi)^3}.
\]

So that finally, we get

\[
\langle \hat{\mathbf{P}}^2 \rangle = V \int k^2 (n_k^2 + n_k^2 - \sigma_k^2) \frac{d \mathbf{k}}{(2\pi)^3}.
\]

The same result can be obtained from the expression

\[
\langle \hat{\mathbf{P}}^2 \rangle = \sum_{k \mathbf{p}} (\mathbf{k} \cdot \mathbf{p}) \langle \hat{n}_k \hat{n}_\mathbf{p} \rangle
\]

using the Wick theorem for

\[
\langle \hat{n}_k \hat{n}_\mathbf{p} \rangle = n_k n_\mathbf{p} + \delta_{\mathbf{k} \mathbf{p}} n_k (1 + n_k) + \delta_{\mathbf{k} \mathbf{p}} \sigma_k^2
\]

and the sum \( \sum k \mathbf{n}_k = 0 \).

In this way, we find

\[
n_s = 1 - \frac{2Q}{3T}, \quad Q \equiv \frac{1}{\rho} \int k^2 (n_k^2 + n_k^2 - \sigma_k^2) \frac{d \mathbf{k}}{(2\pi)^3}.
\]

(134)

It is necessary to stress that here the term containing \( n_k^2 - \sigma_k^2 \) cannot be omitted because, although each of the quantities \( n_k^2 \) and \( \sigma_k^2 \) are of the fourth order with respect to the operators \( a_k \), but the difference \( n_k^2 - \sigma_k^2 \) is effectively of second order. This is explained in section 2.10 showing that in the most important long-wave region the values \( n_k \) and \( |\sigma_k| \) are close to each other, exactly coinciding for the asymptotically small excitation energy. Therefore, the main terms in \( n_k^2 \) and \( \sigma_k^2 \) cancel each other and their difference \( n_k^2 - \sigma_k^2 \) plays the role of a term of the lower order than each of the components.

Such a cancellation is crucial for the calculation of the dissipated heat, where the dangerous terms cancel each other, removing divergences that would exist for each of the terms separately. The sum in the integrand of \( Q \) reads as

\[
n_k + n_k^2 - \sigma_k^2 = \frac{1}{2} \frac{\partial n_k}{\partial \xi_k} - 1 = \frac{\partial n_k}{\partial \xi_k}.
\]

Here we also can use the equality \( \text{cosh} x - 1 = 2 \sinh^2(x/2) \).

The normal density, that is, the density of uncondensed atoms, is

\[
\rho_n = \frac{2Q}{3T} \rho = -\frac{1}{3m} \int k^2 \frac{\partial n_k}{\partial \xi_k} \frac{d \mathbf{k}}{(2\pi)^3}.
\]

In the Bogolubov approximation, the dissipated heat becomes

\[
Q = \frac{1}{8\pi \rho} \int_0^\infty k^4 \frac{d \mathbf{k}}{\cosh(\beta k)} - 1.
\]

Using the change of the variable \( x = \epsilon_k \hbar c^2 \), we get...
Let us study the low-temperature behaviour of the superfluid fraction, when \( T/mc^2 \ll 1 \). Then we use the expansion

\[
\sqrt{\frac{2}{\pi}} \frac{1}{1 + x^2} \quad \approx \quad \frac{1}{2} x^2 - \frac{7}{16} x^4 + \frac{99}{256} x^6
\]

and calculate the integral

\[
\int_{0}^{\infty} \frac{x^\mu dx}{\cosh x + \cos \alpha} = 2\Gamma(1 + \mu) \sum_{k=1}^{\infty} (-1)^{k-1} \sin(k\alpha) \frac{k^{1+\mu}}{k^{1+\mu}},
\]

in which \( \Re \mu > -1 \) and \( |\alpha| < \pi \). The result can be extended to \( \alpha \to \pi \), yielding

\[
\lim_{\alpha \to \pi} \sum_{k=1}^{\infty} (-1)^{k-1} \sin(k\alpha) = \zeta(\mu).
\]

Thus we get the integral

\[
\int_{0}^{\infty} \frac{x^\mu dx}{\cosh x - 1} = 2\Gamma(1 + \mu) \zeta(\mu).
\]

For even powers, this reduces to

\[
\int_{0}^{\infty} \frac{x^{2n} dx}{\cosh x - 1} = (2\pi)^{2n} |B_{2n}|,
\]

with \( B_n \) being the Bernoulli numbers. In this way, we find the expansion for the dissipated heat

\[
\frac{Q}{mc^2} \approx \frac{\rho (mc)^3}{2\pi} \left[ \frac{\pi^2}{15} \left( \frac{T}{mc^2} \right)^5 - \frac{\pi^4}{6} \left( \frac{T}{mc^2} \right)^7 + \frac{3\pi^6}{40} \left( \frac{T}{mc^2} \right)^9 \right].
\]

Then the low-temperature behaviour of the superfluid fraction reads as

\[
n_s \approx 1 - \frac{2\pi^2 (mc)^3}{45 \rho} \left[ \left( \frac{T}{mc^2} \right)^4 - \frac{5\pi^2}{2} \left( \frac{T}{mc^2} \right)^6 + \frac{99\pi^4}{8} \left( \frac{T}{mc^2} \right)^8 \right].
\]

In the limit of zero \( c \), we return to the expressions for the ideal gas,

\[
Q \approx \frac{3}{2} \left( \frac{T}{T_c} \right)^{3/2} \quad , \quad n_s \approx 1 - \left( \frac{T}{T_c} \right)^{3/2}.
\]

The fraction \( n_s \) coincides with \( n_0 \) only in the limit of the ideal gas, when \( c = 0 \). But they are different for any finite \( c \). As has been mentioned above, the limit \( c = 0 \) corresponds to an unstable system. Corrections to the zero-interaction case cannot be derived by the direct expansion of \( Q \) in powers of \( c \), since this leads to divergent terms.

2.15. **Bogolubov theorem**

An important property of Bose systems follows from the investigation of the response induced by local gauge transformations

\[
\hat{U}_c \equiv \exp \left\{ i \int \alpha(\mathbf{r}) \hat{n}(\mathbf{r}) d\mathbf{r} \right\},
\]

where \( \alpha(\mathbf{r}) = \alpha(\mathbf{r}) \) is a real function and \( \hat{n}(\mathbf{r}) \equiv \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \). In particular, this property imposes restrictions specifying the behavior of the spectrum of collective excitations. The mathematical formulation of this property composes the Bogolubov theorem [16, 19].

For any type of statistics, there exist the commutation relations

\[
[\psi(\mathbf{r}), \hat{n}(\mathbf{r}^\prime)] = \psi(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}^\prime),
\]

\[
[\psi(\mathbf{r}), \int \alpha(\mathbf{r}^\prime) \hat{n}(\mathbf{r}^\prime) d\mathbf{r}^\prime] = \alpha(\mathbf{r}) \psi(\mathbf{r}),
\]

from which one has

\[
\psi(\mathbf{r}) \hat{U}_c = e^{i\alpha(\mathbf{r})} \hat{U}_c \psi(\mathbf{r}).
\]

The local gauge transformation is unitary, \( \hat{U}_c \hat{U}_c^\dagger = 1 \). Let us introduce the transformed field operator

\[
\tilde{\psi}(\mathbf{r}) \equiv \hat{U}_c^\dagger \psi(\mathbf{r}) \hat{U}_c = e^{i\alpha(\mathbf{r})} \psi(\mathbf{r}),
\]

with the inverse transformation

\[
\psi(\mathbf{r}) = \hat{U}_c \tilde{\psi}(\mathbf{r}) \hat{U}_c^\dagger = e^{-i\alpha(\mathbf{r})} \tilde{\psi}(\mathbf{r}).
\]

Respectively, for a Hamiltonian \( H \equiv H[\psi] \), we define the transformed Hamiltonian

\[
\tilde{H} \equiv H[\tilde{\psi}] = \hat{U}_c H[\psi] \hat{U}_c^\dagger,
\]

and, similarly, for an operator of observable \( \hat{A} \equiv \hat{A}[\psi] \), the transformed operator

\[
\tilde{A} \equiv \hat{U}_c \hat{A}[\psi] \hat{U}_c^\dagger.
\]

It is straightforward to see that for the averages

\[
\langle \hat{A}[\psi] \rangle_H \equiv \langle \hat{A}[\psi] \rangle \hat{U}_c \hat{U}_c^\dagger \frac{\text{Tr} e^{-\delta H}}{\text{Tr} e^{-H}},
\]

there is the equality

\[
\langle \tilde{A}[\tilde{\psi}] \rangle_{\tilde{H}} = \langle \hat{A}[\psi] \rangle_H.
\]

Owing to this equality, we have

\[
\left\langle \prod_{i} \tilde{\psi}^\dagger(\mathbf{r}_i) \prod_{j} \tilde{\psi}(\mathbf{r}_j) \right\rangle_{\tilde{H}} = \left\langle \prod_{i} \hat{A}^\dagger[\psi(\mathbf{r}_i)] \prod_{j} \hat{A}[\psi(\mathbf{r}_j)] \right\rangle_H.
\]

From direct calculations it follows that

\[
\left\langle \prod_{i} \tilde{\psi}^\dagger(\mathbf{r}_i) \prod_{j} \tilde{\psi}(\mathbf{r}_j) \right\rangle_{\tilde{H}} = \left\langle \prod_{i} \hat{A}^\dagger[\psi(\mathbf{r}_i)] \prod_{j} \hat{A}[\psi(\mathbf{r}_j)] \right\rangle_H \exp \left\{ -i \left( \sum_{i} \alpha(\mathbf{r}_i) - \sum_{j} \alpha(\mathbf{r}_j) \right) \right\}.
\]
Using equation (137), we get
\[
\left\langle \prod_i \psi_i(r) \right\rangle_H = \left\langle \prod_i \psi_i(r) \right\rangle_H \exp \left\{ i \left[ \sum_i \alpha(r_i) - \sum_j \alpha(r_j) \right] \right\}.
\]

Let us consider the infinitesimal transformation, where \( \alpha(r) \to 0 \). Then
\[
\tilde{\psi}(r) = [1 + i\alpha(r)]\psi(r).
\]
And let us define the increment of an operator
\[
\delta(\hat{A}) \equiv \langle \hat{A}[\psi] \rangle_H - \langle \hat{A}[\psi] \rangle_H.
\]
We shall be interested in the increment
\[
\delta \left\langle \prod_i \psi_i(r) \right\rangle_H = i \left[ \sum_i \alpha(r_i) - \sum_j \alpha(r_j) \right].
\]
Consider a uniform system, with the field operators in the momentum space
\[
a_k = \int \varphi_k^\dagger(r) \varphi(r) \, dr,
\]
whose transformed operators are
\[
a_k = \int \varphi_k^\dagger(r) \tilde{\varphi}(r) \, dr.
\]
Let us set \( \alpha(r) = 2 \cos(q \cdot r) \delta \alpha \), with \( \delta \alpha \to 0 \). Then
\[
\tilde{a}_k = a_k + i(a_{k+q} + a_{k-q}) \delta \alpha,
\]
\[
\delta(a_k) = -i(a_{k-q} + a_{k+q}) \delta \alpha.
\]
For a Bose-condensed system, gauge symmetry is broken, because of which
\[
\langle a_k \rangle_H = \sqrt{N_0} \delta \alpha, \quad \delta(a_k) = -i(\delta_{kq} + \delta_{k(-q)}) \sqrt{N_0} \delta \alpha,
\]
\[
\delta(a_k^\dagger a_p) = i(\delta_{k+q}^\dagger \delta_{k+q}^\dagger) a_p - a^\dagger_k a_{p-q} + a^\dagger_k a_{p+q}) \rangle_H \delta \alpha.
\]
With the notation
\[
\langle a_k^\dagger a_p \rangle_H = \delta_{kp} n_k, \quad n_k \equiv \langle a_k^\dagger a_k \rangle_H,
\]
we get
\[
\delta(a_k^\dagger a_p) = i(\delta_{kp+q}^\dagger \delta_{kp+q}^\dagger) a_p - n_k \delta \alpha.
\]
Setting here \( q = k \) gives
\[
\delta(a_k) = -i \sqrt{N_0} \delta \alpha, \quad \delta(a_k^\dagger - a_{-k}) = 2i \sqrt{N_0} \delta \alpha.
\]
The transformed Hamiltonian can be written as \( H[\tilde{\psi}] = H[\psi] + \delta H \), with
\[
\delta H = -\frac{i}{2m} \int \psi^\dagger(r) \left[ \nabla^2 \alpha(r) + 2 \nabla \alpha(r) \cdot \nabla \right] \psi(r) \, dr,
\]
where only the terms linear in \( \alpha \) are left, while containing \( \alpha^2 \) are omitted. Passing to the momentum space, we have
\[
\delta H = H_0 + \frac{i}{2m} \sum_{p} q_p (a^\dagger_{p+q} a_p - a^\dagger_{p+q} a_p).
\]
The latter form is clearly Hermitian, \( H_0 = H_0^\dagger \), and the related increment is
\[
\delta(H_0) = -2Nk^2 \frac{\delta \alpha}{\delta \alpha}.
\]
Now let us use the Kubo formula in the Bogolubov–Tyablikov representation, as is explained in [1]. Then, using the notation for the linear response function \( \chi(\hat{A}, \hat{B}) = \chi(\hat{A}, \hat{B}, 0) \), defined in [1], we obtain
\[
\delta(a_k) = \chi(a_k, H_0) \delta \alpha,
\]
\[
\delta(a_k^\dagger - a_{-k}) = \chi(a_k^\dagger, H_0^\dagger) \delta \alpha,
\]
\[
\delta(H_0) = \chi(H_0, H_0) \delta \alpha.
\]
For the related response functions, we find
\[
|\chi(a_k, H_0)|^2 = N_0, \quad |\chi(a_k^\dagger - a_{-k}, \chi(\hat{B}^\dagger, \hat{B})|^2 = 4N_0, \quad \chi(H_0, H_0) = -2Nk^2 \frac{\delta \alpha}{\delta \alpha}.
\]
The expression \(|\chi(\hat{A}, \hat{B})|^2 \) is a bilinear form, for which the Bogolubov inequality
\[
\langle A, B \rangle \leq \langle A, B \rangle \chi(\hat{A}, \hat{B}) \chi(\hat{B}^\dagger, \hat{B})
\]
is valid (see [1]). In the present case, we have
\[
\langle A, B \rangle \leq \langle A, B \rangle \chi(\hat{A}, \hat{B}) \chi(\hat{B}^\dagger, \hat{B})
\]
\[
\langle A, B \rangle \leq \langle A, B \rangle \chi(\hat{A}, \hat{B}) \chi(\hat{B}^\dagger, \hat{B})
\]
\[
|\chi(a_k, a_{-k})| \geq \frac{mn_0}{2k^2}, \quad |\chi(a_k^\dagger - a_{-k}, a_{-k}^\dagger)| \geq \frac{2mn_0}{k^2}.
\]
(139)
where \( n_0 \equiv N_0/N \) and
\[
\chi(a_k^\dagger - a_{-k}, a_{-k}^\dagger) = \chi(a_k^\dagger, a_k) - \chi(a_k^\dagger, a_{-k}) + \chi(a_{-k}^\dagger, a_{-k}) + \chi(a_k^\dagger, a_{-k}^\dagger).
\]
Another convenient form of the Bogolubov theorem, which is often used, follows from the above inequalities, after introducing the matrix \( [G_{\alpha \beta}(k)] \) composed of the Green functions
\[
G_{11}(k) \equiv \chi(a_k^\dagger, a_k), \quad G_{12}(k) \equiv \chi(a_k^\dagger, a_{-k}), \quad G_{21}(k) \equiv \chi(a_k, a_{-k}), \quad G_{22}(k) \equiv \chi(a_k^\dagger, a_k),
\]
such that
\[
\chi(a_k^\dagger - a_{-k}, a_k - a_{-k}^\dagger) = 2G_{11}(k) + 2G_{22}(k).
\]
The Green functions enjoy the symmetry properties
\[ G_{11}(k) = G_{22}(k), \quad G_{12}(k) = G_{21}(k), \]
\[ G_{00}(-k) = G_{00}(k). \]

Then the Bogolubov theorem acquires the form
\[ |G_{11}(k)| \geq \frac{mn_0}{2k^2}, \quad |G_{11}(k) - G_{12}(k)| \geq \frac{mn_0}{k^2}. \]  
(140)

As will be shown below, this theorem prescribes that the spectrum of collective excitations in a Bose-condensed system has to be gapless.

### 3. Main features

In the theoretical description of Bose-condensed systems there exist several delicate points that have to be taken into account for developing a correct theory. Otherwise, it is easy to come to wrong conclusions having no physical meaning.

#### 3.1. Nonuniqueness of vacuum

As has been explained in the first part of the tutorial [1], the field operators \( \psi_1(\mathbf{r}) \) and \( \psi^\dagger_1(\mathbf{r}) \) are defined on the Fock space \( \mathcal{F}(\psi) \) generated by these field operators from a vacuum state \( |0\rangle \), such that \( \psi_1(\mathbf{r})|0\rangle = 0 \). Any function \( \varphi \in \mathcal{F}(\psi) \) can be constructed from the vacuum by the rule
\[ \varphi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int f_n(r_1, \ldots, r_n) \prod_{i=1}^{n} \psi_i(\mathbf{r}_i) d\mathbf{r}_i |0\rangle, \]
where \( f_n(r_1, \ldots, r_n) \) is a symmetrized function of its arguments.

When accomplishing the Bogolubov shift \( \psi_1(\mathbf{r}) \rightarrow \eta_1(\mathbf{r}) + \psi_1(\mathbf{r}) \), with a nonoperator function \( \eta_1(\mathbf{r}) \) that is not identically zero, one passes from the field operators \( \psi_1(\mathbf{r}) \) to the field operators \( \psi_1(\mathbf{r}) \), both satisfying the Bose commutation relations. The transformation between these field operators can be described by the transformation operator
\[ \hat{C} \equiv \exp \left\{ \int [\eta^*(\mathbf{r}) \psi_1(\mathbf{r}) - \eta_1(\mathbf{r}) \psi^\dagger_1(\mathbf{r})] d\mathbf{r} \right\}, \] 
(141)
whose inverse is
\[ \hat{C}^{-1} = \exp \left\{ -\int [\eta^*(\mathbf{r}) \psi_1(\mathbf{r}) - \eta_1(\mathbf{r}) \psi^\dagger_1(\mathbf{r})] d\mathbf{r} \right\}. \]  
(142)

The transformation operator can be written as
\[ \hat{C} = \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \int [\eta^*(\mathbf{r}) \psi_1(\mathbf{r}) - \eta_1(\mathbf{r}) \psi^\dagger_1(\mathbf{r})] d\mathbf{r} \right\}^n. \]

Using the commutation relation
\[ [\psi_1(\mathbf{r}), \hat{C}] = -\eta_1(\mathbf{r}) \hat{C}, \]
the transformation between the field operators can be represented in the form
\[ \psi_1(\mathbf{r}) = \hat{C} \psi_1(\mathbf{r}) \hat{C}^{-1}, \quad \psi_1(\mathbf{r}) = \hat{C}^{-1} \psi_1(\mathbf{r}) \hat{C}. \]  
(143)

However, the state \( |0\rangle \) is not a vacuum for \( \psi_1(\mathbf{r}) \), since
\[ \psi_1(\mathbf{r})|0\rangle = -\eta_1(\mathbf{r})|0\rangle \neq 0, \]  
(144)
when \( \eta_1(\mathbf{r}) \neq 0 \). In turn, \( |0\rangle \) is not a vacuum for \( \psi_1(\mathbf{r}) \), as far as
\[ \psi_1(\mathbf{r})|0\rangle = \eta_1(\mathbf{r})|0\rangle \neq 0, \]  
(145)
if \( \eta_1(\mathbf{r}) \neq 0 \).

The vacuum for \( \psi_1(\mathbf{r}) \) is the state
\[ |0\rangle \rightarrow \hat{C}^{-1}|0\rangle, \]  
(146)
since \( \psi_1(\mathbf{r})|0\rangle = 0 \). Over this vacuum, one can generate the Fock space \( \mathcal{F}(\psi_1) \) by means of the field operator \( \psi_1(\mathbf{r}) \). But the Fock spaces \( \mathcal{F}(\psi) \) and \( \mathcal{F}(\psi_1) \) are different. Moreover, the spaces \( \mathcal{F}(\psi) \) and \( \mathcal{F}(\psi_1) \) are orthogonal in thermodynamic limit.

To show their orthogonality, we resort to the Baker–Hausdorff formula for the operators \( \hat{A} \) and \( \hat{B} \), for which \( [\hat{A}, \hat{B}] \) commutes with both \( \hat{A} \) and \( \hat{B} \),
\[ [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0. \]
Then we have
\[ e^{\hat{A}\hat{B}} = e^{\hat{B}} e^{\hat{A}} \exp \left\{ \frac{1}{2} [\hat{A}, \hat{B}] \right\}, \]
\[ e^{\hat{A}+\hat{B}} = e^{\hat{A}\hat{B}} \exp \left\{ -\frac{1}{2} [\hat{A}, \hat{B}] \right\}. \]
Operator (142) reads as
\[ \hat{C}^{-1} = \exp \left\{ -\int [\eta^*(\mathbf{r}) \psi_1(\mathbf{r}) - \eta_1(\mathbf{r}) \psi^\dagger_1(\mathbf{r})] d\mathbf{r} \right\} \times \exp \left\{ -\frac{1}{2} \int |\eta_1(\mathbf{r})|^2 d\mathbf{r} \right\}. \]

The action of this operator on the vacuum \( |0\rangle \) is
\[ \hat{C}^{-1}|0\rangle = \exp \left\{ -\frac{1}{2} \int |\eta_1(\mathbf{r})|^2 d\mathbf{r} \right\} \exp \left\{ \int [\eta^*(\mathbf{r}) \psi_1(\mathbf{r}) - \eta_1(\mathbf{r}) \psi^\dagger_1(\mathbf{r})] d\mathbf{r} \right\} |0\rangle. \]

By definition (see [1]) a coherent state \( |\eta\rangle \) is the eigenstate of the destruction operator,
\[ \psi_1(\mathbf{r})|\eta\rangle = \eta(r)|\eta\rangle, \]
with the eigenvalue \( \eta(r) = \langle \psi_1(\mathbf{r}) |\eta\rangle \) called the coherent field. The coherent state can be represented as
\[ |\eta\rangle = n_0 \exp \left\{ \int [\eta^* \psi_1^\dagger \psi_1] d\mathbf{r} \right\} |0\rangle, \]
\[ |\eta_0\rangle = \exp \left\{ -\frac{1}{2} \int |\eta|^2 d\mathbf{r} \right\}. \]
This shows that the vacuum of the Fock space \( \mathcal{F}(\psi_1) \) is the coherent state
\[ |0\rangle \rightarrow \hat{C}^{-1}|0\rangle = |\eta\rangle. \]  
(147)

Considering the scalar product \( \langle 0|0\rangle = \langle 0|\eta\rangle \), we use the equality
\[ \langle 0| \exp \left\{ \int [\eta^* \psi_1^\dagger \psi_1] d\mathbf{r} \right\} |0\rangle = 1. \]
which gives

\[ \langle 0 | \eta \rangle = \exp \left\{ -\frac{1}{2} \int |\eta(r)|^2 \, dr \right\}. \]

The number of condensed particles is given by the integral over the condensate density,

\[ N_0 = \int \rho_0(r) \, dr, \quad \rho_0(r) = |\eta(r)|^2. \]

Therefore

\[ \langle 0 | \eta \rangle = \exp \left\{ -\frac{1}{2} N_0 \right\}. \]

Bose-condensation implies that \( N \propto N \), because of which we see that the vacua \( |0\rangle \) and \( |\eta\rangle \) are asymptotically orthogonal:

\[ \langle 0 | \eta \rangle = 0 \quad (N \to \infty). \]  \tag{148} \]

And all states generated from these vacua are orthogonal to each other, except \( |\eta\rangle \) that is a coherent state in \( \mathcal{F}(\psi) \), and it is the vacuum \( |\eta\rangle = |0\rangle \) in \( \mathcal{F}(\psi_1) \).

The sole intersection between the spaces, containing continuum number of states, is the intersection of zero measure. To eliminate the influence of this intersection, it is possible to impose the orthogonality condition

\[ \int \eta^*(r) \psi(r) \, dr = 0, \quad \int \eta(r) \psi^*(r) \, dr = 0. \]  \tag{149} \]

In this way, we come to the conclusion that the spaces \( \mathcal{F}(\psi) \) and \( \mathcal{F}(\psi_1) \) are asymptotically orthogonal with each other. The spaces have their own vacua that are orthogonal to each other. Thus, a given statistical system may possess several vacua and different orthogonal Fock spaces.

It is also worth noting that the transformation operator \( \hat{C} \) is not defined in one space. The operator \( \hat{C} \) transforms \( \mathcal{F}(\psi_1) \) into \( \mathcal{F}(\psi) \). And the inverse operator \( \hat{C}^{-1} \) transforms \( \mathcal{F}(\psi) \) into \( \mathcal{F}(\psi_1) \). Therefore \( \hat{C} \) is nonunitary, since \( \hat{C}^{-1} \) is not defined on the same space.

Strictly speaking, the Bogolubov shift has to be understood as a replacement \( \psi(r) \rightarrow \hat{\psi}(r) \) of the field operator \( \psi(r) \) by the field operator \( \hat{\psi}(r) \), where

\[ \hat{\psi}(r) \equiv \eta(r) + \psi_1(r), \]  \tag{150} \]

since these operators are defined on different Fock spaces. The operator \( \psi(r) \) is defined on \( \mathcal{F}(\psi) \), but \( \hat{\psi}(r) \) is defined on \( \mathcal{F}(\psi_1) \). The left-hand and right-hand sides of the replacement are defined on different spaces, orthogonal to each other. The same conclusions are valid irrespective to whether the gauge symmetry has been broken by the Bogolubov shift or by infinitesimal sources. More details can be found in [31].

### 3.2. Nonequivalent representations

The Bogolubov shift can be considered as a canonical transformation between the field operators. Although such transformations for operators, enjoying the same commutation relations, are usually written as equalities, they actually are not equalities, but rather are replacements, since the left-hand and right-hand sides of the equalities correspond to operators defined on different Fock spaces. The operators connected by such transformations demonstrate unitary nonequivalent representations of canonical commutation relations or non-equivalent operator representations. The nonequivalent operator representations occur in many commutation relations, not necessarily involving a symmetry breaking.

As an example, let us consider the field operators in the momentum representation. Suppose the field operators \( a_k \) are defined on the Fock space \( \mathcal{F}(a_k) \) generated by \( a_k^\dagger \) and possessing a vacuum \( |0\rangle_a \) such that \( a_k^\dagger |0\rangle_a = 0 \). The Bogolubov canonical transformation

\[ a_k = u_k b_k + v_k^* b_k^\dagger, \quad b_k = u_k^* a_k - v_k^* a_k^\dagger, \]

\[ |u_k|^2 - |v_k|^2 = 1, \]  \tag{151} \]

provides such an example of nonequivalent representations of canonical commutation relations. Note that the coefficient functions here can be chosen as real and symmetric, such that \( u_k^* = u_{-k} \) and \( v_k^* = v_{-k} = v_k \).

Let us introduce the transformation operators

\[ \hat{D} \equiv \exp \left\{ \frac{1}{2} \sum_k \gamma_k (a_k a_{-k} - a_{-k}^\dagger a_k^\dagger) \right\}, \]

\[ \hat{D}^{-1} \equiv \exp \left\{ -\frac{1}{2} \sum_k \gamma_k (a_k a_{-k} - a_{-k}^\dagger a_k^\dagger) \right\}, \]  \tag{152} \]

in which we use the notation

\[ u_k = \cosh \gamma_k, \quad v_k = \sinh \gamma_k, \quad \gamma_k = \ln(u_k + v_k). \]

Because of the commutator

\[ \left[ a_k, \frac{1}{2} \sum_p \gamma_p (a_p a_{-p} - a_{-p}^\dagger a_p^\dagger) \right] = -\gamma_k a_{-k}^\dagger, \]

we have the transformations

\[ a_k = \hat{D} b_k \hat{D}^{-1}, \quad b_k = \hat{D}^{-1} a_k \hat{D}. \]  \tag{153} \]

The state \( |0\rangle_a \) that is a vacuum for \( a_k \) is not a vacuum for \( b_k \), since

\[ b_k |0\rangle_a = -v_k^\dagger b_{-k}^\dagger |0\rangle_a \neq 0. \]

The vacuum for \( b_k \), for which \( b_k |0\rangle_b = 0 \), is

\[ |0\rangle_b = \hat{D}^{-1} |0\rangle_a. \]  \tag{154} \]

This state \( |0\rangle_b \) is not a vacuum for \( a_k \), since

\[ a_k |0\rangle_b = -v_k b_{-k}^\dagger |0\rangle_b \neq 0. \]

The operators \( b_k^\dagger \) generate the Fock space \( \mathcal{F}(b_k) \).

The commutator of the terms in the exponential (152) is

\[ \sum_k \gamma_k^2 (1/2 + a_k^\dagger a_k), \]

which is not proportional to the unity operator. Therefore the Baker–Hausdorff formula does not simplifies, as in the previous section. However, this commutator gives a constant when acting on the vacuum \( |0\rangle_a \). Keeping this in mind, it is possible to use the approximate Baker–Hausdorff formula for \( \hat{D}^{-1} \) acting on \( |0\rangle_a \) omitting higher-order commutators [32]. This gives
\[ \hat{D}^{-1}|0\rangle_a \approx \exp \left( \frac{1}{2} \sum_k \gamma_k a_k^+ a_k \right) \exp \left( -\frac{1}{2} \sum_k \gamma_k a_k^a a_k \right) \times \exp \left\{ -\frac{1}{4} \sum_k \gamma_k^2 (1 + 2a_k^* a_k) \right\} |0\rangle_a. \]

In view of the equality
\[ \exp \left\{ -\frac{1}{4} \sum_k \gamma_k^2 (1 + 2a_k^* a_k) \right\} |0\rangle_a = |0\rangle_a, \]

it follows
\[ |0\rangle_b = \hat{D}^{-1}|0\rangle_a = \exp \left( -\frac{1}{4} \sum_k \gamma_k^2 \right) \exp \left( \frac{1}{2} \sum_k \gamma_k a_k^+ a_k \right) |0\rangle_a. \]

For a macroscopic system
\[ \sum_k \gamma_k^2 = V \int \frac{\gamma_k^2 \, dk}{(2\pi)^3}. \]

Taking into account that
\[ a^\dagger(0) \exp \left( \frac{1}{2} \sum_k \gamma_k a_k^+ a_k \right) |0\rangle_a = 1, \]

we find
\[ a^\dagger(0) |0\rangle_b = \exp \left\{ -\frac{V}{4} \int \gamma_k^2 \, dk (2\pi)^3 \right\}. \]

Since the integral in the exponential is positive, we get
\[ a^\dagger(0) |0\rangle_b \approx 0 \quad (N \to \infty). \tag{155} \]

That is, the vacua are asymptotically orthogonal, hence the spaces \( \mathcal{R}(a_k) \) and \( \mathcal{R}(b_k) \) are also asymptotically orthogonal.

Note that the transformation operator \( \hat{D} \) is not unitary, because \( \hat{D}^\dagger \) is not defined on the same space. Thus, we have a unitary nonequivalent operator representations, where \( \hat{D} \) transforms \( \mathcal{R}(b_k) \) into \( \mathcal{R}(a_k) \) and \( \hat{D}^{-1} \) transforms \( \mathcal{R}(a_k) \) into \( \mathcal{R}(b_k) \). The unitary nonequivalent representation of canonical commutation relations (151), strictly speaking, should be understood as the replacement \( a_k \to a_k + \psi^*_k b_k^\dagger \).

Calculating the averages of operators, it is important to keep in mind the spaces these operators are defined on.

### 3.3. Phase operator

One often defines a phase operator by resorting to the Dirac representation
\[ \psi(\mathbf{r}) \equiv e^{i\phi(\mathbf{r})} \sqrt{\hat{n}(\mathbf{r})}, \]

with \( \phi(\mathbf{r}) \) being the phase operator and \( \hat{n}(\mathbf{r}) \equiv \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \). This representation requires that \( \phi(\mathbf{r}) \) be Hermitian, \( \phi(\mathbf{r}) = \phi^\dagger(\mathbf{r}) \). Then we have
\[ \psi^\dagger(\mathbf{r}) \equiv \sqrt{\hat{n}(\mathbf{r})} e^{-i\phi(\mathbf{r})}, \quad e^{i\phi(\mathbf{r})} = [\phi(\mathbf{r})][\hat{n}(\mathbf{r})]^{-1/2}. \]

Since \([\psi(\mathbf{r}), \hat{n}(\mathbf{r}')] = \psi(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'), \) one has
\[ [e^{i\phi(\mathbf{r})}, \hat{n}(\mathbf{r}')] = e^{i\phi(\mathbf{r})} \delta(\mathbf{r} - \mathbf{r}'), \]

from where one gets the commutation relation
\[ [\hat{n}(\mathbf{r}), \phi(\mathbf{r}')] = i\delta(\mathbf{r} - \mathbf{r}'). \]

But then one comes to the commutator
\[ [\hat{N}, \phi(\mathbf{r})] = i, \quad \hat{N} \equiv \int \hat{n}(\mathbf{r}) \, d\mathbf{r} \]

valid for any \( \mathbf{r} \). This implies that \( \phi(\mathbf{r}) \) does not depend on \( \mathbf{r} \), which is certainly strange.

An operator equality is valid in the weak sense, when it holds for all matrix elements with respect to the functions from the considered space. For the number basis \( \{|n\rangle \} \), such that
\[ \hat{N}|n\rangle = n|n\rangle, \quad (n - n')\langle n|\phi(\mathbf{r})|n'\rangle = i\delta_{nn'}, \]

setting \( n = n' \), we obtain the equality \( i = 0 \), which does not have sense. The conclusion is that such a representation does not exist.

Another often used incorrect representation is
\[ \psi(\mathbf{r}) \equiv \sqrt{\rho_0(\mathbf{r})} e^{iG(\mathbf{r})}, \]

with \( \rho_0(\mathbf{r}) \) being the density of condensed particles. But then
\[ \hat{n}(\mathbf{r}) = \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) = i\rho_0(\mathbf{r}), \quad \hat{N} = \int \rho_0(\mathbf{r}) \, d\mathbf{r} = N_0. \]

From the commutator \([\psi(\mathbf{r}), \hat{N}] = \psi(\mathbf{r}) \), and for \( \hat{N} = N_0 \), one has \( \psi(\mathbf{r}) = 0 \). The conclusion is again that this representation does not exist. The phase operator cannot be introduced by the considered relations.

This does not contradict the possibility of introducing a phase for non-operator functions. For instance, the coherent state, given by the eigenproblem \( \psi(\mathbf{r}) |\eta\rangle = \eta(\mathbf{r}) |\eta\rangle \), defines the coherent field, for which the Madelung form
\[ \eta(\mathbf{r}) = \sqrt{\rho_0(\mathbf{r})} e^{i\theta(\mathbf{r})}, \]

where \( \rho_0(\mathbf{r}) = |\eta(\mathbf{r})|^2 \), can be employed.

The ways of correctly introducing phase operators have been discussed in the review articles [33–36].

### 3.4. Noncommutativity of transformations

As is explained above, canonical transformations can connect operators acting on different Fock spaces. Therefore it is necessary to be careful accomplishing practical calculations. The general rule is to consistently work with one Fock space, accomplishing calculations after canonical transformations.

To illustrate what kind of problems can arise, let us pose the question: is there a difference in the result of the following procedures?

(i) Suppose we, first, realize the Bogolubov shift, that is, we pass from the Fock space \( \mathcal{F}(\psi) \) to the Fock space \( \mathcal{F}(\psi_1) \). Then we accomplish some actions with the operators \( \psi(\mathbf{r}) \) on the space \( \mathcal{F}(\psi_1) \).

(ii) First, we accomplish the equivalent actions with \( \psi(\mathbf{r}) \) on the space \( \mathcal{F}(\psi) \). And then, we realize the Bogolubov shift, hence the transformation from the space \( \mathcal{F}(\psi) \) to the space \( \mathcal{F}(\psi_1) \).

27
The general answer to this question is ‘no’—these actions are not commutative.

All transformations with operators must be accomplished in the same space. As an illustration, let us consider the Bogolubov shift \( \psi(r) \rightarrow \hat{\psi}(r) = \eta(r) + \psi_1(r) \) and the Hartree–Fock–Bogolubov (HFB) approximation. For simplicity, we assume a uniform system, when \( \eta(r) = \eta = \sqrt{\rho_0} \).

Let us be interested in the pair correlation function
\[
g(r_{12}) = \frac{1}{\rho^2} \left( \langle \hat{\psi}^\dagger(r_1) \psi^\dagger(r_1) \psi(r_2) \hat{\psi}(r_2) \rangle_{F(\rho_0)} \right),
\]
where \( r_{12} \equiv r_1 - r_2 \). In what follows, for short, we write \( \langle \ldots \rangle_{F(\rho_0)} \equiv \langle \ldots \rangle \).

Realizing, first, the Bogolubov shift and then the HFB approximation for \( \psi_1(r) \), we have
\[
\langle \psi^\dagger_1(r_1) \psi_1(r_1) \psi_1(r_2) \rangle = \rho_1(\psi_1(r_2)) + \rho_2(\psi^\dagger_1(r_2)) + \sigma(\bar{r}_1, r_2)(\psi^\dagger_1(r_1)),
\]
where the normal and anomalous averages, respectively, are
\[
\rho_1(\bar{r}_1, r_2) \equiv \langle \psi^\dagger_1(r_2) \psi_1(r_1) \rangle, \quad \rho_2(\bar{r}_1, r_2) \equiv \langle \psi_1(r_2) \psi^\dagger_1(r_1) \rangle, \quad \sigma(\bar{r}_1, r_2) \equiv \langle \psi^\dagger_1(r_2) \psi^\dagger_1(r_1) \psi_1(r_2) \psi_1(r_1) \rangle.
\]

In view of the conservation of quantum numbers, \( \langle \psi_1(r) \rangle = 0 \), the HFB approximation gives
\[
\langle \psi_1^\dagger(r_1) \psi_1(r_1) \psi_1(r_2) \rangle = 0.
\]

For the four-operator term, the HFB approximation yields
\[
\langle \psi_1^\dagger(r_1) \psi_1(r_1) \psi_1(r_2) \psi_1(r_2) \rangle = \rho_1^2 + |\rho_1(\bar{r}_1, r_2)|^2 + |\sigma(\bar{r}_1, r_2)|^2.
\]

In this way, we find the pair correlation function
\[
g(r_{12}) = 1 + \frac{2\rho_0}{\rho^2} \text{Re} \left[ \rho_1(\bar{r}_1, r_2) + \sigma(\bar{r}_1, r_2) \right] + \frac{1}{\rho^2} \left( |\rho_1(\bar{r}_1, r_2)|^2 + |\sigma(\bar{r}_1, r_2)|^2 \right).
\]

This function satisfies the correct limit
\[
\lim_{r_{12} \rightarrow \infty} g(r_{12}) = 1 \quad (r_{12} \equiv |r_{12}|).
\]

Now let us, first, use the HFB approximation for \( \psi(r) \) and then, make the Bogolubov shift. This gives
\[
g(r_{12}) \equiv 1 + \frac{2\rho_0}{\rho^2} + \frac{2\rho_0}{\rho^2} \text{Re} \left[ \rho_1(\bar{r}_1, r_2) + \sigma(\bar{r}_1, r_2) \right] + \frac{1}{\rho^2} \left( |\rho_1(\bar{r}_1, r_2)|^2 + |\sigma(\bar{r}_1, r_2)|^2 \right).
\]

The latter correlation function yields the limit
\[
\lim_{r_{12} \rightarrow \infty} g(r_{12}) = 1 + \frac{2\rho_0^2}{\rho^2},
\]
which is not correct when \( \rho_0 \neq 0 \).

Thus the correct order of actions is when, first, one accomplishes the Bogolubov shift and then invokes the HFB approximation for \( \psi_1(r) \). The origin of the noncommutativity of these actions is that the function \( \eta \) does not have the same commutation relations as \( \psi_1(r) \).

### 3.5. Action functional

The evolution equations can be derived in two ways, either by employing the Heisenberg equations of motion or by varying an effective action functional. These two ways are completely equivalent [24, 37]. The variation of an action functional is called the principle of minimal action [28].

For a system with Bose–Einstein condensate, we break the gauge symmetry by accomplishing the Bogolubov shift, thus, passing from the field operator \( \psi_1(r) \), defined on the Fock space \( F(\rho) \), to the operator \( \hat{\psi}(r) \), acting on the space \( F(\nu) \),
\[
\hat{\psi}(r) = \eta(r) + \psi_1(r).
\]

Thus we need to consider the energy Hamiltonian
\[
\hat{H} = \int \psi^\dagger(r) \left( -\frac{\nabla^2_2}{2m} + U \right) \psi(r) dr
+ \frac{1}{2} \int \psi^\dagger(r) \psi^\dagger(r') \Phi_\eta(r-r') \psi(r') \psi^\dagger(r) dr dr',
\]

in which \( U = U(r, t) \) is an external potential, and the interaction potential \( \Phi_\eta(r) = \Phi(r) \) assumed to be integrable.

The Lagrangian is
\[
\hat{L} = \int \psi^\dagger(r) \frac{\partial}{\partial t} \psi(r) dr - \hat{H},
\]

whose time integral gives the action functional. The evolution equations are derived from the conditional extremum of the action functional. Additional constraints, that are to be taken into account, include the normalization condition for the condensate function
\[
N_0 = \int \rho_0(\bar{r}) dr, \quad \rho_0 \equiv |\eta(r)|^2
\]

and the normalization condition for the number of uncondensed atoms
\[
N_1 = \langle \hat{N} \rangle, \quad \hat{N} \equiv \int \psi^\dagger(r) \psi(r) dr, \quad \hat{N} \equiv \langle \hat{N} \rangle.
\]

The total number of particles \( N \) is given by the average
\[
N = \langle \hat{N} \rangle, \quad \hat{N} = \int \psi^\dagger(r) \psi(r) dr,
\]

which can be written as
\[
N = \int \rho(r) dr, \quad \rho(r) \equiv \langle \psi^\dagger(r) \psi(r) \rangle.
\]

All averages are calculated in the space \( F(\nu) \). Because of the orthogonality condition (149), the operator of the total number of atoms is the sum \( \hat{N} = N_0 + N_1 \).

Since the gauge symmetry is broken, it could happen that \( \langle \psi_1(r) \rangle \) could be nonzero, which would imply that quantum numbers, such as spin and momentum, are not conserved and which would contradict the quantum-number conservation.
condition \(\langle \psi_0(r) \rangle = 0\). Therefore it is necessary to impose one more restriction

\[
\langle \hat{A} \rangle = 0, \quad \hat{A} \equiv \int \left[ \lambda(\mathbf{r}) \psi^*_1(\mathbf{r}) + \lambda^*(\mathbf{r}) \psi_1(\mathbf{r}) \right] d\mathbf{r}, \tag{161}
\]

guaranteeing the quantum-number conservation condition (46). Thus the effective action functional, taking into account the above constraints, reads as

\[
A[\eta, \psi_1] = \int \left[ \left( \hat{L}[\psi_1] + \mu_0 N_0 + \mu_1 N_1 + \hat{\Lambda} \right) \right] d\mathbf{r}, \tag{162}
\]

where \(\mu_0, \mu_1, \) and \(\lambda(\mathbf{r})\) are Lagrange multipliers.

Introducing the grand Hamiltonian \(H[\eta, \psi_1]\) as

\[
H[\eta, \psi_1] \equiv \hat{H} - \mu_0 N_0 - \mu_1 N_1 - \hat{\Lambda} \tag{163}
\]

and the effective Lagrangian

\[
L[\eta, \psi_1] = \int \left[ \eta^* \frac{\partial}{\partial t} \eta(\mathbf{r}) + \psi^*_1(\mathbf{r}) \frac{\partial}{\partial t} \psi_1(\mathbf{r}) \right] d\mathbf{r} - H[\eta, \psi_1],
\]

we get the effective action functional

\[
A[\eta, \psi_1] = \int L[\eta, \psi_1] d\mathbf{r}. \tag{164}
\]

The equations of motion for the condensate function and the field operator of uncondensed atoms are given by the extrema of the effective action functional:

\[
\left\{ \frac{\delta A[\eta, \psi_1]}{\delta \eta^* (\mathbf{r}, t)} \right\} = 0, \quad \left\{ \frac{\delta A[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)} \right\} = 0. \tag{165}
\]

The effective action functional correctly represents the considered statistical system only when it takes into account all constraints uniquely defining this system [30, 38].

### 3.6. Grand Hamiltonian

Substituting into the grand Hamiltonian (163) the Bogolubov shift (156) leads to the sum

\[
H[\eta, \psi_1] = \sum_{n=0}^{4} H^{(n)} \tag{166}
\]

of five terms \(H^{(n)}\) arranged according to the number of factors \(\psi_1(\mathbf{r})\) or \(\psi_1^*(\mathbf{r})\) in the operator products entering the corresponding parts. Thus, the zero-order term

\[
H^{(0)} = \int \eta^* (\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) d\mathbf{r}
\]

\[
+ \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}') \left| \eta(\mathbf{r}) \right|^2 \left| \eta(\mathbf{r}') \right|^2 d\mathbf{r}d\mathbf{r}' \tag{167}
\]

contains no operators of uncondensed atoms. Here \(\mu_0\) is the condensate chemical potential guaranteeing the normalization condition (159).

For the quantum-number conservation condition, it is necessary and sufficient that there would be no terms linear in \(\psi_1(\mathbf{r})\), which requires the Lagrange multiplier

\[
\lambda(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left| \eta(\mathbf{r}) \right|^2 \eta(\mathbf{r}') d\mathbf{r}'.
\]

Then the first-order term is zero, \(H^{(1)} = 0\). If the Hamiltonian would contain linear in \(\psi_1(\mathbf{r})\) terms, the average \(\langle \psi_1(\mathbf{r}) \rangle\) would be nonzero [38].

The second-order term is

\[
H^{(2)} = \int \psi_1^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) d\mathbf{r}
\]

\[
+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \eta(\mathbf{r}) \right]^2 \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}') + \eta(\mathbf{r}) \eta(\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r})
\]

\[
+ \frac{1}{2} \eta(\mathbf{r}) \eta(\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + \frac{1}{2} \eta(\mathbf{r}) \eta(\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \right] d\mathbf{r}d\mathbf{r}'. \tag{168}
\]

The third-order term reads as

\[
H^{(3)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \eta(\mathbf{r}) \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}') \psi_1(\mathbf{r})
\]

\[
+ \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \eta(\mathbf{r}) \right] d\mathbf{r}d\mathbf{r}'. \tag{169}
\]

And the fourth-order term is

\[
H^{(4)} = \frac{1}{2} \int \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \Phi(\mathbf{r} - \mathbf{r}' \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r})) d\mathbf{r}d\mathbf{r}'. \tag{170}
\]

The variation of action (165) is equivalent to the equations involving the variation of the grand Hamiltonian. The condensate function is described by the equation

\[
\left\{ \frac{\partial}{\partial t} \right\} \eta(\mathbf{r}, t) = \left\{ \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)} \right\}, \tag{171}
\]

while the equation for the field operator of uncondensed atoms is

\[
\left\{ \frac{\partial}{\partial t} \right\} \psi_1(\mathbf{r}, t) = \left\{ \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)} \right\}. \tag{172}
\]

As has been mentioned above, the variational equation (172) is equivalent to the Heisenberg equation of motion, since

\[
\left\{ \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)} \right\} = [\psi_1(\mathbf{r}, t), H[\eta, \psi_1]]. \tag{173}
\]

Equation (171) results in the condensate-function equation

\[
\left\{ \frac{\partial}{\partial t} \right\} \eta(\mathbf{r}, t) = \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r})
\]

\[
+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \eta(\mathbf{r}) \right]^2 \eta(\mathbf{r}) + \langle \hat{X}(\mathbf{r}, \mathbf{r}') \rangle \right] d\mathbf{r}', \tag{174}
\]

in which \(\eta(\mathbf{r}) \equiv \eta(\mathbf{r}, t), \psi_1(\mathbf{r}) \equiv \psi_1(\mathbf{r}, t), \) with the notation

\[
\hat{X}(\mathbf{r}, \mathbf{r}') \equiv \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \eta(\mathbf{r}) + \psi_1^*(\mathbf{r}) \eta(\mathbf{r}') \psi_1(\mathbf{r})
\]

\[
+ \eta(\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \psi_1(\mathbf{r}) \psi_1(\mathbf{r}).
\]

The field operator of uncondensed atoms satisfies the equation
\[ \frac{\partial}{\partial t} \psi_1(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) \]
\[ + \int \Phi(\mathbf{r} - \mathbf{r}') [\eta(\mathbf{r}')^2 \psi_1(\mathbf{r}) + \eta(\mathbf{r}') \eta(\mathbf{r}) \psi_1(\mathbf{r}')] \, d\mathbf{r}' \]
\[ + \eta(\mathbf{r}') \eta(\mathbf{r}) \psi_1(\mathbf{r}') + \tilde{X}(\mathbf{r}, \mathbf{r}') \] \, d\mathbf{r}' \tag{175} \]

Recall that, after accomplishing the Bogolubov shift, all operators are defined on the Fock space \( \mathcal{F}(\psi_1) \).

### 3.7. Conservation laws

Correctly defining the operators on the Fock space \( \mathcal{F}(\psi_1) \), with broken gauge symmetry, preserves all conservation laws corresponding to the relations between the operators of local observables.

Let us derive the continuity equations. For this purpose, we define the density of current for condensed atoms,

\[ j_\nu(\mathbf{r}) \equiv -\frac{i}{2m} [\eta^*(\mathbf{r}) \nabla \eta(\mathbf{r}) - \eta(\mathbf{r}) \nabla \eta^*(\mathbf{r})], \tag{176} \]

and the density of current for uncondensed atoms,

\[ j_\nu(\mathbf{r}) \equiv -\frac{i}{2m} \{ \psi(\mathbf{r}) \nabla \psi(\mathbf{r}) - [\nabla \psi^*(\mathbf{r})] \psi(\mathbf{r}) \}. \tag{177} \]

Also, we introduce the operator source

\[ \hat{\Gamma}(\mathbf{r}) \equiv \int \Phi(\mathbf{r} - \mathbf{r}') [\tilde{\Xi}(\mathbf{r}, \mathbf{r}') + \tilde{\Xi}^*(\mathbf{r}, \mathbf{r}')] \, d\mathbf{r}', \]

in which

\[ \tilde{\Xi}(\mathbf{r}, \mathbf{r}') = i \eta^*(\mathbf{r}) [\psi^*_1(\mathbf{r}') \eta(\mathbf{r}') + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') + \psi^*_1(\mathbf{r}') \psi_1(\mathbf{r}')] \psi_1(\mathbf{r}). \]

Using these notations, we find the equation connecting the density and current of condensate,

\[ \frac{\partial}{\partial t} \rho_0(\mathbf{r}) + \nabla \cdot j_\nu(\mathbf{r}) = -\hat{\Gamma}(\mathbf{r}), \tag{178} \]

and the operator relation between the operator density of uncondensed atoms and their density of current

\[ \frac{\partial}{\partial t} \tilde{n}_\nu(\mathbf{r}) + \nabla \cdot j_\nu(\mathbf{r}) = \hat{\Gamma}(\mathbf{r}), \tag{179} \]

where \( \tilde{n}_\nu(\mathbf{r}) \equiv \psi^*_1(\mathbf{r}) \psi_1(\mathbf{r}) \).

For the total operator density of atoms and the total density of current

\[ \tilde{n}(\mathbf{r}) \equiv \rho_0(\mathbf{r}) + \tilde{n}_\nu(\mathbf{r}), \quad \tilde{j}(\mathbf{r}) \equiv j_\nu(\mathbf{r}) + j_\nu(\mathbf{r}), \]

we obtain the continuity equation

\[ \frac{\partial}{\partial t} \tilde{n}(\mathbf{r}) + \nabla \cdot \tilde{j}(\mathbf{r}) = 0. \tag{180} \]

Similarly, it is straightforward to derive other relations between the operators of local observables characterizing operator conservation laws.

### 3.8. Condensate function

The condensate function \( \eta(\mathbf{r}, t) \) is the solution to equation (174). Accomplishing there the averaging over the space \( \mathcal{F}(\psi_1) \), we have

\[ \langle \tilde{X}(\mathbf{r}, \mathbf{r}') \rangle = \rho_0(\mathbf{r}) \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') \]
\[ + \langle \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle, \]

where

\[ \rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}), \quad \rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2. \]

\[ \rho_1(\mathbf{r}) \equiv \langle \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \rangle. \]

Then equation (174) becomes

\[ i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) \]
\[ + \int \Phi(\mathbf{r} - \mathbf{r}') \{ \rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') \}
\[ + \sigma(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle \} \, d\mathbf{r}'. \tag{181} \]

In equilibrium, the function \( \eta(\mathbf{r}) \) does not depend on time, which gives the eigenproblem

\[ \mu_0 \eta(\mathbf{r}) = \left[ -\frac{\nabla^2}{2m} + U \right] \eta(\mathbf{r}) \]
\[ + \int \Phi(\mathbf{r} - \mathbf{r}') \{ \rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') \}
\[ + \sigma(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle \} \, d\mathbf{r}'. \tag{182} \]

where \( \mu_0 \) plays the role of an eigenvalue. Generally, this eigenproblem can define the whole spectrum of eigenvalues. The condition of equilibrium implies that \( \mu_0 \) is given by the lowest eigenvalue.

Note that if we would take \( \eta(\mathbf{r}, t) \propto e^{-\imath \lambda t} \), this would be just a redefinition of \( \mu_0 \). So, it is sufficient to accept that in equilibrium the condensate function \( \eta(\mathbf{r}) \) does not depend on time.

In the case of a uniform system, where \( U = 0 \), we have \( \eta(\mathbf{r}) = \eta = \sqrt{\rho_0} \) and \( \rho(\mathbf{r}) = \rho \). The quantities \( \rho_1(\mathbf{r}, \mathbf{r}') \) and \( \sigma(\mathbf{r}, \mathbf{r}') \) depend on \( \mathbf{r} - \mathbf{r}' \). Then equation (182) reduces to

\[ \mu_0 \eta = \rho \Phi \eta + \int \Phi(\mathbf{r}) \{ \rho_1(\mathbf{r}, 0) \eta + \sigma(\mathbf{r}, 0) \eta^* \}
\[ + \langle \psi_1^*(0) \psi_1(0) \psi_1(\mathbf{r}) \rangle \} \, d\mathbf{r}. \tag{183} \]

When we transform these general equations by resorting to the Hartree–Fock–Bogolubov (HFB) approximation, we take into account that in this approximation

\[ \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) = \rho_1(\mathbf{r}') \psi_1(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \psi_1(\mathbf{r}') + \sigma(\mathbf{r}, \mathbf{r}') \psi_1^2(\mathbf{r}') \]

Hence

\[ \langle \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle = 0. \]
The four-operator term takes the form
\[
\psi^\dagger(\mathbf{r}) \psi(\mathbf{r})^\dagger \psi(\mathbf{r}) \psi(\mathbf{r})^\dagger = \rho(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})^\dagger + \rho(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})^\dagger + \rho(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})^\dagger + \sigma(\mathbf{r}, \mathbf{r}') \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}')^\dagger,
\]

Therefore, in the HFB approximation, the condensate-function equation becomes
\[
\frac{\partial}{\partial t} \eta(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \rho(\mathbf{r}) \eta(\mathbf{r}') + \rho(\mathbf{r}) \eta(\mathbf{r}') + \sigma(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') \right] d\mathbf{r}'.
\]

And the equation for the field operator of uncondensed atoms is
\[
\frac{\partial}{\partial t} \psi(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \rho(\mathbf{r}) \psi(\mathbf{r}') + \rho(\mathbf{r}) \psi(\mathbf{r}') + \sigma(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \right] d\mathbf{r}'.
\]

In the latter equation, the terms quadratic in \( \psi(\mathbf{r}) \) are omitted.

For an equilibrium system in the HFB approximation, we have the equation
\[
\mu_0 \eta(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \rho(\mathbf{r}) \eta(\mathbf{r}') + \rho(\mathbf{r}) \eta(\mathbf{r}') + \sigma(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') \right] d\mathbf{r}'.
\]

In equilibrium, this reduces to the eigenproblem
\[
\int | \eta(\mathbf{r}) |^2 d\mathbf{r} = N_0
\]
is assumed.

The mathematical structure of equations (188) and (189) corresponds to the general nonlinear Schrödinger (NLS) equations [39], while (190) is the stationary NLS equation. Such equations are employed for modelling many problems, for instance, surface waves on a deep fluid [40], electromagnetic waves in fiber optics [41, 42], and Bose–Einstein condensates [43–46].

The most general form (188) of the equation for Bose systems was, first, advanced by Bogolubov during his lectures in the Moscow State University and Kiev State University and published in 1949 in his famous Lectures on Quantum Statistics [47]. Since then, these lectures have been republished numerous times, e.g. in [16, 18, 19]. Bogolubov analyzed in detail the particular case of equilibrium uniform systems [8, 9, 16, 18, 19] as well as the general case of nonequilibrium systems exhibiting superfluid hydrodynamics [48].

Equations (188) and (189) were investigated by Gross in a series of papers [49–53] and different nonuniform solutions were found, including periodic and vortex solutions.

Note that the Ginzburg-Landau equation [54, 55] for superconductors has also the structure of the NLS equation and reduces to the above equations under zero vector potential. Abrikosov [56] found vortex solutions for the Ginzburg-Landau equation. Therefore, such solutions should also exist for the NLS equations (188) and (189), for which the vortex solutions were found as well [52, 53, 57–59]. The role
of vortices in superfluid hydrodynamics was emphasized by Iordanskii [60].

Comparing the equations for the condensate function (181) and (188), we see that the vacuum state can be approximately achieved in a physical system, when practically all atoms are condensed, which requires asymptotically low temperature and asymptotically weak interactions.

In an equilibrium system at finite temperature, the condensate function $\eta(\mathbf{r})$ realizes a minimum of the grand thermodynamic potential

$$\Omega = -T \ln \text{Tr}_{\mathcal{F}(\psi)} \exp\{-\beta H[\eta, \psi_1]\}.$$  

The extremum condition

$$\frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} = \left\langle \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r})} \right\rangle = 0$$

is in agreement with the evolution equation (171) for an equilibrium system, when the condensate function does not depend on time. Thermodynamic stability conditions guarantee that this extremum is a minimum. The so minimized grand potential $\Omega$ characterizes an absolutely stable equilibrium system.

3.9. Thermodynamic self-consistency

Statistical ensemble is a pair of the Fock space describing the system and a statistical operator. The Fock space for a Bose-condensed system is $\mathcal{F}(\psi)$. The statistical operator for an equilibrium system can be found from the principle of minimal information [1, 61] that implies conditional maximization of entropy [62, 63].

Statistical conditions for an equilibrium system are as follows. The statistical operator is normalized, such that $1 = \langle \hat{1} \rangle = \text{Tr}\hat{\rho}$, where $\hat{1}$ is the unity operator in the space $\mathcal{F}(\psi)$. The internal energy is $E = \langle \hat{H} \rangle = \text{Tr}\hat{\rho}\hat{H}$. The number of condensed atoms is $N_0 = \langle \hat{N}_0 \rangle$, with $\hat{N}_0 \equiv \hat{N}_0 \hat{1}$. The number of uncondensed atoms is $N_1 = \langle \hat{N}_1 \rangle$. And the quantum-number conservation condition reads as $\langle \hat{\lambda} \rangle = 0$. This defines the information functional,

$$I[\hat{\rho}] = \text{Tr}\hat{\rho}\ln \hat{\rho} + \lambda_0(\text{Tr}\hat{\rho} - 1) + \beta(\text{Tr}\hat{\rho}\hat{H} - E)$$

$$- \beta \mu_0(\text{Tr}\hat{\rho}\hat{N}_0 - N_0) - \beta \mu_1(\text{Tr}\hat{\rho}\hat{N}_1 - N_1) - \beta \text{Tr}\hat{\rho}\hat{\lambda}.$$  

(191)

The minimization of the information functional yields the statistical operator

$$\hat{\rho} = \frac{1}{Z} \exp\{-\beta H[\eta, \psi_1]\},$$

(192)

with the same grand Hamiltonian as in the evolution equations and with the partition function

$$Z \equiv \text{Tr}\exp\{-\beta H[\eta, \psi_1]\}.$$  

Both dynamic and equilibrium properties are governed by the same grand Hamiltonian.

For an equilibrium system, the Bogolubov–Ginibre condition

$$\frac{\partial \Omega}{\partial N_0} = \left\langle \frac{\partial H[\eta, \psi_1]}{\partial N_0} \right\rangle = 0$$

holds, since

$$\frac{\partial \Omega}{\partial N_0} = \int \left[ \frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} \frac{\partial \eta^*(\mathbf{r})}{\partial N_0} + \frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} \frac{\partial \eta^*(\mathbf{r})}{\partial N_0} \right] d\mathbf{r}$$

and

$$\frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} = 0.$$  

The free energy $F = \Omega + \mu_0 N_0 + \mu_1 N_1$, under the total number of particles $N$ being fixed, can also be written as $F = \Omega + \mu N$, where $\mu$ is the system chemical potential. Comparison of these expressions gives the system chemical potential

$$\mu = \mu_0 n_0 + \mu_1 n_1.$$  

(194)

Free energy and grand potential are connected through the differential relations

$$dF = -SdT + PdV + \mu dN, \quad d\Omega = -SdT + PdV - Nd\mu.$$  

It is easy to show that the thermodynamic and Gibbs entropies coincide,

$$S = -\frac{\partial \Omega}{\partial T} = -\text{Tr}\hat{\rho}\ln \hat{\rho}.$$  

For the particle variance, we have

$$\text{var}(\hat{N}) = T \frac{\partial N}{\partial \mu}.$$  

(195)

This can be proved as follows. From the equations

$$N_0 = -\frac{\partial \Omega}{\partial \mu_0}, \quad N_1 = -\frac{\partial \Omega}{\partial \mu_1}, \quad N = -\frac{\partial \Omega}{\partial \mu} = N_0 + N_1$$  

we get

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial \Omega}{\partial \mu_0} + \frac{\partial \Omega}{\partial \mu_1}.$$  

Differentiating again leads to the relation

$$\frac{\partial^2 \Omega}{\partial \mu^2} = \frac{\partial^2 \Omega}{\partial \mu_0^2} + \frac{\partial^2 \Omega}{\partial \mu_1^2} + 2\frac{\partial^2 \Omega}{\partial \mu_0 \partial \mu_1}.$$  

By direct calculations, we find

$$\frac{\partial^2 \Omega}{\partial \mu_0^2} = -\beta \text{var}(\hat{N}_0), \quad \frac{\partial^2 \Omega}{\partial \mu_1^2} = -\beta \text{var}(\hat{N}_1),$$

$$\frac{\partial^2 \Omega}{\partial \mu_0 \partial \mu_1} = -\beta \text{cov}(\hat{N}_0, \hat{N}_1).$$  

Hence,

$$\frac{\partial N}{\partial \mu} = -\frac{\partial^2 \Omega}{\partial \mu^2} = \beta \text{var}(\hat{N}),$$  

which gives equation (195).

32
In this way, it is straightforward to show that all thermodynamic relations are valid \[24, 30, 38\].

3.10. Nonuniform matter

The HFB approximation can be used for the general case of a nonuniform system. Defining the normal and anomalous averages

\[
\rho(r, r') \equiv \langle \psi^\dagger(r') \psi(r) \rangle, \quad \sigma(r, r') \equiv \langle \psi^\dagger(r') \psi(r) \rangle, \quad (196)
\]

we remember that the field operators depend on time, \(\psi_t(r, t)\), while time is not explicitly shown. So that, in general, the consideration of the present section is applicable to nonequilibrium systems as well.

We use the notation

\[
\rho_0(r) = |\psi(r)|^2, \quad \rho_1(r) = \rho_1(r, r), \quad \rho_2(r) = \rho_2(r) + \rho_2(r, r), \quad (197)
\]

and keep in mind that \(\langle \psi(r) \rangle = 0\).

If the Hamiltonian would contain linear in \(\psi(r)\) terms, then \(\langle \psi^\dagger(r) \psi(r) \rangle\) would not be zero. Therefore the Lagrange multiplier \(\lambda(r)\) is chosen so that to kill the linear in \(\psi(r)\) terms. Then in the HFB approximation, we have \(H^{(3)} = 0\), implying that all matrix elements of this term are zero.

In the HFB approximation, Hamiltonian (166) becomes

\[
H_{\text{HFB}} = E_{\text{HFB}} + \int \psi^\dagger(r)\left(-\frac{\nabla^2}{2m} + U - \mu_1\right)\psi(r)dr + \int \Phi(r - r')\left[\rho_1(r')\psi_1(r) + \rho_1(r)\psi_1^\dagger(r')\right]drdr' + \frac{1}{2}\sigma(r, r')\psi_1(r)\psi_1^\dagger(r) + \frac{1}{2}\sigma(r', r')\psi_1^\dagger(r')\psi_1(r)drdr',
\]

where

\[
E_{\text{HFB}} = H^{(0)} - \frac{1}{2} \int \Phi(r - r')\left[\rho_1(r')\rho_1(r) + |\rho_1(r, r')|^2\right]drdr',
\]

(198)

For a nonuniform system, the Bogolubov canonical transformations read as

\[
\psi_1(r) = \sum_k [u_k(r)b_k + v_k^*(r)b_k^*], \\
\psi_1^\dagger(r) = \sum_k [u_k^*(r)b_k^* + v_k(r)b_k],
\]

(200)

where \(b_k = b_k(t)\) and \(k\) is a set of quantum numbers. The inverse transformations are

\[
b_k = \int [v_k^*(r)\psi_1^\dagger(r) - v_k^*(r)\psi_1(r)] dr, \\
b_k^* = \int [u_k^*(r)\psi_1^\dagger(r) - u_k^*(r)\psi_1(r)] dr.
\]

The requirement that \(b_k^*\) and \(b_k\) be Bose operators yields the equations

\[
\sum_k [u_k(r)v_k^*(r') - v_k^*(r)u_k(r')] = 0,
\]

\[
\sum_k [u_k(r)\tilde{u}_k^*(r') - \tilde{v}_k^*(r)u_k(r')] = \delta(r - r'),
\]

\[
\int [u_k(r)v_k^*(r) - v_k^*(r)u_k(r)] dr = 0,
\]

\[
\int [u_k^*(r)\tilde{u}_k(r') - \tilde{v}_k(r)\tilde{u}_k^*(r')] dr = \delta_{pp'}.
\]

We introduce the quantities

\[
\omega(r, r') \equiv \left[\frac{-\nabla^2}{2m} + U(r) - \mu_1 + \int \Phi(r - r')\rho(r')dr\right] \delta(r - r') + \Phi(r - r')\rho(r, r'),
\]

(202)

and

\[
\Delta(r, r') \equiv \Phi(r - r')\sigma(r, r').
\]

(203)

Requiring that the resulting Hamiltonian be diagonal imposes the Bogolubov diagonalization equations

\[
\int [\omega(r, r')u_k^*(r') + \Delta(r, r')v_k(r')] dr' = \varepsilon_k u_k(r),
\]

\[
\int [\omega(r, r')v_k^*(r') + \Delta(r, r')u_k(r')] dr' = -\varepsilon_k v_k(r).
\]

(204)

The same equations can be obtained by substituting the transformations for \(\psi_1(r)\) and \(\psi_1^\dagger(r)\) into their equations of motion within the \(H_{\text{HFB}}\) approximation, that is the linearized equation for \(\psi(r)\).

Employing the Bogolubov equations (204) transforms Hamiltonian (198) into the diagonal Hamiltonian

\[
H_B = E_0 + \sum_k \varepsilon_k b_k^\dagger b_k, \quad E_0 = E_{\text{HFB}} - \sum_k \varepsilon_k \int |v_k(r)|^2 dr.
\]

(205)

The operators \(b_k\) represent collective excitations called bogolons.

The Hamiltonian \(H_B\) is defined on the space \(\mathcal{F}(b_k)\), with the averages \(\langle \ldots \rangle\) implying the averaging in the space \(\mathcal{F}(b_k)\) with \(H_B\). This leads to the bogolon distribution

\[
\pi_k \equiv \langle b_k^\dagger b_k \rangle = (e^{\varepsilon_k} - 1)^{-1},
\]

(206)

while \(\langle b_k b_k^\dagger \rangle = 0\). The single-particle density matrix of uncondensed atoms reads as

\[
\rho_0(r, r') = \sum_k [\pi_k u_k^*(r)u_k^\dagger(r') + (1 + \pi_k)v_k^2(r)v_k(r')],
\]

(207)

the related atomic density being

\[
\rho_\lambda(r) = \sum_k [\pi_k |u_k(r)|^2 + (1 + \pi_k)|v_k(r)|^2].
\]

(208)

The anomalous density matrix

\[
\sigma_\lambda(r, r') = \sum_k [\pi_k u_k(r)\tilde{u}_k(r') + (1 + \pi_k)u_k^2(r)u_k(r')]
\]

(209)
gives the anomalous average
\[
\sigma_{\mathbf{r}}(\mathbf{r}) \equiv \sigma_{\mathbf{r}}(\mathbf{r}, \mathbf{r}) = \sum_{k} (1 + 2\eta_{k}) u_{k}(\mathbf{r}) v_{k}^{*}(\mathbf{r}).
\] (210)

The concrete nature of the quantum numbers \(k\) and the explicit expressions for the coefficient functions \(u_{k}\) and \(v_{k}\) in the Bogolubov equations (204) depend on the form of the external potential \(U(\mathbf{r})\).

### 3.11. Uniform system

When there is no external potential, \(U(\mathbf{r}) = 0\), a large system is uniform. Then one expands the field operators in plane waves,
\[
\psi_{1}(\mathbf{r}) = \sum_{k} a_{k}\phi_{k}(\mathbf{r}), \quad \phi_{k}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}.
\]
The condensate function does not depend on spatial variables and, in equilibrium, can be chosen to be real, such that \(\eta(\mathbf{r}) = \eta = \eta^{*} = \sqrt{\rho_{0}}\). The normal and anomalous single-particle density matrices can be written as the expansions
\[
\rho_{1}(\mathbf{r}, \mathbf{r}) = \sum_{k} n_{k}\phi_{k}(\mathbf{r})\phi_{k}^{*}(\mathbf{r}), \quad n_{k} \equiv \langle a_{k}^{\dagger}a_{k} \rangle,
\]
\[
\sigma_{1}(\mathbf{r}, \mathbf{r}) = \sum_{k} \sigma_{k}\phi_{k}(\mathbf{r})\phi_{k}^{*}(\mathbf{r}), \quad \sigma_{k} \equiv \langle a_{k}^{\dagger}a_{-k} \rangle.
\] (211)

And the density matrices (197) become
\[
\rho(\mathbf{r}, \mathbf{r}) = \rho_{0} + \rho_{1}(\mathbf{r}, \mathbf{r}), \quad \sigma(\mathbf{r}, \mathbf{r}) = \rho_{0} + \sigma_{1}(\mathbf{r}, \mathbf{r}),
\]
with the total density \(\rho(\mathbf{r}) = \rho = \rho_{0} + \rho_{1}\). The interaction potential is assumed to enjoy the Fourier transform
\[
\Phi_{k} = \int \Phi_{r} e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}.
\]

The grand Hamiltonian (166) is the sum of five terms, with the zero-order term
\[
H^{(0)} = \left(\frac{1}{2} \rho_{0}\Phi_{0} - \mu_{0}\right) N_{0}.
\] (212)

The first-order term is exactly zero, \(H^{(1)} = 0\), because of the orthogonality of the plane waves with \(k \neq 0\) and \(k = 0\). The second-order term is
\[
H^{(2)} = \sum_{k} \left\{ \frac{k^{2}}{2m} + \rho_{0}(\Phi_{0} + \Phi_{k}) - \mu_{1} \right\} a_{k}^{\dagger}a_{k} + \frac{1}{2} \sum_{k} \rho_{0}\Phi_{k} a_{k}^{\dagger}a_{k} + \frac{1}{2} \sum_{k} \sigma_{k} a_{k}^{\dagger}a_{k}.
\] (213)

The third-order term reads as
\[
H^{(3)} = \frac{\rho_{0}}{\sqrt{V}} \sum_{p,q} \Phi_{p} a_{p}^{\dagger}a_{q}^{\dagger}a_{-p-m_{q}} + \frac{1}{2} \sum_{k} \sigma_{k} a_{k}^{\dagger}a_{k}.
\] (214)

where the prime implies that \(p \neq 0, q \neq 0\), and \(p - q = 0\). The fourth-order term takes the form
\[
H^{(4)} = \frac{1}{2V} \sum_{k} \sum_{p,q} \Phi_{q} a_{p}^{\dagger}a_{q}^{\dagger}a_{k}^{\dagger}a_{-p-m_{q}}.
\] (215)
in which \(p \neq 0, q \neq 0, k + p = 0\), and \(k - q = 0\).

In the HFB approximation, we have
\[
\begin{align*}
\langle a_{k}^{\dagger}a_{q} \rangle & = \langle a_{k}^{\dagger}a_{q} \rangle, \\
\langle a_{p}a_{q} \rangle & = \langle a_{p}a_{q} \rangle + \langle a_{k}^{\dagger}a_{p} \rangle + \langle a_{q}a_{k} \rangle - \langle a_{p} \rangle \langle a_{q} \rangle - \langle a_{k}^{\dagger}a_{p} \rangle - \langle a_{q}a_{k} \rangle,
\end{align*}
\]
and
\[
\begin{align*}
\langle a_{k}a_{q} \rangle & = \langle a_{k}a_{q} \rangle, \\
\langle a_{p} \rangle & = \langle a_{p} \rangle. 
\end{align*}
\]

This gives \(H^{(3)} = 0\) in the HFB approximation, since \(\langle a_{k} \rangle = 0\) for \(k \neq 0\).

Employing the HFB approximation to the fourth-order term, we use the quantum number conservation condition,
\[
\langle a_{k}^{\dagger}a_{p} \rangle = \delta_{kp}(\langle a_{1} \rangle), \quad \langle a_{p}a_{k} \rangle = \delta_{kp}(\langle a_{-1} \rangle).
\]

Then we get
\[
\begin{align*}
H^{(4)} & = \sum_{k} \rho_{1} \Phi_{k} \left( a_{k}^{\dagger}a_{k} - \frac{1}{2} \mu_{1} \right) \\
& + \frac{1}{V} \sum_{p,q} \Phi_{q} \left[ n_{p}a_{p}^{\dagger}a_{p}^{\dagger} + \frac{1}{2} \left( \sigma_{k}^{*}a_{p}^{\dagger}a_{p}^{\dagger} + \sigma_{k}^{*}a_{p}^{\dagger}a_{p} \right) - \frac{1}{2} (n_{p}a_{p}^{\dagger}a_{p}^{\dagger}) \right],
\end{align*}
\] (216)

Let us introduce the notations
\[
\omega_{k} \equiv \frac{k^{2}}{2m} + \rho_{0}\Phi_{k} + \frac{1}{V} \sum_{p=0}^{\infty} n_{p} \Phi_{k+p} - \mu_{1}
\] (217)
and
\[
\Delta_{k} \equiv \rho_{0}\Phi_{k} + \frac{1}{V} \sum_{p=0}^{\infty} \sigma_{p}\Phi_{k+p}.
\] (218)

These are related to the general nonuniform case by the expansions
\[
\begin{align*}
\omega(\mathbf{r}, \mathbf{r}) & = \sum_{k} \omega_{k}(\mathbf{r}) \phi_{k}(\mathbf{r})^{2}, \\
\omega_{k} & = \int \phi_{k}(\mathbf{r})^{2}(\omega(\mathbf{r}, \mathbf{r})) \phi_{k}(\mathbf{r}) d\mathbf{r}^{*}, \\
\Delta(k, \mathbf{r}, \mathbf{r}) & = \sum_{k} \Delta_{k}(\mathbf{r}) \phi_{k}(\mathbf{r})^{2}, \\
\Delta_{k} & = \int \phi_{k}(\mathbf{r})^{2}(\Delta(k, \mathbf{r}, \mathbf{r})) \phi_{k}(\mathbf{r}) d\mathbf{r}^{*}.
\end{align*}
\]

Thus the grand Hamiltonian of a uniform system in the HFB approximation reduces to
\[
H_{\text{HFB}} = E_{\text{HFB}} + \sum_{k=0}^{\infty} \omega_{k} a_{k}^{\dagger}a_{k} + \frac{1}{2} \sum_{k=0}^{\infty} \Delta_{k} a_{k}^{\dagger}a_{-k} + a_{-k}a_{k},
\] (219)
with
\[
E_{\text{HFB}} = H^{(0)} - \frac{1}{2} \rho_{0}\Phi_{0} N_{0} - \frac{1}{2V} \sum_{k=0}^{\infty} \Phi_{k+p}(n_{p}a_{p}^{\dagger}a_{p}).
\] (220)

Substituting to equations (204) the functions \(u_{k}(\mathbf{r}) = u_{k}\phi_{k}(\mathbf{r})\) and \(v_{k}(\mathbf{r}) = v_{k}\phi_{k}(\mathbf{r})\) yields the Bogolubov diagonalization equations.
\[ (\omega_k - \varepsilon_k)u_k + \Delta_k v_k = 0, \quad \Delta_k u_k + (\omega_k + \varepsilon_k)v_k = 0, \quad (221) \]

where

\[ \varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2} \]

is the spectrum of collective excitations.

The condition of the condensate existence

\[ \lim_{k \to 0} \varepsilon_k = 0, \quad \varepsilon_k \gg 0 \]

defines

\[ \mu_1 = \rho \Phi_0 + \frac{1}{V} \sum_{p=0} \Phi_p (n_p - \sigma_p). \]

The condensate chemical potential \((187)\) becomes

\[ \mu_0 = \rho \Phi_0 + \frac{1}{V} \sum_{p=0} (n_p + \sigma_p) \Phi_p. \]

As is evident, \(\mu_0\) and \(\mu_1\) are different,

\[ \mu_0 - \mu_1 = \frac{2}{V} \sum_{p=0} \sigma_p \Phi_p. \]

In the dilute-gas approximation, we have

\[ \mu_0 = (\rho + \rho_1 + \sigma_1) \Phi_0, \quad \mu_1 = (\rho + \rho_1 - \sigma_1) \Phi_0. \]

Hamiltonian \((219)\) is diagonalized by the Bogolubov canonical transformation \(a_k = u_k b_k + v_k^* b_k^\dagger\) similarly to this procedure in the Bogolubov approximation, but with different \(\omega_k\) and \(\Delta_k\) defined in equations \((217)\) and \((218)\). For the coefficient functions, we now have

\[ u_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta_k^2} + \varepsilon_k}{2\varepsilon_k}, \quad v_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta_k^2} - \varepsilon_k}{2\varepsilon_k}, \]

\[ u_k^2 - v_k^2 = 1, \quad u_k v_k = -\frac{\Delta_k}{2\varepsilon_k}, \]

\[ \frac{u_k^2 + v_k^2}{\varepsilon_k} = \frac{\omega_k}{\varepsilon_k}. \]

The normal and anomalous averages, in the momentum representation, are

\[ n_k = \frac{\sqrt{\varepsilon_k^2 + \Delta_k^2}}{2\varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right) - \frac{1}{2}, \quad \sigma_k = -\frac{\Delta_k}{2\varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right). \]

(227)

At small excitation energy, such that \(\varepsilon_k \ll \Delta_k\) and \(\varepsilon_k \ll T\), these averages behave as

\[ n_k \approx \frac{T \Delta_k}{\varepsilon_k} + \frac{\Delta_k}{12T} + \frac{T}{2\Delta_k} - \frac{1}{2} + \left( \frac{\Delta_k}{3T} - \frac{T}{\Delta_k} - \frac{\Delta_k^3}{90T^3} \right) \frac{\varepsilon_k^2}{8\Delta_k^2}. \]

While at high excitation energy, when \(\varepsilon_k \gg \Delta_k\) and \(\varepsilon_k \gg T\), their asymptotic forms are

\[ n_k \approx \left( \frac{\Delta_k}{2\varepsilon_k} \right)^2 - \left( \frac{\Delta_k}{2\varepsilon_k} \right)^4 + e^{-\beta \varepsilon_k}, \quad \sigma_k \approx -\frac{\Delta_k}{2\varepsilon_k} (1 + 2e^{-\beta \varepsilon_k}). \]

Comparing these expressions, we see that the anomalous average \(\sigma_k\) is of order or larger than the normal average \(n_k\), hence \(\sigma_k\) can never be neglected \([26]\).

Diagonalizing Hamiltonian \((219)\), we come to the Bogolubov Hamiltonian

\[ H_B = E_B + \sum_{k=0} \varepsilon_k b_k^\dagger b_k, \]

(228)

in which

\[ E_B = E_{\text{HFB}} - \frac{1}{2} \sum_{k=0} (\omega_k - \varepsilon_k). \]

Here \(\omega_k\) is expression \((217)\) that can be written as

\[ \omega_k = \frac{k^2}{2m} + \Delta + \rho_0 (\Phi_k - \Phi_0) + \frac{1}{V} \sum_{p=0} n_p (\Phi_{k+p} - \Phi_p). \]

(229)

where

\[ \Delta \equiv \lim_{k \to 0} \Delta_k = \rho_0 \Phi_0 + \frac{1}{V} \sum_{p=0} \sigma_p \Phi_p. \]

In the long-wave limit \(k \to 0\), we have the following expansions:

\[ \Phi_{p+k} \approx \Phi_p + \frac{1}{2} \Phi_p'' k^2, \quad \Phi_p'' \equiv \frac{\partial^2 \Phi_p}{\partial p^2}, \]

\[ \omega_k \approx \Delta + \frac{1}{2} \left( \frac{1}{m} + \rho_0 \Phi_p'' + \frac{1}{V} \sum_{p=0} n_p \Phi_p'' k^2, \right) \]

\[ \Delta_k \approx \Delta + \frac{1}{2} \left( \rho_0 \Phi_p'' + \frac{1}{V} \sum_{p=0} \sigma_p \Phi_p'' k^2. \right) \]

Using these expansions, it is straightforward to show that, in the long-wave limit \(k \to 0\), the spectrum of collective excitations \((222)\) is phonon-like,

\[ \varepsilon_k \approx ck, \quad c \equiv \frac{\Delta}{\sqrt{m^*}}, \]

(231)

with the sound velocity \(c\), in which

\[ m^* \equiv \frac{m}{1 + \frac{m}{V} \sum_{p=0} (n_p - \sigma_p) \Phi_p^2} \]

is effective mass.

The HFB Hamiltonian \((219)\) as well as the Bogolubov Hamiltonian \((228)\) are quadratic in the field operators \(a_k\) or \(b_k\). Therefore, calculating observable quantities, we have to limit such calculations by the terms of second order in the field.
operators. Thus, calculating \( \text{var}(\hat{N}) \), we have to keep only the terms of second order with respect to \( \rho_0 \). The variance \( \text{var}(\hat{N}) \) is an important quantity characterizing the system stability. The variance can be represented as

\[
\text{var}(\hat{N}) = N \left\{ 1 + \rho \int [g(r) - 1] \, dr \right\},
\]

with the pair correlation function

\[
g(r) = 1 + \frac{2\rho_0}{\rho^2} \text{Re} \left[ \rho_0(0,0) + \sigma(0,0) \right]
\]

in second order with respect to the field operators. Because of the equations \( n_k^+ = n_{-k} = n_k \) and \( \sigma_k^+ = \sigma_{-k} = \sigma_k \), the expressions \( \rho_0(r,0) \) and \( \sigma(r,0) \) are real and have the form

\[
\rho_0(r,0) = \frac{1}{V} \sum_{k=0} \rho_0 e^{ik \cdot r}, \quad \sigma(r,0) = \frac{1}{V} \sum_{k=0} \sigma_k e^{ik \cdot r}.
\]

This gives the pair correlation function

\[
g(r) = 1 + \frac{2\rho_0}{\rho^2} \int (n_k + \sigma_k) e^{ik \cdot r} \, dk \frac{d}{(2\pi)^3}.
\]

Since

\[
\int [g(r) - 1] \, dr = \frac{2\rho_0}{\rho^2} \lim_{k \to 0} (n_k + \sigma_k),
\]

we get

\[
\text{var}(\hat{N}) = \frac{N}{1 + \rho} \lim_{k \to 0} (n_k + \sigma_k),
\]

Under the condition \( \rho_0/\rho \approx 1 \), we find

\[
\text{var}(\hat{N}) = N \left\{ 1 + 2 \lim_{k \to 0} (n_k + \sigma_k) \right\},
\]

\[
\lim_{k \to 0} (n_k + \sigma_k) = \frac{1}{2} (\frac{T}{\Delta} - 1),
\]

where

\[
\Delta = \rho_0 \Phi_0 + \int \sigma_k \Phi_k \, dk \frac{d}{(2\pi)^3} = m^* c^2.
\]

It is again worth stressing the importance of the anomalous average \( \sigma_k \), without which \( \text{var}(\hat{N})/N \) would be divergent. But calculating the variance correctly, we find the latter and, respectively, compressibility in the form

\[
\text{var}(\hat{N}) = \frac{T}{m^* c^2}, \quad \kappa_T = \frac{\text{var}(\hat{N})}{N \rho T} = \frac{1}{\rho m^* c^2}.
\]

The particle fluctuations are thermodynamically normal for all \( T < T_c \) and the system is stable.

When temperature approaches the critical temperature, \( T \to T_c \), then \( \rho_0 \to 0 \), \( \sigma_k \to 0 \) and \( c \to 0 \). At the critical point, the compressibility \( \kappa_T \to \infty \), which is natural for a second-order phase transition.

The equation for the superfluid fraction in the dilute-gas approximation enjoys the same form

\[
n_s = \frac{1 - \frac{2Q}{3T}}{\sqrt{\pi}},
\]

as in the Bogolubov approximation (134), but with the new sound velocity \( c \) defined in (231). At the critical temperature \( T_c \), the superfluid fraction \( n_s \to 0 \) together with the condensate fraction \( n_0 \).

The condensation temperature \( T_c \) can be found from the expression for the average density, under the conditions \( \rho_0 = 0 \), \( \rho_1 = \rho \), \( \Delta = 0 \), and \( \epsilon_k = k^2/2m \). In the case of local interactions, the average density at the critical temperature reads as

\[
\rho = \frac{1}{2} \int \left[ \coth \left( \frac{k^2}{2mT_c} \right) - 1 \right] \, dk \frac{d}{(2\pi)^3}.
\]

Taking the integral

\[
\int_0^\infty \left( \coth x - 1 \right) \, dx = \frac{1}{2} \left( \pi \sqrt{\frac{3}{2}} \right),
\]

we obtain

\[
T_c = \frac{2\pi m}{\left( \frac{\rho}{\zeta(3/2)} \right)^{2/3}}.
\]

This is the same expression as for the ideal Bose gas, which is caused by the use of the local delta-function interaction potential (102) corresponding to the dilute-gas approximation.

3.12. Nonlocal interactions

If the interaction potential is not local, the critical temperature is different. To find out how the nonlocal interactions influence the transition temperature, let us consider the approach to \( T_c \) from above. For \( T > T_c \), we can use the Hartree–Fock approximation, when the single-particle spectrum is

\[
\omega_k = \frac{k^2}{2m} + \rho \Phi_0 + \frac{1}{V} \sum_p n_p \Phi_{k+p} - \mu.
\]

For the occurrence of Bose–Einstein condensation, it is necessary that

\[
\lim_{k \to 0} \omega_k = 0 \quad (T = T_c + 0).
\]

This defines the chemical potential at the transition temperature

\[
\mu = \rho \Phi_0 + \frac{1}{V} \sum_p n_p \Phi_p,
\]

which gives

\[
\omega_k = \frac{k^2}{2m} + \frac{1}{V} \sum_p n_p (\Phi_{k+p} - \Phi_p), \quad (T = T_c).
\]

Calculating the sums over momentum, containing the distribution \( n_k \), we can take into account that this distribution is maximal at zero \( k \), hence the main contribution comes from the long-wave limit \( k \to 0 \). Therefore it is admissible to invoke the approximation

\[
\sum_k \longrightarrow \int \frac{dk}{(2\pi)^3}
\]
Then spectrum (236) reads as
\[ \omega_k = \frac{k^2}{2m} + \rho(\Phi_0 + \Phi_k) - \mu. \]
And the chemical potential at the transition point becomes \( \mu = \frac{2}{\rho} \Phi_0 \), which yields
\[ \omega_k = \frac{k^2}{2m} + \rho(\Phi_k - \Phi_0). \] (239)

To find the long-wave limit of the Fourier transform
\[ \Phi_k = \int \Phi(r)e^{-ik\cdot r}dr \]
for a potential depending on \( r \equiv |r| \), we substitute into the integral the expansion
\[ e^{-ik\cdot r} \approx 1 - ik \cdot r - \frac{1}{2} (k \cdot r)^2. \]
The integral of the linear term is zero. Hence
\[ \Phi_k \approx \Phi_0 - \frac{1}{2} \int \Phi(r)(k \cdot r)^2 dr. \]
Defining the effective interaction radius \( r_{\text{eff}} \) by the equation
\[ r_{\text{eff}}^2 = \int \Phi(r)^2 dr = \frac{4\pi}{\Phi_0} \int \rho^4 \Phi(r)^2 dr, \] (240)
we obtain
\[ \Phi_k \approx \left(1 - \frac{1}{12} \frac{k^2 r_{\text{eff}}^2}{\rho} \right) \Phi_0. \]
Thus for the long-wave limit of spectrum (239), we have
\[ \omega_k \approx \frac{k^2}{2m^*}(k \to 0), \] (241)
with the effective mass
\[ m^* = \frac{m}{1 - m r_{\text{eff}}^2/\rho \Phi_0 / 6}. \] (242)

As is seen, for repulsive interactions, the effective mass is larger than \( m \).

The critical temperature \( T_c \) is found from the integral
\[ \rho = \int n_k \frac{dk}{(2\pi)^3}, \quad n_k = (e^{\omega_k/T_c} - 1)^{-1}, \]
which results in
\[ T_c \approx \frac{2\pi}{m^*} \left[ \frac{\rho}{\xi(3/2)} \right]^{2/3}. \] (243)

To explicitly compare the transition temperature \( T_c \) with the condensation temperature \( T_0 \) of ideal gas, one introduces the relative difference
\[ \frac{\Delta T_c}{T_0} \equiv \frac{T_c}{T_0} - 1 = \left( \frac{2\pi}{m^*} \left[ \frac{\rho}{\xi(3/2)} \right]^{2/3} \right). \] (244)
This gives
\[ \frac{\Delta T_c}{T_0} = \frac{m^*}{m} - 1 \approx -\frac{1}{6} m r_{\text{eff}}^2/\rho \Phi_0. \] (245)

A nonlocal interaction potential leads to a lower critical temperature, as compared to the condensation temperature for a gas with local interactions, \( T_c < T_0 \). Notice that for a local potential, proportional to \( \delta(r) \), the effective interaction radius \( r_{\text{eff}} = 0 \), as a result of which \( m^* = m \) and \( T_c \) reduces to \( T_0 \).

As a nonlocal interaction potential, one often takes the Gaussian potential
\[ \Phi(r) = A \exp\left( -\frac{r^2}{2b^2} \right). \]
Its Fourier transform is
\[ \Phi_k \equiv \int \Phi(r)e^{-ik\cdot r}dr = \frac{4\pi}{k} \int_{-\infty}^{\infty} r \sin(kr)\Phi(r)dr = \Phi_0 \exp\left( -\frac{k^2 b^2}{2} \right). \]
The Born-type normalization
\[ \Phi_0 \equiv \int \Phi(r)dr = 4\pi \frac{a_s}{m}, \]
yields
\[ \Phi_0 = (2\pi)^{3/2} Ab^3, \quad A = \sqrt{\frac{2}{\pi \rho b^2}}. \]
Using the integral
\[ \int_0^{\infty} x^n e^{-\alpha x^2} dx = \frac{1}{2} \left( \frac{n+1}{2} \right) \frac{1}{2^{(n+1)/2}}, \]
for the effective interaction radius, defined in (240), we get \( r_{\text{eff}} = \sqrt{3} b \).

3.13. Condensate and superfluid

Let us consider in more detail the condensate and superfluid fractions for a uniform system with local interactions, in the HFB approximation. For the condensate fraction we have
\[ n_0 = 1 - \frac{\rho_1}{\rho}, \quad \rho_1 = \int n_k \frac{dk}{(2\pi)^3}. \] (246)

While the superfluid fraction is
\[ n_s = 1 - \frac{2Q}{3T}, \quad Q = \frac{\text{var}(\hat{P})}{2mN}. \] (247)

For an equilibrium system,
\[ \langle \hat{P} \rangle = 0, \quad Q = \frac{(\hat{P})^2}{2mN}. \]
And for a uniform system,
\[ \langle \hat{P} \rangle^2 = \sum_{kp} (k \cdot p) \langle \hat{n}_k \hat{n}_p \rangle \quad (\hat{n}_k \equiv a_k^\dagger a_k). \]
In the Hartree–Fock–Bogolubov approximation,
\[ \langle \hat{n}_i \hat{n}_p \rangle = n_in_p + \delta_{ip} n_i (1 + n_k) - \delta_{ip} \sigma_k^2. \]

Therefore
\[ Q = \frac{1}{\rho} \int \frac{k^2}{2m} (n_k + n_k^2 - \sigma_k^2) \frac{dk}{(2\pi)^3}. \]

Using the equality \( \cosh x - 1 = 2 \sinh^2(x/2) \), we have
\[ n_k + n_k^2 - \sigma_k^2 = \frac{1}{4} \sinh^2(\beta k/\mathcal{E}). \]

Then the dissipated heat becomes
\[ Q = \frac{1}{(4\pi)^3 m \rho} \int_0^\infty \frac{k^4 dk}{\sinh^2(\beta k/\mathcal{E})}. \quad (248) \]

In the case of local interactions,
\[ \omega_k = \frac{k^2}{2m} + mc^2, \quad \Delta_k = mc^2, \]
and the spectrum of collective excitations takes the form
\[ \varepsilon_k = \sqrt{(\omega_k)^2 + \left(\frac{k^2}{2m}\right)^2}. \quad (249) \]

The sound velocity \( c \) is defined by the equation
\[ mc^2 = \langle \rho_0 + \sigma_1 \rangle \Phi_0, \quad (250) \]

with the anomalous average
\[ \sigma_1 = \int \frac{\sigma_1 dk}{(2\pi)^3}. \]

The density of uncondensed atoms can be reduced to the integral
\[ \rho_1 = \frac{(mc)^2}{3\pi^2} \times \left\{ 1 + \frac{3}{2\sqrt{2}} \int_0^\infty \left( \sqrt{1 + x^2} - 1 \right)^{1/2} \left[ \coth \left( \frac{mc^2}{2T} \right) - 1 \right] dx \right\}. \quad (251) \]

And the anomalous average writes as
\[ \sigma_1 = - \int \frac{m c^2}{2 \varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right) \frac{dk}{(2\pi)^3}. \quad (252) \]

This integral diverges for any finite \( c \) and requires to be regularized. In any type of regularization, the following properties must hold for \( \sigma_1 \). The anomalous average has to be zero for the ideal Bose gas. Hence there should exist the ideal-gas condition:
\[ \sigma_1 \to 0 \quad (\Phi_0 \to 0). \quad (253) \]

The anomalous average is nonzero together with \( \rho_0 \) since both of them are caused by the gauge symmetry breaking. When the gauge symmetry is restored, \( \sigma_1 \) must be zero, which is the symmetry-restoration condition
\[ \sigma_1 \to 0 \quad (\rho_0 \to 0). \quad (254) \]

For temperatures outside of the critical region, when \( T \ll T_c \), the following regularization can be done. Notice that at zero temperature, \( \sigma_1 \) reduces to the form
\[ \sigma_{\text{eff}} = -mc^2 \int \frac{dk}{(2\pi)^3}. \quad (255) \]

We separate in integral (252) the zero-temperature form by adding and subtracting one, which gives
\[ \sigma_1 = \sigma_{\text{eff}} - \int \frac{m c^2}{2 \varepsilon_k} \left[ \coth \left( \frac{\varepsilon_k}{2T} \right) - 1 \right] \frac{dk}{(2\pi)^3}. \quad (256) \]

The integral in \( \sigma_{\text{eff}} \) is ultraviolet divergent, so that a regularization is needed. The regularization resorting to nonlocal interactions involves complicated equations. The cutoff regularization essentially depends on the chosen cutoff momentum, whose choice is ambiguous. We resort to the dimensional regularization, that is asymptotically exact in the region of weak interactions, and then we accomplish an analytic continuation to finite interactions. Dimensional regularization yields
\[ \int \frac{1}{(2\pi)^3} \frac{dk}{2 \varepsilon_k} \equiv - \frac{m^2 c_{\text{eff}}^2}{\pi^2}, \]

where \( c_{\text{eff}} \) is to be defined.

It is convenient to introduce the dimensionless anomalous averages
\[ \sigma_0 \equiv \frac{\sigma_{\text{eff}}}{\rho}, \quad \sigma \equiv \frac{\sigma_1}{\rho}, \quad (257) \]

and the dimensionless Bogolubov sound velocity
\[ s_B \equiv \frac{mc_B}{\rho^{1/3}}, \quad c_B \equiv \sqrt{\frac{\rho}{m}} \Phi_0. \quad (258) \]

Then the anomalous average \( \sigma_0 \) can be written in the form
\[ \sigma_0 = \frac{s_B m c_{\text{eff}}}{\pi^2 \rho^{1/3}} \left( \Phi_0 \to 0 \right). \quad (259) \]

Equation (250) for the sound velocity can be written as
\[ c = c_B \sqrt{n_0 + \sigma}. \quad (260) \]

In order to analytically continue the anomalous average (259) from weak to finite interactions, we combine it with expression (260) in the form of the iterative equation
\[ \sigma_{0,(n+1)} = \frac{s_B^3}{\pi} \sqrt{n_0 + \sigma_{0,(n)}}. \quad (261) \]

This shows that \( c_{\text{eff}} \) is defined by expression (260) with the appropriate iteration for \( \sigma \). Starting the iteration from the zero approximation \( \sigma_0 = 0 \), we get the first approximation \( \sigma_{0,(1)} = (s_B^3/\pi^2) \sqrt{n_0} \). The second approximation reads as
\[ \sigma_{0,(2)} = \frac{s_B^3}{\pi} \left( n_0 + \frac{s_B^3}{\pi} \sqrt{n_0} \right)^{1/2}. \quad (262) \]

This form satisfies the ideal-gas and symmetry-restoration conditions.

In this way, at finite temperatures outside of the critical region, the anomalous average (256) can be transformed to
\[ \sigma_i = \sigma_{ii} - \frac{(mc)^3}{2\sqrt{2} \pi^2} \int_0^\infty \frac{(\sqrt{1+x^2} - 1)^{1/2}}{\sqrt{1+x^2}} \left[ \coth \left( \frac{mc^2}{2T} x \right) - 1 \right] dx. \]  

(263)

The dissipated heat (248), at any temperature, reduces to

\[ Q = \frac{(mc)^5}{\sqrt{2}(2\pi)^3m} \int_0^\infty \frac{1}{1+x^2} \left[ \frac{1}{\sqrt{1+x^2}} \right] dx \]

(264)

From the above expressions, we can find the behavior of all fractions below the transition temperature, where \( T \ll T_c \). For instance, at low temperatures, such that \( T/mc^2 \ll 1 \), we have the density of uncondensed atoms

\[ \rho_i = \frac{(mc)^3}{3\pi^2} + \frac{(mc)^3}{12} \left( \frac{T}{mc^2} \right)^2, \]

the anomalous average

\[ \sigma_i \approx \sigma_{ii} - \frac{(mc)^3}{12} \left( \frac{T}{mc^2} \right)^2, \]

and the dissipated heat

\[ Q \approx \frac{\pi^2(mc)^5}{15\rho} \left( \frac{T}{mc^2} \right)^5. \]

This yields the condensate fraction

\[ n_0 \approx 1 - \frac{(mc)^3}{3\pi^2 \rho} - \frac{(mc)^3}{12\rho} \left( \frac{T}{mc^2} \right)^2, \]

(265)

and the superfluid fraction

\[ n_s \approx 1 - \frac{2\pi^2(mc)^3}{45\rho} \left( \frac{T}{mc^2} \right)^4. \]

(266)

Numerical investigation [64] shows that the condensate fraction as a function of the interaction strength is in good agreement with Monte Carlo simulations [65].

When temperature tends to the critical \( T_c \), it is necessary to take a different form of the anomalous average (252), instead of the noncritical expression (256). Returning to the initial expression (252) of the anomalous average, we rewrite it as

\[ \sigma_i = -\frac{(mc)^3}{2\sqrt{2} \pi^2} \int_0^\infty \frac{1}{\sqrt{1+x^2}} \coth \left( \frac{mc^2}{2T} x \right) dx. \]

From here, taking into account that \( c \to 0 \) when \( T \to T_c \), and using the integral

\[ \int_0^\infty \frac{(\sqrt{1+x^2} - 1)^{1/2}}{x\sqrt{1+x^2}} dx = \frac{\pi}{\sqrt{2}}, \]

we come to the expression

\[ \sigma_i \approx -\frac{m^2cT}{2\pi}, \quad (T \to T_c). \]

(267)

There is a temptation to consider the critical behavior in the vicinity of \( T_c \) by expanding the corresponding expressions in powers of \( mc^2/T_c \ll 1 \). Then, in the zero order, when \( c = 0 \), we come to the same behavior as in the case of the ideal Bose gas. However, in higher orders, we confront divergent integrals. Hence, such an expansion is not appropriate. Numerical solution proves [66] that the condensate and superfluid fractions continuously tend to zero at \( T_c \), which implies the second order phase transition.

It is important to stress that the described above self-consistent theory is unique, providing, in the mean-field approximation [64], good agreement of the condensate fraction with Monte Carlo simulations [65] for arbitrarily strong interactions and correctly characterizing the Bose–Einstein condensation as a second-order phase transition occurring together with the superfluid transition [66].

### 3.14. Gas parameter

For numerical analysis, it is convenient to employ dimensionless quantities. For this purpose, let us introduce the gas parameter

\[ \gamma \equiv \rho^{1/3}a_s = \frac{a}{a}, \]

(268)

characterizing the interaction strength, the dimensionless sound velocity

\[ s \equiv \frac{mc}{\rho^{1/3}}, \]

(269)

and the dimensionless temperature

\[ t \equiv \frac{mT}{\rho^{1/3}}. \]

(270)

Note that for the ideal-gas critical temperature \( T_c \), given by expression (235),

\[ t_c \equiv \frac{2\pi}{\rho^{1/3}} = \frac{2\pi}{(3\pi/2)^{1/3}} = 3.312498. \]

The condensate fraction now reads as

\[ n_0 = 1 - \frac{s^3}{3\pi^2} \int_0^\infty \frac{x(x^2 + 1)^{1/2}}{\sqrt{1+x^2} \sinh(2sx/2T)} dx. \]

(271)

And the superfluid fraction is

\[ n_s = 1 - \frac{s^3}{6\sqrt{2} \pi^2} \int_0^\infty \frac{x(x^2 + 1)^{1/2}}{\sqrt{1+x^2} \sinh(2sx/2T)} dx. \]

(272)

We use the dimensionless anomalous density \( \sigma \equiv \sigma_i/\rho \) and the local interaction potential with the strength \( \Phi_0 = 4\pi a_s/m \). Then we find

\[ \sigma = \sigma_0 - \frac{s^3}{2\sqrt{2} \pi^2} \int_0^\infty \frac{(\sqrt{1+x^2} - 1)^{1/2}}{\sqrt{1+x^2} \coth (sx/2T) - 1} dx. \]

(273)
Formula (250) gives for the dimensionless sound velocity the equation

\[ s^2 = 4\pi\gamma(n_0 + \sigma). \]  

(274)

Let us consider the case of zero temperature. At zero \( T = 0 \), the above equations simplify to

\[ n_0 = 1 - \frac{s^3}{3\pi}, \quad n_s = 1, \quad \sigma = \sigma_0. \]  

(275)

Here \( \sigma_0 \) is defined by formula (262). For weak interactions, when \( \gamma \to 0 \), we get

\[ n_0 \approx 1 - \frac{8}{3\sqrt{\pi}} \gamma^{3/2} - \frac{64}{3\pi} \gamma^3 - \frac{256}{9\pi^{3/2}} \gamma^{9/2}, \]

\[ s \approx \sqrt{4\pi\gamma} + \frac{16}{3} \gamma^{2/3} - \frac{64}{9\sqrt{\pi}} \gamma^{7/2} - \frac{4480}{27\pi} \gamma^3, \]

\[ \sigma \approx \frac{8}{\sqrt{\pi}} \gamma^{3/2} + \frac{64}{3\pi} \gamma^3 - \frac{1408}{9\pi^{3/2}} \gamma^{9/2}. \]

If the interactions are strong, so that \( \gamma \to \infty \), then

\[ n_0 \approx 4 \times 10^{-5} \frac{1}{\gamma^{13}}, \quad s \approx (3\pi^{2/3})^{1/3} - \left(\frac{\pi}{3}\right)^{2/3} n_0, \]

\[ \sigma \approx \frac{(9\pi)^{1/3}}{4} \gamma^{-1} - n_0. \]

These strong-interaction asymptotic expressions should be understood as corresponding to a metastable uniform system, since under such strong interactions the system would crystallize.

Recall that in the Bogolubov approximation, the condensate fraction is given by the form

\[ n_B = 1 - \frac{8}{3\sqrt{\pi}} \gamma^{3/2} \]

and the sound velocity is \( s_B = 2\sqrt{\gamma} \). The condensate depletion becomes total, with \( n_B = 0 \) and \( s_B = 0 \) at the gas parameter

\[ \gamma_B = \frac{(9\pi)^{1/3}}{4} = 0.761618. \]

For superfluid \(^4\)He, the helium atoms can be represented by hard spheres of diameter \( a_s = 2.203 \) Å. At saturated vapour pressure, \( \rho a_s^3 = 0.21 \), which corresponds to \( \gamma_{He} = 0.594 \). This gives the condensate fraction about 3\%. Experiments suggest for the condensate fraction the values in the range between 2\% and 10\%. The most recent data [67] give the zero-temperature condensate fraction around 7\%.

The ground-state energy is the internal energy \( E \equiv \langle H \rangle + \mu N \) at zero temperature (\( T = 0 \)). Then

\[ \langle H \rangle = E_B = E_{HF} + N \int \frac{\varepsilon_k - \omega_k}{2\rho} \frac{d\mathbf{k}}{(2\pi)^3}. \]  

(276)

The last integral is divergent, but can be regularized by dimensional regularization,

\[ \int \frac{\varepsilon_k - \omega_k}{2\rho} \frac{d\mathbf{k}}{(2\pi)^3} = \frac{8(mc)^2}{15\pi^2 m \rho}. \]

Defining the dimensionless ground-state energy

\[ E_0 = \frac{2mE}{\rho^{3/2} N}. \]  

(277)

we obtain

\[ E_0 = 4\pi\gamma \left( 1 + n_0^2 - 2n_1 - \sigma^2 + \frac{4\pi^5}{15\pi^2 \gamma^2} \right). \]  

(278)

For weak interactions, when \( \gamma \ll 1 \), the ground-state energy becomes

\[ E_0 \approx 4\pi\gamma \left( 1 + n_0^2 - 2n_1 - \sigma^2 + \frac{4\pi^5}{15\pi^2 \gamma^2} \right). \]  

(279)

First two terms here exactly coincide with the Lee–Huang–Yang formula [68, 69].

As has been mentioned above, the strong-interaction expansion does not have much sense, since at about \( \gamma \approx 0.65 \) the system crystalizes [65]. The formula for finite \( \gamma \) can be obtained from expansion (279) by means of the self-similar factor approximants [70–72], which give

\[ E_0 = 4\pi\gamma(1 + 2.934\gamma^{3/2})^{1.641}. \]  

(280)

This expression reproduces the Lee–Huang–Yang energy at small \( \gamma \ll 1 \) and is in good agreement with the Monte Carlo simulations [65] up to \( \gamma \approx 0.6 \).

### 3.15. Conservation of particles

Spontaneous gauge symmetry breaking is the necessary and sufficient condition for Bose–Einstein condensation [10, 22, 24]. But if gauge symmetry is broken, then the number of atoms, generally, is not conserved in the process of calculations. However, there is no contradiction with the fact that the total number of atoms in the system can be fixed. This is because when one requires that the number of particles be prescribed, this concerns the observable quantity, that is, the average number of atoms in the system can be fixed. Actually, any conditions imposed on the number of particles in the system are senseful only with respect to observable quantities that are defined as statistical averages.

Recall that in the grand canonical ensemble, the number of particles is not fixed, independently whether gauge symmetry is broken or not. Moreover, when employing the field-operator representation, the number of particles is not conserved under the action of field operators [1, 73–75]. But any such a nonconservation on the operator level does not contradict the conservation of the number of particles as an observable quantity.

Let us show in what sense the number of particles is conserved, when gauge symmetry is broken by means of infinitesimal sources and the observable quantities are defined through quasiaverages.

Usually, the operator of the number of particles \( \hat{N} = \int \psi^*(\mathbf{r})\psi(\mathbf{r})d\mathbf{r} \) commutes with the Hamiltonian, \( [\hat{N}, \hat{H}] = 0 \). The field operator can be represented as an expansion over a
basis of natural orbitals \( \{ \varphi_k(r) \} \), where it is possible to separate a term corresponding to Bose condensate:

\[
\psi(r) = \psi_0(r) + \psi_1(r), \quad \psi_0(r) = a_0 \varphi_0(r), \\
\psi_1(r) = \sum_{k>0} a_k \varphi_k(r).
\]

Here \( k \) is a multi-index labelling quantum states.

The gauge symmetry is broken by adding to the Hamiltonian a symmetry-breaking term, for instance, by defining the Hamiltonian

\[
H_c \equiv H - \varepsilon \sqrt{\rho_0} \int_V [\psi_0^*(r) + \psi_0(r)] \, \mathrm{d}r.
\]

The operator

\[
\hat{N}_0 \equiv \int \psi_0^*(r) \psi_0(r) \, \mathrm{d}r
\]

is the number-of-particle operator of condensed atoms. Because of the commutation relations

\[
[\psi_0(r), \psi_0^*(r')] = \varphi_0(r) \varphi_0^*(r'), \\
[\psi_0(r), \hat{N}_0] = \psi_0(r), \\
[\psi_0^*(r), \hat{N}_0] = -\psi_0^*(r),
\]

we have

\[
\frac{i}{\varepsilon} \frac{d\hat{N}}{dt} = [\hat{N}, H_c] = \varepsilon \sqrt{\rho_0} \int_V [\psi_0^*(r) - \psi_0(r)] \, \mathrm{d}r.
\]

This tells us that \( \hat{N} \) is not an integral of motion.

However, the observable quantity is the average number of particles, for which we get

\[
\frac{d}{dt} \langle \hat{N}_c \rangle = \varepsilon \sqrt{\rho_0} \int_V \langle \psi_0^*(r) - \psi_0(r) \rangle \, \mathrm{d}r.
\]

Quasiaverages in the Bogolubov theory \([18, 19]\) are introduced as the averages under the Hamiltonian, containing the symmetry-breaking source, for which then the thermodynamic limit \( N \to \infty \) is taken, after which the source is removed, \( \varepsilon \to 0 \).

The order of the limits cannot be interchanged. Taking into account that in the Bogolubov theory \( \langle \psi_0(r) \rangle_c \approx \eta(r) \), we find

\[
\frac{d}{dt} \langle \hat{N}_c \rangle = \varepsilon \sqrt{\rho_0} \int_V \langle \eta^*(r) - \eta(r) \rangle \, \mathrm{d}r.
\]

Considering the reduced quantities, with respect to \( N \equiv N(0) \), we come to the equation

\[
\frac{d}{dt} \langle \hat{N}_c \rangle = \varepsilon \sqrt{\rho_0} \frac{1}{N} \int_V \langle \eta^*(r) - \eta(r) \rangle \, \mathrm{d}r.
\]

If the system is uniform, so that \( \eta(r) \approx \sqrt{\rho_0} \) for \( N \to \infty \), then

\[
\lim_{N \to \infty} \frac{d}{dt} \langle \hat{N}_c \rangle \frac{1}{N} = 0.
\]

Hence, the average number of atoms is conserved.

In the general case of any kind of a system whether nonuniform or uniform, equilibrium or nonequilibrium, the Cauchy–Schwarz inequality is valid:

\[
\left| \int_V \eta(r) \, \mathrm{d}r \right| \leq \sqrt{\langle \hat{N}_c \rangle} \sqrt{V}.
\]

Therefore

\[
\left| \frac{d}{dt} \langle \hat{N}_c \rangle \right| \leq 2 \varepsilon \rho_0.
\]

Since the condensate fraction is \( n_0 \equiv \lim_{N \to \infty} N_0 / N \), we see that

\[
\lim_{N \to \infty} \frac{d}{dt} \langle \hat{N}_c \rangle = 0.
\]

That is, the average number of particles is a well defined quantity and, being an observable, it is conserved on average.

The same conclusion, that the observable number of particles is conserved, being a well defined fixed quantity, can be derived in the case where the gauge symmetry is broken by means of the Bogolubov shift. Then the operator of the total number of particles

\[
\hat{N}[\eta, \psi] \equiv \int \phi^*(r) \phi(r) \, \mathrm{d}r
\]

commutes with the Hamiltonian \( H[\eta, \psi] \). The symmetry is broken not by adding infinitesimal terms, but in the Fock space \( \mathcal{F}[\psi] \) that now is not gauge symmetric.

In the case of the Bogolubov shift, the operator of condensed atoms \( \hat{N}_0 \) becomes a nonoperator quantity \( N_0 \). This implies that the condensate fluctuations are negligible, since

\[
\lim_{N \to \infty} \text{var}(\hat{N}_0) / N = 0.
\]

The observable number of atoms remains well defined fixed quantity \( N = \langle \hat{N} \rangle \).

4. Trapped atoms

The trapping of atoms is described by external confining potentials. In the presence of such potentials, the system becomes nonuniform, which induces novel properties of Bose systems and requires to resort to different methods of description.

4.1. Trapping potentials

An atom consists of a nucleus and electrons, which produce a magnetic dipole moment \( \vec{\mu} \) or an electric dipole moment \( \vec{d} \). So, even neutral atoms can be manipulated by external magnetic or electric fields to be confined inside a trap. There exist magnetic traps, optical traps, and their combinations. It is not our aim to describe here the details of experimental atomic trapping, which requires separate consideration and can be found in other publications, e.g. in the book by Letokhov [46]. But we only briefly mention the physical origin of the trapping fields.
As is clear from their name, magnetic traps are based on the action of external magnetic fields on the atomic magnetic moments. An atom possesses a nuclear spin $\mathbf{I}$, with the largest eigenvalue $I$, and an electron spin $\mathbf{S}$, with the largest eigenvalue $S$. There also exists an electron angular momentum $\mathbf{L}$, with the largest eigenvalue $L$. The total electron momentum $\mathbf{J}$ is the sum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. And the total atomic momentum (total atomic spin) $F$ is $\mathbf{F} = \mathbf{J} + \mathbf{I}$. The total electron momentum $J$ is the sum $J = L + S$. And the total atomic momentum (total atomic spin) $F$ is $F = J + I$. The total electron momentum $J$ is the sum $J = L + S$. And the total atomic momentum (total atomic spin) $F$ is $F = J + I$.

The atomic magnetic dipole moment is $\mu = \mu_B \mathbf{g} \mathbf{F}$, where $\mu_B = |e|/2m_e$ is the Bohr magneton and $g_F$ is the atomic Landé factor

$$g_F = g_J \frac{F(F + 1) + J(J + 1) - I(I + 1)}{2F(F + 1)},$$

$$g_F = 1 + \frac{J(J + 1) + S(S + 1) - L(L + 1)}{2J(J + 1)}.$$

An external magnetic field $\mathbf{B}(\mathbf{r}, t)$ creates the magnetic potential

$$U_B(\mathbf{r}, t) = -\mu \cdot \mathbf{B}(\mathbf{r}, t)$$

acting on the atom. The required configuration of the total magnetic field is formed by magnetic coils.

In optical traps, an electric laser field $\mathbf{E}(\mathbf{r}, t)$ creates an electric potential

$$U_E(\mathbf{r}, t) = -\mathbf{d}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t).$$

The electric dipole moment is composed of an internal dipole moment $\mathbf{d}_0$ and an induced dipole moment $\mathbf{d}_{ind}(\mathbf{r}, t) = \alpha \mathbf{E}(\mathbf{r}, t)$, where $\alpha$ is the dipole polarizability. Thus, $\mathbf{d}(\mathbf{r}, t) = \mathbf{d}_0 + \mathbf{d}_{ind}(\mathbf{r}, t)$.

The characteristic variation frequencies of external electric and magnetic fields are much larger than the typical frequencies of the atomic motion. Therefore an atom feels an effective potential corresponding to temporal and quantum-mechanical averaging. The atom lifetime in a trap is much longer than the times of field variations. Thus, the effective trapping potential, acting on an atom, is

$$U(\mathbf{r}) = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau (U_B(\mathbf{r}, t) + U_E(\mathbf{r}, t))dt.$$
\[ \mathbf{d}k \rightarrow \frac{2 \pi^{d/2}}{\Gamma(d/2)} k^{d-1} \mathbf{d}k \quad (k \equiv |\mathbf{k}|). \]

Then
\[ \int \frac{\mathbf{d}k}{(2\pi)^d} = \frac{2}{(4\pi)^{d/2}\Gamma(d/2)} \int_0^\infty k^{d-1} \mathbf{d}k \quad (285) \]
for any \( d \geq 1 \).

The quasiclassical momentum \( k(\varepsilon, \mathbf{r}) \) is defined as the solution of the equation \( \varepsilon \mathbf{p} = \mathbf{E} \), giving \( k = k(\varepsilon, \mathbf{r}) \). In view of the Schrödinger equation, we get
\[ k(\varepsilon, \mathbf{r}) = \sqrt{2m[\varepsilon - U(\mathbf{r})]} \quad (286) \]
for \( \varepsilon \) non-negative, which defines the volume \( \mathcal{V}_\varepsilon \) available for quasiclassical motion,
\[ \mathcal{V}_\varepsilon = \{ \mathbf{r} | U(\mathbf{r}) \leq \varepsilon \}. \] (287)

Using \( \mathbf{d}k = (\partial k(\varepsilon, \mathbf{r})/\partial \varepsilon) \mathbf{d}\varepsilon \), we get
\[ \int \frac{\mathbf{d}k}{(2\pi)^d} \mathbf{d}\varepsilon = \frac{2}{(4\pi)^{d/2}\Gamma(d/2)} \int_0^\infty \varepsilon \mathbf{d}\varepsilon \]
The density of states is defined as
\[ \rho(\varepsilon) = \frac{2}{(4\pi)^{d/2}\Gamma(d/2)} \int_\mathcal{V}_\varepsilon k^{d-1}(\varepsilon, \mathbf{r}) \frac{\partial k}{\partial \varepsilon} \mathbf{d}\varepsilon \quad (288) \]

Taking into account the replacement
\[ \int \frac{\mathbf{d}k}{(2\pi)^d} \rightarrow \int_0^\infty \rho(\varepsilon) \mathbf{d}\varepsilon \]
and the derivative \( \partial k(\varepsilon, \mathbf{r})/\partial \varepsilon = m/k(\varepsilon, \mathbf{r}) \), we obtain the density of states
\[ \rho(\varepsilon) = \frac{(2\pi)^d}{(4\pi)^{d/2}\Gamma(d/2)} \int_\mathcal{V}_\varepsilon \varepsilon \partial U(\mathbf{r})/\partial \varepsilon \mathbf{d}\varepsilon \quad (289) \]
for any dimensionality \( d \geq 1 \).

In particular, for the one-dimensional case, with the available volume
\[ \mathcal{V}_\varepsilon = \{ x | -x_c \leq x \leq x_c \}, \]
where \( x_c \) is found form the equality \( U(x_c) = \varepsilon \), the density of states reads as
\[ \rho(\varepsilon) = \frac{\sqrt{2m}}{2\pi} \int_{x_c}^{x_c} \frac{dx}{\sqrt{\varepsilon - U(x)}} \quad (d = 1). \]

An important situation is when the system is confined in a box of volume \( V \), with no potential inside, \( U(\mathbf{r}) \rightarrow 0 \). Then, in one dimension \( (d = 1) \), the turning points are given by \( x_c = L/2 \), with \( L \) being the system length. The density of states becomes
\[ \rho(\varepsilon) = \frac{\sqrt{2m}}{2\pi} L \varepsilon^{-1/2} \quad (d = 1). \]

In the general \( d \)-dimensional case, the density of states for a system in a box is
\[ \rho(\varepsilon) = \frac{(2\pi)^{d/2}}{(4\pi)^{d/2}\Gamma(d/2)} V \varepsilon^{d/2-1} \quad (d \geq 1). \] (290)

Here the available volume coincides with the box volume \( V = \int_\mathcal{V}_\varepsilon \mathbf{d}\varepsilon \).

### 4.3. Power-law potentials

A very general situation is when atoms are trapped by power-law potentials of the form
\[ U(\mathbf{r}) = \sum_{\alpha=1}^d \frac{\omega_\alpha}{l_\alpha} r_\alpha^{n_\alpha} \quad (291) \]
with \( l_\alpha \) being the effective trap length in the \( \alpha \)-direction. The parameters \( \omega_\alpha \) and \( n_\alpha \) are positive.

As an example, consider a one-dimensional trap \( (d = 1) \), with the potential
\[ U(x) = \frac{\omega_0}{2} \left| \frac{x}{l_0} \right|^n. \]

Then
\[ U(x_c) = \varepsilon, \quad x_c = \left( \frac{2\varepsilon}{\omega_0} \right)^{1/n} l_0. \]

and the available region corresponds to \( -x_c \leq x \leq x_c \). The density of states takes the form
\[ \rho(\varepsilon) = \frac{\varepsilon^{s-1}}{\pi n} \frac{2}{\omega_0} \int_0^1 \frac{y^{-1+1/n}}{\sqrt{1-y}} \mathbf{d}y \quad (d = 1), \]

where the notation
\[ s \equiv \frac{1}{2} + \frac{1}{n} \]
is used, having the meaning of an effective confining dimension.

To reorganize the above integral, recall the definition of the beta function, or Euler integral of the first kind,
\[ B(\mu, \nu) \equiv \int_0^1 x^{\mu-1}(1-x)^{\nu-1} \mathbf{d}x, \]
where \( \text{Re} \ \mu > 0 \) and \( \text{Re} \ \nu > 0 \). The beta function enjoys the property
\[ B(\mu, \nu) = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} = B(\nu, \mu). \]

Using this, we find the density of states
\[ \rho(\varepsilon) = \frac{\varepsilon^{s-1}}{\gamma_l \Gamma(s)} \quad (d = 1), \]
in which
\[ \gamma_l \equiv \frac{\sqrt{\pi}}{\Gamma(1+1/n)} \left( \frac{\omega_0}{2} \right)^{1/n}. \]

In the general case of \( d \gg 1 \), we have
The density of states becomes
\[
\rho(\varepsilon) = \frac{2^{d-1}}{\pi^{d/2} \Gamma(d/2) \prod_{n=1}^{d} \omega_{n}^{1/2 + 1/n_{a}}}
\times \int \left( 1 - \varepsilon \right)^{d/2} \prod_{a=1}^{d} \frac{\gamma_{a}^{-1 + 1/n_{a}}}{\gamma_{a}} \, d\gamma_{a}.
\]

Here, the confining dimension is
\[
s \equiv \frac{d}{2} + \sum_{a=1}^{d} \frac{1}{n_{a}}.
\]

For \( \text{Re} \mu > 0 \) and \( \text{Re} \nu > 0 \), and any \( d \geq 1 \), one has
\[
\prod_{a=1}^{d} \left( \frac{1}{n_{a}} \right) \frac{d}{2} + \sum_{i=1}^{d} \frac{1}{n_{i}} = \frac{\Gamma(d/2)}{\Gamma(s)} \prod_{a=1}^{d} \frac{1}{n_{a}}
\]
In that way, we find the density of states
\[
\rho(\varepsilon) = \frac{\varepsilon^{d-1}}{\gamma_{d} \Gamma(s)} \quad (d \geq 1),
\]
where
\[
\gamma_{d} \equiv \frac{\pi^{d/2} \prod_{a=1}^{d} \omega_{a}^{1/2 + 1/n_{a}}}{2^{d} \prod_{n=1}^{d} \Gamma(1 + 1/n_{a})} \quad (d \geq 1).
\]

For a one-dimensional system \((d = 1)\), we have \( \gamma_{1} \) defined above.

The case of a system in a box of volume \( V \) is recovered, when
\[
n_{a} \longrightarrow \infty, \quad \prod_{a=1}^{d} 2l_{a} \longrightarrow V, \quad s \longrightarrow \frac{d}{2}, \quad l_{0} \longrightarrow \frac{L}{2},
\]
\( V = L^{d} \).

Here and in what follows we use the notations
\[
l_{0} \equiv \left( \prod_{a=1}^{d} l_{a} \right)^{1/2}, \quad \omega_{0} \equiv \left( \prod_{a=1}^{d} \omega_{a} \right)^{1/2}.
\]

A very often met potential describes harmonic traps, when \( n_{a} = 2 \). Then \( s = d \) and \( \gamma_{d} = \omega_{0}^{d} \) for all \( d \geq 1 \). The density of states becomes
\[
\rho(\varepsilon) = \frac{\varepsilon^{d-1}}{\Gamma(d) \omega_{0}^{d}} \quad (n_{a} = 2, s = d \geq 1).
\]

In that way, it is straightforward to calculate any required sum over momenta by means of the replacement
\[
\sum_{k} \longrightarrow \int_{0}^{\infty} \rho(\varepsilon) \, d\varepsilon.
\]

### 4.4. Condensation in traps

To illustrate the possibility of Bose–Einstein condensation inside a trap, let us consider ideal trapped Bose gas. An important quantity for such a gas is the Bose–Einstein integral function \((48)\). The lower limit in this integral, for a large uniform system, is zero, corresponding to zero minimal energy. Bose–Einstein condensation in power-law potentials with the integral function \((48)\) has been studied in Refs. [76–79].

However, when atoms are confined in a trap, the lower energy is not zero, but a finite positive quantity \( \varepsilon_{\min} \). Therefore the lower limit of integral \((48)\) has to be \( u_{\min} \equiv \beta \varepsilon_{\min} \). Thus for trapped atoms, it has been suggested \([80]\) to introduce the generalized integral
\[
g_{s}(\varepsilon) \equiv \frac{1}{\Gamma(n)} \int_{u_{\min}}^{\infty} \frac{z^{n-1}}{e^{\beta u} - 1} \, du.
\]

As is shown below, this generalization is principally important for trapped atoms.

The total number of atoms of ideal Bose gas writes as
\[
N = N_{0} + \int n_{k} \frac{dk}{(2\pi)^{d}} \, dr,
\]
with \( n_{k} = [e_{k}(a_{k} - 1) - 1]^{-1} \). In the generalized semiclassical approximation \([80]\), this takes the form
\[
\int n_{k}(r) \frac{dk}{(2\pi)^{d}} \, dr = \int_{u_{\min}}^{\infty} n(\varepsilon) \rho(\varepsilon) \, d\varepsilon,
\]
with the distribution \( n(\varepsilon) = [e_{k}(a_{k} - 1) - 1]^{-1} \). Changing the variable to \( u = \beta \varepsilon \) gives
\[
N = N_{0} + T^{s} \int_{u_{\min}}^{\infty} \frac{z^{s}}{e^{\beta u} - 1} \, du,
\]
where \( z \equiv e^{\beta_{0}} \) is fugacity and \( u_{\min} \equiv \beta \varepsilon_{\min} \). For the power-law potential, this becomes
\[
N = N_{0} + T^{s} g_{s}(\varepsilon).
\]

At the point of condensation, \( \mu \to 0 \) and \( z \to 1 \), while \( N_{0} = 0 \), which yields the condensation temperature
\[
T_{c} = \left[ \frac{\gamma_{d}N}{g_{s}(1)} \right]^{1/s}.
\]

Bose–Einstein condensation of ideal gas in power-law potentials has been studied \([76–79]\) using the semiclassical approximation employing the standard definition of the Bose–Einstein integral function \((48)\), with zero lower limit. Expression \((48)\) for \( g_{s}(1) \) is finite for \( s > 1 \) and diverges for \( s \leq 1 \), which would imply that condensation can occur only for \( s > 1 \). In particular, condensation could not happen in a one-dimensional harmonic trap \([76, 77]\). But the situation is different if the more correct generalized form \((296)\) is employed. The difference arises in those cases where the standard form \((48)\) diverges, that is, for \( s \leq 1 \). When it is finite, that is, for \( s > 1 \), the lower limit can be replaced by zero. In this way, we need to attentively consider what happens for \( s \leq 1 \).

Let us study one-dimensional Bose gas in a harmonic trap, when \( n = 2 \) and \( d = 1 \), hence \( s = 1 \). Taking into account that the trap houses a finite, although large, number of atoms \( N \gg 1 \), we need to evaluate the integral

\[
\int_{0}^{\infty} \rho(\varepsilon) \, d\varepsilon.
\]
$$g_1(1) = \int_{u_{\text{min}}}^{\infty} \frac{du}{e^u - 1} \quad (u_{\text{min}} \ll 1).$$

For small $u_{\text{min}}$, we have $g_1(1) \approx -\ln u_{\text{min}}$. In the considered case of ideal gas, its spectrum is $\varepsilon = k^2/2m$. Hence $u_{\text{min}} = \beta k^2/2m$. The minimal wave vector is limited by the inverse effective trap size defined by the expressions

$$l_0 \equiv \left( \prod_{n=1}^{d} l_n \right)^{1/d}, \quad \omega_0 \equiv \left( \prod_{n=1}^{d} \omega_n \right)^{1/d} = \frac{1}{m l_0^2}.$$

Therefore the lower limit in the integral $g_1(1)$ is given by the formula

$$u_{\text{min}} = \frac{\omega_0}{2T} \left( k_{\text{min}} = \frac{1}{l_0} \right). \quad (299)$$

This yields

$$g_1(1) \approx \ln \left( \frac{2T}{\omega_0} \right) \left( \frac{\omega_0}{T} \ll 1 \right).$$

For the case $n = 2$ and $s = 1$, parameter (294) is $\gamma_1 = \omega_0$. Then expression (298) gives the equation

$$T_c = \frac{N \omega_0}{\ln(2T_c/\omega_0)} \quad (d = 1, n = 2, s = 1). \quad (300)$$

This equation exactly coincides with that derived in purely quantum-mechanical calculation [81]. We can rewrite equation (300) in the equivalent form as

$$T_c = \frac{N \omega_0}{\ln(2N) - \ln(2T_c/\omega_0)}.$$

Using the inequality

$$\frac{T_c}{\omega_0} \ll e^{2N} \quad (N \gg 1),$$

we obtain the condensation temperature

$$T_c = \frac{N \omega_0}{
\ln(2N)} \quad (d = 1, n = 2, s = 1). \quad (301)$$

To illustrate the correctness of the inequality used above, we notice that

$$\frac{T_c}{\omega_0} = \frac{N}{\ln(2N)} \ll e^{2N} \quad (N \gg 1).$$

The validity of the semiclassical approximation is preserved, since

$$\frac{\omega_0}{T_c} = \frac{\ln(2N)}{N} \ll 1 \quad (N \gg 1).$$

The existence of the finite condensation temperature (301) suggests that Bose condensation could occur in a one-dimensional harmonic trap.

And what happens in a one-dimensional trap for powers higher than harmonic? Then, for $d = 1$ and $n > 2$, one has $1/2 < s < 1$. Integral (296) is estimated as

$$g_1(1) \approx \frac{1}{\Gamma(s)} \int_{u_{\text{min}}}^{\infty} \frac{du}{u^{2-s}} \quad (0 < s < 1).$$

This leads to

$$g_1(1) \approx \frac{u_{\text{min}}^{s-1}}{(1-s)\Gamma(s)} \left( 2T/\omega_0 \right)^{1-s}. \quad (301)$$

As a result, we obtain the condensation temperature

$$T_c = \frac{\sqrt{\pi} (1-s) \Gamma(s)}{2T(1+1/n)} N \omega_0 \quad (0 < s < 1). \quad (302)$$

This formula tells us that, it seems, Bose–Einstein condensation could occur in any one-dimensional ($d = 1$) trap for all $n$.

The behavior of the condensate fraction follows from equation (297) that can be represented as

$$\frac{N_0}{N} = \frac{g_1(z)}{g_1(1)} \left( T/T_c \right)^{s}. \quad (303)$$

Let us specify the condensation temperature for harmonic traps, when $n = 2, s = d$, and

$$\gamma_d = \omega_0^d \quad (n = 2, s = d).$$

For a one-dimensional harmonic trap, the condensation temperature is given by expression (301). For harmonic traps of higher dimensionality, we have

$$T_c = \omega_0 \left[ \frac{N}{\zeta(d)} \right]^{1/d} \quad (d \gg 2, n = 2, s = d). \quad (304)$$

For the dimensionality two and three, we should substitute here $\zeta(2) = \pi^2/6$ and $\zeta(3) = 1.202 057$, respectively.

Above the transition temperature, $T > T_c$, there is no condensate, $N_0 = 0$, the fugacity $z < 1$, and the chemical potential $\mu$ is defined from the equation

$$g_1(z)T^s = N \gamma_d \quad (T > T_c). \quad (305)$$

For $T \gg T_c$, the fugacity is small, $z \ll 1$, and we can use the estimate $g_1(z) \approx z$. Then

$$\mu \approx -T \ln \left( \frac{T^s}{N \gamma_d} \right) \quad (T \gg T_c).$$

Employing the relation $N \gamma_d = g_1(1)T_c^s$ transforms the chemical potential to

$$\mu \approx -T \ln \left[ \frac{1}{g_1(1)} \left( \frac{T}{T_c} \right)^s \right] \quad (T \gg T_c).$$

In the case of harmonic traps, the high-temperature chemical potential reads as

$$\mu \approx -T \ln \left( \frac{1}{N} \frac{T}{\omega_0} \right)^d \quad (T \gg T_c, n = 2).$$

In this way, it looks like Bose–Einstein condensation of ideal gas can occur in low-dimensional traps, contrary to the
case of uniform Bose gas, for which the condensation in one-dimensional space \((d = 1)\) is impossible at all, the condensation temperature for two-dimensional gas is \(T_c = 0\), and finite-temperature condensation can exist only for \(d > 2\). However, before concluding on the possibility of condensation, it is worth remembering that the uniform ideal Bose gas also formally displays a transition temperature, but, actually, it does not exist below this temperature, being unstable. A formal occurrence in theory of a transition temperature does not guarantee that the condensation can be real, if below this temperature the system is unstable. Recall that the problem of stability requires the investigation of susceptibilities in thermodynamic limit.

### 4.5. Thermodynamic limit

For finite systems, there are no first- or second order phase transitions, but only crossovers can exist [1]. First- or second order transitions require the consideration of thermodynamic limit. But how thermodynamic limit can be defined for trapped atoms?

The physical meaning of thermodynamic limit for any statistical system, including trapped atoms, can be formulated as follows [80]. This limit assumes that the number of atoms tends to infinity, \(N \to \infty\). At the same time, extensive observable quantities \(A_N\), that are statistical averages of self-adjoint operators, increase proportionally to \(N\). Hence, the ratio of extensive observables to the number of atoms tends to a constant,

\[
\lim_{N \to \infty} \frac{A_N}{N} = \text{const.} \quad (306)
\]

Taking, as an observable quantity, internal energy \(E\), it is required that \(E \propto N\) for all \(T\), under \(N \to \infty\). In other words, thermodynamic limit implies that

\[
\lim_{N \to \infty} \frac{E}{N} = \text{const.,}
\]

where a finite constant is assumed. Thus, thermodynamic limit can be defined by the conditions

\[
N \to \infty, \quad E \to \infty, \quad \frac{E}{N} \to \text{const.} \quad (307)
\]

In the case of power-low confining potentials,

\[
E = \int_0^\infty \varepsilon n(\varepsilon) \rho(\varepsilon) d\varepsilon, \quad \frac{E}{N} = \frac{s g_{s+1}(z)}{N \gamma_d} T_c^{s+1}.
\]

Hence thermodynamic limit can be presented in the form

\[
N \to \infty, \quad \gamma_d \to 0, \quad N \gamma_d \to \text{const.}\n\]

Since \(N \gamma_d = g_s(1) T_c^s\), thermodynamic limit means that \(g_s(1) T_c^s \to \text{const.}\), when \(N \to \infty\).

To illustrate these conditions in more detail, let us consider the case of **equipower traps**, for which \(n_n = n\). The characteristic frequencies \(\omega_n\) can be different, so that the system can be anisotropic. The confining dimension is

\[
s = \left(\frac{1}{2} + \frac{1}{n}\right) d, \quad (308)
\]

being always larger than one-half, \(s \geq 1/2\). For an equipower potential in \(d\)-dimensional space, parameter (294) is

\[
\gamma_d = \frac{\pi^{d/2}}{\Gamma(d+1/2)} \frac{\omega_0}{2} \quad (d \geq 1).
\]

As is seen, \(\gamma_d \propto \omega_0^d\) for any \(d \geq 1\). Therefore thermodynamic limit for such potentials takes the form

\[
N \to \infty, \quad \omega_0 \to 0, \quad \omega_0 \to \text{const.} \quad (310)
\]

This shows that \(\omega_0 \propto N^{-1/s} \to 0\), as \(N \to \infty\). Consequently, \(l_0 \propto \omega_0^{-1/s} \propto N^{1/2s}\).

These properties confirm the validity of the semiclassical approximation, since, for \(N \gg 1\), one finds

\[
\begin{align*}
\frac{\omega_0}{T_c} &\propto \frac{1}{N} \quad (s < 1), \\
\frac{\omega_0}{T_c} &\propto \frac{\ln N}{N} \quad (s = 1), \\
\frac{\omega_0}{T_c} &\propto \frac{1}{N^{1/2}} \quad (s > 1).
\end{align*}
\]

The behavior of the critical temperatures, under \(N \to \infty\), is as follows:

\[
T_c \to \text{const.} \quad (s > 1), \quad T_c \propto \frac{1}{\ln N} \to 0 \quad (s = 1), \quad T_c \propto N^{1-1/s} \to 0 \quad (s < 1).
\]

For **harmonic traps**, we get

\[
T_c \propto \frac{1}{\ln N} \to 0 \quad (d = 1), \quad T_c \to \text{const.} \quad (d \geq 2).
\]

Thus, in thermodynamic limit, finite critical temperatures exist only for \(s > 1\).

### 4.6. Specific heat

Specific heat is one of the susceptibilities characterizing the system stability with respect to thermal energy fluctuations [1]. For a system with a fixed number of atoms \(N\), the specific heat is defined as

\[
C_N = \frac{\text{var}(\dot{H})}{N T^2} = \frac{1}{N} \frac{\partial E}{\partial T} \quad (311)
\]

The number of particles is kept fixed, since the volume is not defined for a system in a confining potential. Keeping in mind power-law potentials, we get

\[
C_N = \frac{s T^s}{N \gamma_d} \left[ (s + 1) g_{s+1}(z) + g_s(z) \frac{\partial \ln z}{\partial \ln T} \right].
\]

Above the transition temperature, \(T > T_c\), we have \(\mu < 0\), hence \(z < 1\), and \(s \geq 1/2\). The chemical potential \(\mu = \mu(T)\) is a function of temperature above \(T_c\). Differentiating equation (305) over \(\mu\) gives

\[
\frac{\partial \ln z}{\partial \ln T} = -s \frac{g_s(z)}{g_{s-1}(z)} \quad (T > T_c).
\]
This yields the specific heat
\[ C_N = s(s + 1) \frac{g_{z+1}(z)}{g_z(z)} - s^2 \frac{g_{z+1}(z)}{g_{z-1}(z)} \quad (T > T_c). \] (312)

Note that \( \lim_{N \to \infty} C_N = s. \)

Taking into account that for \( z < 1 \) all integrals \( g_z(z) \) are finite, because \( s \geq 1/2 \), we see that \( C_N \) is finite for all \( N \). That is, thermal fluctuations are thermodynamically normal everywhere above \( T_c \).

Below the condensation temperature, \( T \leq T_c \), we have \( \mu = 0 \), hence \( z = 1 \). Then
\[ C_N = \frac{s(s + 1)}{N} g_{z+1}(1) T^s \quad (T < T_c). \]
The other form of the specific heat for \( T < T_c \) is
\[ C_N = s(s + 1) \frac{g_{z+1}(1)}{g_z(1)} \left( \frac{T}{T_c} \right)^s \quad (T < T_c). \] (313)

As we see, \( C_N \) is finite for all \( N \), including \( N \to \infty \), since \( s \geq 1/2 \). The finiteness of positive \( C_N \) means that thermal fluctuations of energy are thermodynamically normal. Therefore the system is thermally stable.

At the condensation point \( T_c \), the specific heat experiences a discontinuity that is characterized by a finite value of the difference
\[ \Delta C_N \equiv C_N(T_c + 0) - C_N(T_c - 0), \]
for which we get
\[ \Delta C_N = -s^2 \frac{g_1(g_z(1))}{g_1(1)}. \] (314)

For finite systems, the specific heat is always discontinuous, with the following jumps, depending on the confining dimension:
\[ \Delta C_N = -s^2 \frac{\zeta(s)}{\zeta(s-1)} \quad (s > 2), \]
\[ \Delta C_N = -\frac{2\pi^2}{3 \ln(2T_c/\omega_0)} \quad (s = 2), \]
\[ \Delta C_N = -s^2 \zeta(s)(2 - s)\Gamma(s - 1) \left( \frac{\omega_0}{2T_c} \right)^{2-s} \quad (1 < s < 2), \]
\[ \Delta C_N = -\frac{\omega_0}{2T_c} \ln \left( \frac{2T_c}{\omega_0} \right) \quad (s = 1), \]
\[ \Delta C_N = -s^2(2 - s)\Gamma(s - 1)\omega_0 \quad (s < 1). \]

Here, for \( s = 1 \), we use the relation
\[ g_0(1) = \lim_{z \to 1} \frac{\partial}{\partial z} g_z(z), \quad g_0(1) \approx \frac{2T_c}{\omega_0} - \frac{\omega_0}{2T_c}. \]

The jump is negative, \( \Delta C_N < 0 \), for \( s \geq 1 \) and positive, \( \Delta C_N > 0 \), for \( s < 1 \), since \( \Gamma(s - 1) < 0 \) for \( 1/2 \leq s < 1 \). Thus, for finite systems, \( C_N \) is always discontinuous:
\[ C_N(T_c - 0) > C_N(T_c + 0) \quad (s \geq 1), \]
\[ C_N(T_c - 0) < C_N(T_c + 0) \quad (s < 1). \]

The values of the jumps in thermodynamic limit, when \( N \to \infty \), tend to zero for \( s < 2 \), but tend to a finite value for \( s > 2 \). When \( s > 2 \), then \( T_c \) const. and
\[ \Delta C_N \propto \text{const.} < 0 \quad (s > 2). \]

For \( s = 2 \), we have \( T_c \propto \text{const.} \) and \( \omega_0 \propto N^{-1/2} \), which gives
\[ \Delta C_N \propto -\frac{1}{\ln N} \to -0 \quad (s = 2). \]

When \( 1 < s < 2 \), then \( T_c \propto \text{const.} \) and \( \omega_0 \propto N^{-1/s} \), hence
\[ \Delta C_N \propto -N^{1-2/s} \to -0 \quad (1 < s < 2). \]

For \( s = 1 \), one has \( T_c \propto 1/\ln N \) and \( \omega_0 \propto 1/N \), from where
\[ \Delta C_N \propto -\frac{(\ln N)^2}{N} \to -0 \quad (s = 1). \]

Finally, if \( s < 1 \), then \( T_c \propto N^{1-1/s} \) and \( \omega_0 \propto N^{-1/s} \), which results in
\[ \Delta C_N \propto \frac{1}{N} \to +0 \quad (s < 1). \]

In the case of harmonic traps, \( \Delta C_N \) for \( d = 1 \) is the same as the value for \( s = 1 \) above and \( \Delta C_N \) for \( d = 2 \) is the same as for \( s = 2 \). And for a three-dimensional harmonic trap, we find
\[ \Delta C_N = -\frac{54}{\pi^2} \zeta(3) \quad (d = 3). \] (315)

### 4.7. Particle fluctuations

Particle fluctuations are characterized by the number-of-particles dispersion that define the isothermal compressibility
\[ \kappa_T = \var_{\bar{N}}(\bar{N}) \frac{1}{\rho TN} \left( \frac{\partial \bar{N}}{\partial \mu} \right) \] (316)

where \( \rho \) is average density of atoms in a trap and
\[ \var(\bar{N}) \equiv \left( \bar{N}^2 \right) - \left( \bar{N} \right)^2 = T \frac{\partial N}{\partial \mu} \left( \frac{\partial \rho}{\partial \mu} \right) \]

If Bose condensate is possible, then the operator of the total number of atoms is the sum \( \hat{N} = \hat{N}_0 + \hat{N}_t \). Employing the Bogolubov shift fixes the number-of-particle operator of condensed atoms as a nonoperator quantity, \( \hat{N}_o = N_0 \). Thence
$\text{var}(N_0) = 0$. As a result, $\text{var}(\hat{N}) = \text{var}(\hat{N}_1)$. So we need to calculate the dispersion for the number-of-particle operator of uncondensed atoms

$$\text{var}(\hat{N}) = \text{var}(\hat{N}_1) = T \frac{\partial N_1}{\partial \mu}. \quad \text{(317)}$$

For power-law potentials,

$$N_1 = \frac{T^s}{\gamma_d} g_d(z),$$

giving

$$\text{var}(\hat{N}_1) = \frac{T^s}{\gamma_d} g_{d-1}(z),$$

which also can be written as

$$\text{var}(\hat{N}_1) = N \frac{g_{d-1}(z)}{g_d(1)} \left( \frac{T}{T_c} \right)^s. \quad \text{(317)}$$

Above the critical temperature, $T > T_c$, where $z < 1$, the integral $g_d(z)$ is finite for $n > 0$ and $z < 1$. The integral $g_{d-1}(z)$ is finite for $s > 1$. For $s = 0$, we have

$$g_0(z) = \frac{z}{1-z} \quad (n = 0, z < 1),$$

which also is finite for $z < 1$. Thus we come to the conclusion that

$$\text{var}(\hat{N}_1) \propto N \quad (s \geq 1, T > T_c), \quad \text{(318)}$$

which implies thermodynamically normal fluctuations, with $\kappa_T$ being finite for $N \to \infty$. Hence the system is stable.

However for $s < 1$, we confront the integral

$$g_n(z) \simeq \frac{z}{(1-z)^n} \Gamma(n) \frac{2T}{\omega_0} \left( \frac{2T}{\omega_0} \right)^n \quad (n \leq 0, z < 1),$$

which leads to the variance

$$\text{var}(\hat{N}_1) = \frac{zT}{(1-z)(1-s)\Gamma(s-1)} \frac{2}{\omega_0} \left( \frac{2T}{\omega_0} \right)^{1-s} \quad (s < 1, z < 1).$$

By using the relation

$$\Gamma(-x)\Gamma(x) = -\frac{x}{\pi \sin(\pi x)},$$

we find that $\Gamma(s-1) < 0$ for $s < 1$. Therefore the compressibility

$$\kappa_T \propto -N^{-1+1/s} \to -\infty \quad (s < 1, T > T_c) \quad \text{(319)}$$
is divergent and negative, hence the system is unstable.

In that way, above $T_c$, the system can be stable only for $s \geq 1$. In particular, a one-dimensional trapped gas with $n > 2$ is unstable, which means that it cannot form a stable equilibrium system.

In the case of harmonic traps, when $s = d$, the ideal gas is always stable above $T_c$, for any $d \geq 1$. Below the condensation temperature, $T < T_c$, when $z \to 1$, we obtain

$$\text{var}(\hat{N}_1) = \frac{T^s}{\gamma_d} g_{d-1}(1).$$

From here, we find

$$\text{var}(\hat{N}_1) = \frac{N}{\zeta(s)} \left( \frac{T}{T_c} \right)^s \ln \left( \frac{2T}{\omega_0} \right) \quad (s = 2),$$

$$\text{var}(\hat{N}_1) = \frac{N}{(2-s)\zeta(s)\Gamma(s-1)} \left( \frac{2T}{\omega_0} \right)^{2-s} \left( \frac{T}{T_c} \right)^2 \quad (1 < s < 2),$$

$$\text{var}(\hat{N}_1) = \frac{2}{\omega_0} \left( \frac{T}{\omega_0} \right)^2 \quad (s = 1).$$

And for $s < 1$, we get the same dispersion as for $s < 2$. However, for $s < 1$, the variance $\text{var}(\hat{N}_1)$ becomes negative, since $\Gamma(s-1) < 0$ for $1/2 < s < 1$.

In thermodynamic limit, we find

$$\text{var}(\hat{N}_1) \propto N \quad (s > 2), \quad \text{var}(\hat{N}_1) \propto N \ln N \quad (s = 2),$$

$$\text{var}(\hat{N}_1) \propto N^{2/s} \quad (1 < s < 2),$$

$$\text{var}(\hat{N}_1) \propto N^2 \quad (s = 1), \quad \text{var}(\hat{N}_1) \propto -N^{2/s} \quad (s < 1).$$

This leads to the following behavior of compressibility:

$$\kappa_T \propto \text{const.} \quad (s > 2), \quad \kappa_T \propto N \ln N \quad (s = 2),$$

$$\kappa_T \propto N^{-1+2/s} \quad (1 < s < 2),$$

$$\kappa_T \propto N \quad (s = 1), \quad \kappa_T \propto -N^{-1+2/s} \quad (s < 1).$$

Such an asymptotic behavior shows that the ideal gas, trapped in a power-law potential becomes unstable below the formal condensation temperature for all $s \leq 2$. The condensed system can be stable only for $s > 2$, which gives the stability condition

$$\frac{d}{2} + \sum_{a=1}^{d} \frac{1}{n_a} > 2. \quad \text{(320)}$$

While thermodynamically anomalous density fluctuations and divergent compressibility mean that equilibrium cannot be reached in a trapped system with $s \leq 2$.

In the particular case of harmonic traps, when $n_a = 2$, $s = d$, and $\gamma_d = \omega_0^d$, we obtain

$$\text{var}(\hat{N}_1) = g_{d-1}(1) \left( \frac{T}{\omega_0} \right)^d.$$ 

This results in

$$\text{var}(\hat{N}_1) = 2 \left( \frac{T}{\omega_0} \right)^2 \quad (d = 1),$$
The density of atoms is the sum of condensed and uncondensed atoms. In the case of ideal gas in a harmonic trap, density fluctuations are rather strong, destroying equilibrium Bose-condensed gas. But for dimensional harmonic traps, density fluctuations are rather thermodynamically normal [82].

Respectively, the behavior of the compressibility is as follows,

\[ \kappa_T \propto N \quad (d = 1), \quad \kappa_T \propto \ln N \quad (d = 2), \quad \kappa_T \propto \text{const.} \quad (d = 3). \]

This tells us that a harmonically trapped ideal Bose gas below \( T_c \) is stable only for \( d = 3 \). In one-dimensional and two-dimensional harmonic traps, density fluctuations are rather strong, destroying equilibrium Bose-condensed gas. But for the three-dimensional harmonic potential, fluctuations are thermodynamically normal [82].

### 4.8. Quantum limit

In order to show that the generalized semiclassical approximation [80] leads to the same conclusions as the purely quantum treatment of trapped gases, let us consider Bose gas in a one-dimensional harmonic trap, using quantum mechanical description [81]. This case is of interest, since the condensation temperature does not exist, if the standard semiclassical approximation is involved [77], while it exists when the generalized semiclassical approximation is employed [80].

The case of interest corresponds to \( d = 1 \) and \( n = 2 \). The quantum-mechanical spectrum is

\[ \epsilon_j = \left( j + \frac{1}{2} \right) \omega \quad (j = 0, 1, 2, \ldots), \]

where \( \omega = \omega_0 \). The distribution of atoms over the energy levels \( n_j = \text{exp}(\epsilon_j - \mu) - 1 \) can be written as

\[ n_j = \frac{z}{e^{\beta \omega} - z}, \quad z \equiv \exp\left\{ \left( \mu - \frac{1}{2} \omega \right) \right\}. \]

The total number of atoms

\[ N = \sum_{j=0}^{\infty} n_j = N_0 + N_1 \]

can be separated into two terms describing the ground-state population and the population of excited states,

\[ N_0 = \frac{z}{1 - z}, \quad N_1 = \sum_{j=1}^{\infty} \frac{z}{e^{\beta \omega} - z}. \]

Condensation occurs when \( \mu \to \omega/2 \) and \( z \to 1 \). Replacing the summation over \( j \) by integration, we get

\[ N_1 \approx \int_{1/2}^{\infty} \frac{zd\epsilon}{e^{\beta \omega} - z}. \]

For \( \beta \omega \ll 1 \), it has been checked numerically [81] that a good approximation of the above integral is

\[ N_1 \approx \frac{1}{2\beta \omega} \ln(1 - ze^{-\beta \omega/2}). \]

For \( N_1 = N \), this gives the equation for the critical temperature \( T_c \),

\[ N = \frac{T_c}{\omega} \ln \left( \frac{2T_c}{\omega} \right). \]

which coincides with the equation (300) in the generalized semiclassical approximation.

Studying particle fluctuations, we use the derivative

\[ \frac{\partial N_1}{\partial \mu} = \frac{z}{\omega} e^{\beta \omega/2} - z, \]

which, under \( \beta \omega \ll 1 \) and \( z \to 1 \), yields

\[ \text{var}(N_1) = 2 \left( \frac{T_c}{\omega} \right)^2 (T \ll T_c). \]

Again, this variance exactly coincides with the corresponding expression in the generalized semiclassical approximation.

In this way, in the region of applicability of the generalized semiclassical approximation, the latter is equivalent to quantum calculations, at the same time being essentially simpler.

### 4.9. Density distributions

The density of atoms is the sum \( \rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) \) of the density of condensed atoms \( \rho_0(\mathbf{r}) = |\eta(\mathbf{r})|^2 \) and of the density \( \rho_1(\mathbf{r}) \) of uncondensed atoms. In the case of ideal gas in a harmonic trap, the condensate function is the ground-state wave function of a \( d \)-dimensional harmonic oscillator

\[ \eta(\mathbf{r}) = \sqrt{N_0} \left( \frac{m \omega_0}{\pi} \right)^{d/4} \exp\left( -\frac{m}{2} \sum_{\alpha=1}^{d} \omega_{\alpha} r_{\alpha}^2 \right). \]

That is, the real-space density of condensed atoms is

\[ \rho_0(\mathbf{r}) = N_0 \left( \frac{m \omega_0}{\pi} \right)^{d/2} \exp\left( -m \sum_{\alpha=1}^{d} \omega_{\alpha} r_{\alpha}^2 \right). \]

Recall that

\[ \int \rho_0(\mathbf{r})d\mathbf{r} = N_0, \quad \omega_{\alpha} \equiv \left( \prod_{\alpha=1}^{d} \frac{\omega_{\alpha}}{\omega} \right)^{1/d}. \]

At the trap center \( \mathbf{r} = 0 \), we have

\[ \rho_0(0) = N_0 \left( \frac{m \omega_0}{\pi} \right)^{d/2}. \]

When \( T \) diminishes, \( N_0 \) increases. In thermodynamic limit, when \( N \to \infty \), so that \( N_0 \propto N \) and \( \omega_0 \propto N^{-1/d} \), the central density is

\[ \rho_0(0) \propto \sqrt{N} \quad (d \geq 1). \quad (321) \]

The distribution of uncondensed atoms in the semiclassical approximation, valid for arbitrary trapping potentials, reads as
\[ n_k(r) = \frac{1}{\exp[\beta \epsilon_k(r) - \mu]} - 1. \]

In the case of ideal gas, the spectrum is
\[ \epsilon_k(r) = \frac{k^2}{2m} + U(r). \]

The real-space distribution of uncondensed atoms writes as
\[ \rho_1(r) = \int n_k(r) \frac{dk}{(2\pi)^d} = \frac{1}{\lambda_T^d} g_{d/2}(z(r)) \quad (d \geq 1), \]
where
\[ z(r) \equiv \exp[\beta \mu - U(r)], \quad \lambda_T = \frac{2\pi}{mT}. \]

The normalization conditions are
\[ N_1 = \int n_k(r) \frac{dk}{(2\pi)^d} \, dr = \int \rho_1(r) \, dr. \]

Below the condensation temperature, \( T \lesssim T_c \), we can set \( \mu = U(0) = 0 \). Then the density of uncondensed atoms at the center of the trap \( r = 0 \) is given by the expression
\[ \rho_1(0) = \frac{1}{\lambda_T^d} g_{d/2}(1) \quad (d \geq 1), \]
in which, according to the generalized semiclassical approximation [80],
\[ g_{d/2}(1) \approx 2 \left( \frac{2T}{\pi \omega_0} \right)^{d/2}, \quad g_1(1) \approx \ln \left( \frac{2T}{\omega_0} \right). \]

Thus, for arbitrary trapping potentials, the central density of uncondensed atoms is
\[ \rho_1(0) = \frac{2}{\lambda_T^d} \left( \frac{2T}{\pi \omega_0} \right)^{d/2} \quad (d = 1), \]
\[ \rho_1(0) = \frac{1}{\lambda_T^d} \ln \left( \frac{2T}{\omega_0} \right) \quad (d = 2), \]
\[ \rho_1(0) = \frac{1}{\lambda_T^d} \left( \frac{3}{2} \right) \quad (d = 3). \] (322)

When \( T \to 0 \), then \( \rho_1(0) \to 0 \). But at any finite temperature \( T > 0 \), when \( N \to \infty \) and \( \omega_0 \propto N^{-1/2} \), then the central density of uncondensed atoms behaves as
\[ \rho_1(0) \propto N^{d/2} \quad (d = 1), \quad \rho_1(0) \propto \ln N \quad (d = 2), \]
\[ \rho_1(0) \propto \text{const.} \quad (d = 3). \] (323)
This shows that, for dimensionality \( d = 1, 2 \) and large \( N \), uncondensed atoms would collapse to the trap center.

Comparing the central densities of uncondensed and condensed atoms for harmonic traps at large \( N \to \infty \), we get
\[ \frac{\rho_1(0)}{\rho_0(0)} \to \text{const.} \quad (d = 1); \quad \frac{\rho_1(0)}{\rho_0(0)} \to 0 \quad (d \geq 2). \]

As we see, for one-dimensional traps, the condensate density at the trap center cannot be distinguished from the density of uncondensed atoms. This is connected with the instability of the condensed gas in one-dimensional harmonic traps, caused by anomalous particle fluctuations.

Let us consider the momentum distribution of uncondensed atoms
\[ n_k \equiv \int n_k(r) \, dr \]
for ideal gas in a harmonic trap. Then we find
\[ n_k = \left( \frac{2\pi \omega_0^d}{\lambda_T} \right)^{d/2} g_{d/2}(z_k) \quad (d \geq 1), \]
where
\[ z_k \equiv \exp \left\{ \beta \mu - \frac{k^2}{2m} \right\}. \]

Below the condensation temperature of ideal gas in a harmonic trap of arbitrary anisotropy, \( \mu = 0 \) for \( T \lesssim T_c \).

Let us consider the zero-momentum value of \( n_k \) at \( k = 0 \) denoted as
\[ \tilde{n}_k(0) \equiv \lim_{k \to 0} n_k. \]

For different dimensionalities, we find
\[ \tilde{n}_1(0) = 4t_0 \left( \frac{T}{\omega_0} \right) \quad (d = 1), \]
\[ \tilde{n}_2(0) = 2\pi t_0^2 \left( \frac{T}{\omega_0} \right) \ln \left( \frac{2T}{\omega_0} \right) \quad (d = 2), \]
\[ \tilde{n}_3(0) = \left( \frac{3}{2} \right)^2 3^{3/2} t_0^3 \left( \frac{2\pi}{\omega_0} \right)^{3/2} \quad (d = 3). \] (324)

When \( T \to 0 \), the zero-momentum density \( \tilde{n}_1(0) \to 0 \).

However, for any finite \( T \), in thermodynamic limit \( N \to \infty \), when \( \omega_0 \propto N^{-1/d} \), we obtain
\[ \tilde{n}_1(0) \propto N^{3/2} \quad (d = 1), \quad \tilde{n}_2(0) \propto N \ln N \quad (d = 2), \]
\[ \tilde{n}_3(0) \propto N \quad (d = 3). \] (325)
This demonstrates that the zero-momentum density of uncondensed atoms is anomalously large for dimensionality \( d = 1, 2 \).

The momentum distribution of condensed atoms is \( n_0 \theta_{k_0} \).
Comparing \( \tilde{n}_k(0) \), for harmonic traps, with the zero-momentum density of condensed atoms \( N_0 \theta_{k_0} \), in thermodynamic limit \( N \to \infty \), we have
\[ \tilde{n}_1(0) \propto N^{1/2} \quad (d = 1); \quad \tilde{n}_2(0) \propto N \ln N \quad (d = 2); \]
\[ \tilde{n}_3(0) \propto \text{const.} \quad (d = 3). \]

We see that the zero-momentum density of uncondensed atoms, in low-dimensional harmonic traps of dimensionality
\(d = 1, 2\), is much larger than the zero-momentum density of condensed atoms. Such an anomalous situation is connected with the instability of ideal condensed gas in these traps.

4.10. Finite-size corrections

The generalized semiclassical approximation \([80]\) makes it possible to explicitly estimate corrections caused by the finite number of atoms in a trap. Recall that in this approximation the Bose–Einstein integral (48) is replaced by the generalized integral

\[
g_n(z) = \frac{1}{\Gamma(n)} \int_{u_{\text{min}}}^{\infty} \frac{zw^{n-1}}{e^w - z} dw,
\]

with the nonzero lower limit

\[
u_{\text{min}} = \frac{\beta k_{\text{min}}^2}{2m} = \frac{\omega_0^2}{2T} \left( k_{\text{min}} = \frac{1}{l_0} \right).
\]

This integral can be split in two parts as

\[
\int_{u_{\text{min}}}^{\infty} \frac{zw^{n-1}}{e^w - z} dw = g_n^{(0)}(z) - \frac{1}{\Gamma(n)} \int_0^{u_{\text{min}}} \frac{zw^{n-1}}{e^w - z} dw,
\]

where \(g_n^{(0)}(z)\) is given by integral (48) with zero lower limit.

Taking into account that \(u_{\text{min}} \ll 1\) and setting in the second term \(z \approx 1\), we get

\[
\int_0^{u_{\text{max}}} \frac{zw^{n-1}}{e^w - z} dw \approx \frac{u_{\text{min}}^{n-1}}{n-1} (n > 1).
\]

Therefore, we have

\[
g_n(z) = g_n^{(0)}(z) - \frac{u_{\text{min}}^{n-1}}{(n - 1)\Gamma(n)}.
\]

Let us consider power-law potentials. Then, taking into consideration that \(g_n^{(0)}(1) = \zeta(s)\) for \(s > 1\), so that \(g_n(1) \rightarrow \zeta(s)(1 - \phi)\), we define the coefficient of finite-size corrections

\[
\phi \equiv \frac{u_{\text{min}}^{s-1}}{(s - 1)\Gamma(s)\zeta(s)},
\]

we find the condensation temperature

\[
T_c = \frac{\gamma_0 \zeta(s)(1 - \phi)}{\zeta(s)(1 - \phi)}. \tag{326}
\]

This temperature should be compared with the condensation temperature

\[
T_0 = \left[ \frac{\gamma_0 \zeta(1)}{\zeta(1)} \right]^{1/s}
\]

without finite-size corrections. Their ratio is

\[
\left( \frac{T_c}{T_0} \right)^s \approx 1 + \phi \quad (\phi \ll 1).
\]

For small \(\phi\), we have

\[
\frac{T_c}{T_0} = \frac{1}{s} \phi \quad (\phi \ll 1).
\]

Introducing the relative temperature shift

\[
\frac{\Delta T_c}{T_0} \equiv \frac{T_c - T_0}{T_0},
\]

we obtain

\[
\frac{\Delta T_c}{T_0} = \frac{1}{s(s - 1)\Gamma(s)\zeta(s)} \left( \frac{\omega_0}{2T_0} \right)^{s-1} (s > 1). \tag{327}
\]

For large \(N\), one has \(\omega_0 \propto N^{-1/s}\), because of which

\[
\frac{\Delta T_c}{T_0} \propto \frac{1}{N^{-1/s}} (s > 1).
\]

For power-law potentials, with a confining dimension \(s > 1\), the shift of the condensation temperature is positive.

In the case of harmonic traps, the temperature shift, caused by finite-size corrections, is

\[
\frac{\Delta T_c}{T_0} = \frac{1}{d(d - 1)\Gamma(d)2^{d-1}} |\zeta(d)|^{1/d} N^{1-1/d} \tag{328}
\]

In particular, for a two-dimensional harmonic trap, the shift is

\[
\frac{\Delta T_c}{T_0} = \frac{1}{4\sqrt{\zeta(2)}N^{1/2}} (d = 2). \tag{329}
\]

while for a three-dimensional trap,

\[
\frac{\Delta T_c}{T_0} = \frac{1}{48(\zeta(3))^{1/3}N^{2/3}} (d = 3). \tag{330}
\]

Thus, for harmonic traps, finite-size corrections shift the transition temperature upward.

4.11. Quantum corrections

In the approximations above, it has been assumed that at the condensation point the chemical potential of ideal Bose gas becomes zero. However, strictly speaking, for finite quantum systems, the chemical potential becomes not zero, but tends to the lowest energy level in the trap, \(\mu \rightarrow \varepsilon_0 \equiv \min_\alpha \varepsilon_\alpha\). The energy \(\varepsilon_0\) is the quantum lowest energy of the spectrum related to the Schrödinger equation. For example, for a one-dimensional harmonic oscillator, \(\varepsilon_0 = \omega_0/2\). For a \(d\)-dimensional harmonic oscillator

\[
\varepsilon_0 = \frac{1}{d} \sum_{\alpha=1}^d \omega_\alpha = \frac{d}{2} \omega_\varepsilon \quad (\omega_\varepsilon \equiv \frac{1}{d} \sum_{\alpha=1}^d \omega_\alpha)
\]

In the general case of power-law potentials, the fraction of uncondensed atoms is
m = \frac{N_{1}}{N} = \frac{g_{s}(z) \left( \frac{T}{T_{0}} \right)^{s}}{g_{s}(1)}, \quad N_{1} = \frac{T_{0}}{\gamma_{d}^{1/2}} g_{s}(z) \quad (z \equiv e^{i\phi}).

When temperature tends to the condensation temperature, \( T \to T_{c} \), then \( \mu \to \epsilon_{0} \), with this lowest energy being much smaller than \( T_{c} \), because of which
\[ g_{s}(z) \simeq g_{s}(1) + g_{s-1}(1)\delta_{0} \quad \left( \frac{\epsilon_{0}}{T_{c}} \ll 1 \right). \]

Introducing the coefficient of quantum corrections
\[ \phi_{\epsilon} \equiv \frac{g_{s-1}(1)\epsilon_{0}}{g_{s}(1)T_{0}} = \frac{g_{s-1}(1)\epsilon_{0}}{(\gamma_{d}N)^{1/2}|g_{s}(1)|^{1-1/s}}, \]
we get the fraction of uncondensed atoms
\[ m = \left( \frac{T}{T_{0}} \right)^{s} + \phi_{\epsilon} \left( \frac{T}{T_{0}} \right)^{s-1}, \quad (331) \]
in which \( T_{0} \) is the condensation temperature without quantum corrections. Respectively, the fraction of condensed atoms \( n_{0} \equiv 1 - n_{1} \) reads as
\[ n_{0} = 1 - \left( \frac{T}{T_{0}} \right)^{s} - \phi_{\epsilon} \left( \frac{T}{T_{0}} \right)^{s-1}. \quad (332) \]

At the condensation temperature, \( T = T_{c} \), we have \( n_{0} = 0 \) and \( n_{1} = 1 \). Then formula (332) leads to the equation
\[ \epsilon_{c} + \phi_{\epsilon} \epsilon_{c}^{s-1} - 1 = 0 \quad \left( \epsilon_{c} \equiv \frac{T_{c}}{T_{0}} \right) \]
for the condensation temperature. The quantum-correction coefficient is assumed to be small, \( |\phi_{\epsilon}| \ll 1 \). For the relative shift of the condensation temperature we get
\[ \Delta T_{c} = - \frac{\epsilon_{0}}{\omega_{0}} \ln(2N) \quad (s = 1), \]
\[ \Delta T_{c} = \frac{2\epsilon_{0}}{s\omega_{0}} \ln \frac{4N}{\zeta(2)} \quad (s = 2), \]
\[ \Delta T_{c} = \frac{2\epsilon_{0}}{s\omega_{0}} \ln \frac{4N}{\zeta(2)} \quad (s = 3). \]

Recall that in the generalized semiclassical approximation [80], we have the following Bose integrals
\[ g_{1}(1) = \zeta(s) \quad (s > 1), \quad g_{s}(1) \simeq \ln \left( \frac{2T}{\omega_{0}} \right) \quad (s = 1), \]
\[ g_{s}(1) \simeq \frac{(2T_{c}/\omega_{0})^{1-s}}{(1-s)\Gamma(s)} \quad (0 < s < 1), \quad g_{0}(1) \simeq \frac{2T}{\omega_{0}} \quad (s = 0). \]

Using these expressions and the property \( \Gamma(s) = (s-1)\Gamma(s-1) \), we obtain the condensation-temperature shifts, caused by quantum corrections,
\[ \frac{\Delta T_{c}}{T_{0}} = - \frac{\epsilon_{0}}{s\zeta(2)\omega_{0}} \ln \frac{4N}{\zeta(2)} \quad (d = 2), \]
\[ \frac{\Delta T_{c}}{T_{0}} = - \frac{\epsilon_{0}}{2\zeta(2)\omega_{0}} \ln \frac{4N}{\zeta(2)} \quad (d = 3). \]

Quantum corrections reduce the condensation temperature.

The influence of quantum corrections has been studied for a three-dimensional harmonic trap by Grossmann and Holthaus [83, 84]. For a spherical harmonic trap, for which \( \omega_{0} = \omega_{0} \), they found the coefficient exactly coinciding with the coefficient in the last of shifts (333) that equals
\[ \frac{\zeta(2)}{2\zeta(3)} = 0.727504. \]

For anisotropic traps, \( \omega > \omega_{0} \), and the temperature shift is larger than for the isotropic case.

For increasing number of atoms \( N \to \infty \) in a harmonic trap, the behavior of the shifts is as follows:
\[
\Delta T_c \propto -\frac{1}{\ln N} \quad (d = 1),
\]
\[
\Delta T_c \propto -\frac{\ln N}{\sqrt{N}} \quad (d = 2),
\]
\[
\Delta T_c \propto -\frac{1}{N^{d/3}} \quad (d = 3).
\]

For harmonic traps, quantum corrections are larger than finite-size corrections considered in the previous section. Also the quantum corrections to the condensation temperature are of opposite sign, as compared to the finite-size corrections. But the quantum corrections are more important.

4.12. Finite box

For a finite system, boundary conditions can play role. Thus, let us consider ideal Bose gas in a finite box of volume \( V = L^d \). When using periodic boundary conditions, the wave vector is quantized so that \( k_a = (2\pi/L) n_a \), with \( n_0 = 0, 1, 2, \ldots \) Hence the minimal wave vector is \( k_0 \to 0 \) and the minimal energy is \( \epsilon_0 \to 0 \). This corresponds to a uniform system for which there are neither finite-size nor quantum corrections.

But for atoms, confined in a finite box, more appropriate is the zero boundary condition

\[ \psi_0(r) = 0 \quad (r_0 = 0, L) \]

for a wave function labelled by the multi-index \( n \equiv \{ n_a \} \), with \( n_0 = 1, 2, 3, \ldots \). The wave function is

\[ \psi_n(r) = \left( \frac{2}{L} \right)^{d/2} \prod_{a=1}^d \sin \left( \frac{\pi n_a}{L} \right) r \quad (r = (r_a)). \]

It enjoys the symmetry property \( |\psi_n(-r)| = |\psi_n(r)| \). The energy spectrum reads

\[ \epsilon_n = \frac{\pi^2}{2mL^2} \sum_{a=1}^d n_a^2, \quad \epsilon_0 = \frac{\pi^2 d}{2mL^2}. \]

Because of the wave-function symmetry under the inversion \( r \to -r \), it is sufficient to consider only positive coordinates.

Deriving the density of states, we have to keep in mind that not all parts of the box volume are available for the particle motion. Thus a \( d \)-dimensional cube has \( 2^n \) planes on which the wave function is zero, hence these planes are not available for motion. Therefore from the total density of states in the box, we need to subtract \( \rho_{\text{sub}}(\epsilon) \) corresponding to the density of states on the surface \( 2d (L/2)^{d-1} \). In that way, the density of states is

\[
\rho(\epsilon) = \frac{(2m)^d L^d}{(4\pi)^{d/2} \Gamma(d/2)} e^{\epsilon(d-2)/2} - \frac{(2m)^{d-1} L^d}{(4\pi)^{(d-1)/2} \Gamma(d/2 - 1/2)} e^{\epsilon(d-3)/2}. \tag{336}
\]

For a three-dimensional box, this gives

\[
\rho(\epsilon) = \frac{(2m)^3 L^3}{(4\pi)^{3/2} \Gamma(3/2)} e^{\epsilon/2} - \frac{3mL^2}{4\pi} \quad (d = 3). \tag{337}
\]

The total number of atoms is

\[ N = N_0 + \int_{\epsilon_0}^{\infty} n(\epsilon) \rho(\epsilon) d\epsilon, \]

where

\[ n(\epsilon) = \frac{z}{e^z - 1} \quad (z = e^{\beta \epsilon}). \]

Note that, in agreement with the generalized semiclassi-

For temperature approaching \( T_c \), we have \( \mu \to 0 \). Taking this into account makes it straightforward to evaluate the integrals

\[ \frac{1}{\Gamma(3/2)} \int_{u_0}^{\infty} \frac{z^{3/2}}{e^z - 1} du = \frac{3}{2\rho L^2} \int_{u_0}^{\infty} \frac{z}{e^z - 1}, \]

where \( u_0 \equiv \beta \epsilon_0 \ll 1 \).

For temperature approaching \( T_c \), we have \( \mu \to 0 \). Taking this into account makes it straightforward to evaluate the integrals

\[ \frac{1}{\Gamma(3/2)} \int_{u_0}^{\infty} \frac{z^{3/2}}{e^z - 1} du = \frac{4 \sqrt{\pi} u_0}{\pi}, \quad T - T_0 \equiv \beta \epsilon_0 \ll -\ln u_0. \]

Then for the fraction of condensed particles near \( T_c \), we find

\[ n_0 = 1 - \frac{1}{2\rho L^2} \left[ g_{3/2}(z) - 4 \sqrt{\pi} u_0 + \frac{3\lambda_L^2}{2L} \ln u_0 \right]. \]

Since \( z \approx 1 + u_0 \), as \( T \to T_c \), we have

\[ g_{3/2}(z) \approx g_{3/2}(1) + 1/2(u_0), \quad g_{3/2}(1) \approx \frac{2}{\sqrt{\pi} u_0}, \]

which gives

\[ g_{3/2}(z) \approx \left( \frac{3}{2} \right)^2 \left( \frac{3}{2} \right)^2 \frac{1}{\sqrt{\pi}} \ln u_0. \]

At \( T_c \) the condensate fraction \( n_0 \to 0 \). Then the equation for the condensate fraction leads to the equation

\[ \left( \frac{3}{2} \right)^2 - 2 \sqrt{\pi} u_0 + \frac{3\lambda_L^2}{2L} \ln u_0 = \rho \lambda_L^3. \]

From here, introducing the notation

\[ \lambda_0 \equiv \sqrt{\frac{2\pi}{m \Gamma(3/2)}} = \left( \frac{\zeta(3/2)}{\rho} \right)^{1/3}, \quad T_0 = \frac{2\pi}{m} \left( \frac{\rho}{\zeta(3/2)} \right)^{2/3}, \]

we get

\[ \left( \frac{T_c}{T_0} \right)^{3/2} = 1 - \frac{2\sqrt{\pi} u_0}{\sqrt{\pi} \zeta(3/2)} + \frac{3\lambda_0}{2\zeta(3/2)} \ln u_0. \]

Using the smallness of \( u_0 \ll 1 \), we derive from the previous equation the shift of the condensation temperature, caused by the finiteness of the box.
Above the condensation temperature $T_c$, in the semiclassical Hartree–Fock approximation, reads
\[ \varepsilon_k(r) = \frac{k^2}{2m} + U(r) + 2\Phi_0 \rho(r), \]
where we keep in mind local interactions (102) with the interaction strength $\Phi_0 = 4\pi a/m$. The semiclassical atomic distribution can be written in the form
\[ n_k(r) = \frac{z_{\text{int}}(r)}{\exp(\beta\varepsilon_k - 2m) - z_{\text{int}}(r)}. \]

with the notation
\[ z_{\text{int}}(r) \equiv z(r) \exp\{-2\beta\Phi_0 \rho(r)\}, \quad z(r) = \exp\{-\beta(\varepsilon_k - U(r))\}. \]

The atomic spatial density is
\[ \rho(r) = \int n_k(r) \frac{dk}{(2\pi)^d} = \frac{1}{\lambda_T^d} g_{d/2}(z_{\text{int}}(r)). \]

Here we take into account only interaction corrections, caused by weak interactions, and neglect quantum corrections considered in section 4.11. Therefore $\mu \to 2\Phi_0 \rho(0)$, when $T \to T_c$.

Interactions are assumed to be weak, such that
\[ \left| \frac{\Phi_0 \rho(0)}{T_c} \right| \ll 1 \] (341)
for all $N$. Then we can employ the approximation
\[ g_{d/2}(z_{\text{int}}(r)) \simeq g_{d/2}(z(r)) - 2\beta\Phi_0 \rho(r) g_{d/2-1}(z(r)). \]

As a result, the normalization condition for the total number of atoms can be represented in the form
\[ N = \int \rho(r) \, dr = \frac{T}{\gamma_T} \int g_{d/2}(z(r)) \, dr, \]
with $z = e^{\beta\varepsilon_k}$. At the transition point, where $\mu = 2\Phi_0 \rho(0)$, we can write
\[ g_d(z) \simeq g_d(1) + g_{d-1}(1) 2\beta\Phi_0 \rho(0), \quad \rho(0) = \frac{1}{\lambda_T^d} g_{d/2}(1), \]
and the spatial density in the integrand is
\[ \rho(r) = \frac{1}{\lambda_T^d} g_{d/2}(e^{-\beta\varepsilon_k}), \]
with $U = U(r)$.

In order that $g_{d-1}(1)$ be limited at large $N$, the confining dimension should be $s > 2$. This is in agreement with the fact that the Bose-condensed state of trapped atoms is unstable when the confining dimension $s$ is smaller than 2, as is found in section 4.7. The stability condition (320) requires that $s > 2$, since for $s$ smaller than or equal to 2, particle fluctuations are thermodynamically anomalous. In the present case, interactions yield small corrections for all $N$ only when $s > 2$ and $d > 2$.

For power-law trapping potentials, the condensation temperature $T_0$ of ideal gas is defined by the relation
\(\gamma s N = T_0^0 \delta(1)\). Our aim is to find out how this temperature changes when interactions are switched on.

For what follows, we introduce the interaction-correction coefficient

\[
\phi_{\text{int}} \equiv \frac{2\Phi_0}{g_s(1)T_0^0} \left[ G_d/2(1)g_{s-1}(1) - S_d(s) \right],
\]

in which the notation

\[
S_d(s) \equiv \gamma_s \frac{d}{dT} \int \frac{g_d/2(e^{-\beta U})g_{d-2}(1)e^{-\beta U})dr}{dtrs}
\]

is used and

\[
\lambda_0 \equiv \sqrt{\frac{2\pi}{mT_0^0}}.
\]

The above normalization condition for the total number of atoms, at \(T = T_c\), can be written in the form

\[
t_c^0 + \phi_{\text{int}} s^{-1} - 1 = 0 \quad \left( t_c \equiv \frac{T_c}{T_0^0} \right).
\]

By assumption, the interactions are weak, such that the interaction-correction coefficient is small, \(|\phi_{\text{int}}| \ll 1\). Then for the relative condensation-temperature shift, we have

\[
\frac{\Delta T_c}{T_0^0} = -\frac{1}{s} \phi_{\text{int}}.
\]

Evaluating the interaction-correction coefficient \((342)\) we keep in mind the power-law confining potential

\[
U(r) = \sum_{\alpha=1}^{d} \frac{\omega_{\alpha}}{2} \left| \frac{r_\alpha}{l_\alpha} \right|^p \left( \frac{l_\alpha}{\sqrt{m\omega_{\alpha}}} \right),
\]

we take the integral

\[
\int_0^\infty \exp(-x^p)dx = \frac{1}{\nu} \Gamma \left( \frac{1}{\nu} \right) \quad (\text{Re} \nu > 0),
\]

and use the representations

\[
S_d(s) = \sum_{m,n=1}^{\infty} \frac{n}{(mn)^{d/2}(m+n)^{d/2}} \quad g_{d}(z) = \sum_{j=1}^{\infty} \frac{z^j}{j}
\]

Since we deal with the case \(d > 2\) and \(s > 2\), we take \(d = 3\). The relative condensation-temperature shift \((343)\) becomes

\[
\frac{\Delta T_c}{T_0^0} = -c_3(s) \frac{a_s}{\lambda_0},
\]

where \(a_s\) is scattering length and

\[
c_3(s) \equiv \frac{4}{\zeta(3)} \left[ 3 \zeta(3) - S_3(s) \right].
\]

Taking into account that

\[
\zeta(s - 1) \simeq \frac{1}{s - 2} \quad (s \to 2), \quad \zeta(s - 1) < 0 \quad (s < 2)
\]

we find that \(S_3(s)\) logarithmically diverges as \(s \to 2\), and

\[
c_3(s) \simeq \frac{12\zeta(3/2)}{\pi^2(s - 2)} \to \infty \quad (s \to 2).
\]

This is in agreement with the fact that trapped Bose-condensed system with \(s < 2\) is unstable.

Let us consider a three-dimensional harmonic trap, when \(s = d = 3\). Then

\[
S_3(3) = 1.2084708, \quad c_3(3) = 3.426032.
\]

And the shift of the condensation temperature \(T_c\) of weakly interacting Bose gas, with respect to that of the ideal gas, using the notations

\[
\lambda_0 \equiv \sqrt{\frac{2\pi}{mT_0^0}} \quad T_0 = \omega_0 \left[ \frac{N}{\zeta(3)} \right]^{1/3},
\]

becomes

\[
\frac{\Delta T_c}{T_0} = -3.426032 \frac{\omega_0 a_s}{\lambda_0},
\]

in agreement with the result of Pitaevskii and Stringari \([44]\).

We may study the interaction corrections for increasing confining dimension \((s \to \infty)\), when \(\zeta(s) \to 1\) and \(S_3(s) \to 0\). Then

\[
c_3(s) \simeq \frac{4}{3} \zeta \left( \frac{3}{2} \right) \quad (s \to \infty).
\]

The limit \(s \to \infty\) implies that \(n_s \to 0\), if \(d\) is fixed. Taking into account that

\[
\gamma_d \simeq \frac{\pi d^{d/2}}{\Gamma(s/d)} \left( \frac{\omega_0}{2} \right)^{s/d},
\]

and

\[
\Gamma(z) \simeq \frac{2\pi}{z} z^e \quad (|z| \gg 1),
\]

we have

\[
T_0 \simeq \frac{\omega_0 N^{1/3}}{2s}, \quad \lambda_0 \simeq \frac{4\pi s}{m\omega_0 N^{1/3}}.
\]

Since \(\omega_0 \propto N^{-1/3}\), then \(\omega_0 N^{1/3}\) is finite. In this way, we come to the conclusion that

\[
\frac{\Delta T_c}{T_0} \propto -\frac{1}{\sqrt{s}} \to 0 \quad (s \to \infty).
\]

The temperature shift tends to zero because the limit \(n_s \to 0\), under fixed \(d\), effectively removes the trapping potential, making the system uniform. And for a uniform system, the condensation temperature of Bose gas, in mean-field approximation, coincides with that of ideal Bose gas.

### 4.14. Thomas–Fermi approximation

In the general case of interacting atoms at finite temperature, trapped in a confining potential \(U(r)\), we have to employ the techniques of section 3.10 treating nonuniform matter.

For dilute gas, one accepts local interactions, with the delta-function potential \(\Phi(r) = \Phi_0 \delta(r)\). Resorting to the Hartree–Fock–Bogolubov approximation for a nonuniform matter, as in section 3.10, for the local potential, we have
\[ \omega(r, r') = \omega(r) \delta(r - r'), \]
\[ \omega(r) = -\frac{\nabla^2}{2m} + U(r) + 2\Phi_0 \rho(r) - \mu_1, \] (346)
and
\[ \Delta(r, r') = \Delta(r) \delta(r - r'), \quad \Delta(r) = \Phi_0 [\rho_0(r) + \sigma_1(r)]. \] (347)
Here the local densities are
\[ \rho(r) = \rho_0(r) + \rho_1(r), \quad \rho_0(r) = \frac{|\eta(r)|^2}{m}. \]
The Bogolubov equations (204) become
\[ \omega(r) u_k(r) + \Delta(r) v_k(r) = \varepsilon_k u_k(r), \]
\[ \omega^*(r) v_k(r) + \Delta^*(r) u_k(r) = -\varepsilon_k v_k(r). \] (348)
Since \( \omega(r) \) is real, \( \Delta(r) \) also can be treated as real. Additional conditions for the coefficient functions \( u_k(r) \) and \( v_k(r) \) are as in section 3.10.

The condensate-function equation for an equilibrium system (186) reduces to
\[ \left[ -\frac{\nabla^2}{2m} + U(r) + \Phi_0 \frac{[|\eta(r)|^2 \eta(r)]}{m} + 2\rho_0(r) \eta^*(r) + \sigma_1(r) \eta^*(r) \right] = \mu_0 \eta(r). \] (349)
For an equilibrium system, the functions \( \Delta(r), \sigma_1(r), \) and \( \eta(r) \) can be considered to be real.

The condensate chemical potential \( \mu_0 \) can be found from the normalization condition
\[ N_0 = \int |\eta(r)|^2 \, dr. \]
The density of uncondensed atoms \( \rho_0(r) \) and the anomalous average \( \sigma_1(r) \) are defined in section 3.10. The condition of condensate existence
\[ \min_k \varepsilon_k = 0 \quad (\varepsilon_k \geq 0) \]
defines \( \mu_1 \). The number of condensed atoms is connected with the total number of atoms by the relation
\[ N_0 = N - N_1, \quad N_1 = \int \rho_1(r) \, dr. \]
If the interaction term in the condensate-function equation (349) is much larger than the kinetic-energy term, the latter can be omitted, which is named the Thomas–Fermi approximation. Then we get the condensate density
\[ \rho_0(r) = \frac{\mu_0 - U(r)}{\Phi_0} - 2\rho_1(r) - \sigma_1(r). \] (350)
This expression is valid for the Fermi region, where the density \( \rho_0(r) \) is non-negative. And outside the Fermi region, one sets \( \rho_0(r) = 0 \).

4.15. Local-density approximation

The local-density approximation is similar to the semiclassical approximation. It is applicable for slowly varying in space external potentials \( U(r) \), that is, for weakly nonuniform matter. The meaning of the slow spatial variation is defined below.

Considering the Hartree–Fock–Bogolubov approximation for nonuniform matter in section 3.10, one can look for the solutions of the Bogolubov equations in the form
\[ u_k(r) = u(k, r) \varphi_k(r), \quad v_k(r) = v(k, r) \varphi_k(r), \]
with the plane wave \( \varphi_k(r) \equiv e^{ik \cdot r} \sqrt{V} \). The latter is assumed to be a fast varying function of the spatial variable \( r \), as compared to the slowly varying functions \( u(k, r) \) and \( v(k, r) \).

Upon differentiating the coefficient functions, one has
\[ \nabla u_k(r) = \varphi_k(r)(\nabla + i\kappa) u(k, r), \quad \nabla v_k(r) = \varphi_k^*(r) \times (\nabla + i\kappa) v(k, r). \]
The coefficient functions are slowly varying in \( r \) in the case of weak system nonuniformity, so that
\[ [\nabla u(k, r)] \ll k \rho_0(k, r), \quad [\nabla v(k, r)] \ll k \varphi(k, r)]. \]
The trapping potential \( U(r) \) and density \( \rho(r) \) are slowly varying functions of \( r \), such that the dependence on the spatial variable in all quantities comes from these functions. Then it is possible to use the expressions appearing for uniform systems, with replacing the average density \( \rho \) by the local density \( \rho(r) \). To this end, for a dilute gas with local interactions, \( \omega_k \) changes to
\[ \omega(k, r) = \frac{k^2}{2m} + U(r) + 2\Phi_0 \rho(r) - \mu_1, \] (351)
\( \Delta_k \) changes to
\[ \Delta(k, r) = \Phi_0 [\rho_0(r) + \sigma_1(r)], \] (352)
and \( \varepsilon_k \) changes to \( \varepsilon(k, r) \). As a result, the Bogolubov equations read as
\[ [\omega(k, r) - \varepsilon(k, r)] u(k, r) + \Delta(k, r) v(k, r) = 0, \]
\[ \Delta(k, r) u(k, r) + [\omega^*(k, r) + \varepsilon(k, r)] v(k, r) = 0. \] (353)

With \( \omega(k, r) \) being real, one can treat \( \sigma_1(r) \) as real, hence \( \Delta(k, r) \) is also real. Therefore one can look for real solutions \( u(k, r) \) and \( v(k, r) \). Similarly to the case of a uniform system, we have
\[ u^2(k, r) - v^2(k, r) = 1. \]
The local spectrum of collective excitations is
\[ \varepsilon(k, r) = \sqrt{\omega^2(k, r) - \Delta^2(k, r)}. \]
And, analogously to the uniform case, we find
\[ u^2(k, r) = \frac{\omega(k, r) + \varepsilon(k, r)}{2\varepsilon(k, r)}, \quad v^2(k, r) = \frac{\omega(k, r) - \varepsilon(k, r)}{2\varepsilon(k, r)}. \]
Quasiparticle excitation distribution \( \pi \equiv \langle b_k^\dagger b_k \rangle \) changes to
\[ \pi(k, r) = \{ \exp \left[ \beta \omega(k, r) \right] - 1 \}^{-1}. \]
The condition of condensate existence, in the local-density interpretation, is
The spectrum of collective excitations takes the local form

$$\epsilon(k, r) = \sqrt{c^2(k^2) + \left(\frac{k^2}{2m}\right)^2}.$$  \hfill (358)

Following this way, we replace \(n(k, r)\) by \(n(k, r)\) and \(\sigma(k, r)\) by \(\sigma(k, r)\), defined by the expressions

$$n(k, r) = \frac{\omega(k, r)}{2\epsilon(k, r)} \coth \left(\frac{\epsilon(k, r)}{2T}\right) - \frac{1}{2},$$

$$\sigma(k, r) = -\frac{mc^2(k, r)}{2\epsilon(k, r)} \coth \left(\frac{\epsilon(k, r)}{2T}\right).$$ \hfill (359)

The local density of uncondensed atoms and the anomalous average are given by the integrals

$$\rho_1(r) = \int n(k, r) \frac{dk}{(2\pi)^3}, \quad \sigma_1(r) = \int \sigma(k, r) \frac{dk}{(2\pi)^3}.$$ \hfill (360)

Thus, almost all main equations, derived for uniform systems, can be straightforwardly transformed for weakly nonuniform systems, employing the local-density approximation.

5. Coherent states

The phenomenon of coherence possesses two sides, state coherence and transition coherence. The state coherence characterizes correlations between static properties of the considered objects, while the transition coherence describes correlated dynamical processes \[86\]. Generally, these two sides are interconnected.

5.1. Coherence characteristics

The appearance of Bose–Einstein condensate implies the appearance of coherent properties in the system. One can say that Bose–Einstein condensate is the coherent fraction of the considered system. In that sense, the condensate fraction \(n_0 = N_0/N\) plays the role of coherence measure for the system as a whole.

Generally, coherent phenomena in space and time can be described by means of correlation functions. The so-called first-order coherence is characterized by the first-order correlation function

$$C(r, t, r', t') = \frac{\rho(r, t, r', t')}{\sqrt{\rho(r, t) \rho(r', t')}}.$$ \hfill (361)

in which

$$\rho(r, t, r', t') \equiv \langle \psi^*(r', t') \psi(r, t) \rangle, \quad \rho(r, t) \equiv \langle \psi^*(r, t) \psi(r, t) \rangle.$$

By means of this correlation function, one can describe the spatial features of coherence.

For an isotropic system, one can define the coherence radius \(r_{coh}\) by the expression

$$r_{coh}^2 = \frac{\int r^2 C(r, t, 0, 0) dr}{\int C(r, t, 0, 0) dr},$$ \hfill (362)

with the integration over the system volume. Generally speaking, this radius depends on time.

For a cylindrically symmetric system, with the symmetry axis \(z\), it is possible to introduce two characteristic lengths, the transverse coherence radius \(r_{coh}\) given by the relation

$$r_{coh}^2 = \frac{\int r^2 C(r, t, 0, 0) dr}{\int C(r, t, 0, 0) dr},$$

where \(r_\perp = \sqrt{x^2 + y^2}\), and the coherence length \(l_{coh}\), defined by the formula

$$l_{coh}^2 = \frac{\int r^2 C(r, t, 0, 0) dr}{\int C(r, t, 0, 0) dr}.$$ \hfill (363)

For nonequilibrium systems, one can introduce the coherence time \(t_{coh}\) by the equation

$$t_{coh}^2 = \frac{\int t^2 C(r, t, 0, 0) dr}{\int C(r, t, 0, 0) dr},$$

with the integration over time from \(t = 0\) to \(t = t_{obs}\) where \(t_{obs}\) is the observation time. The latter, in particular, can tend to infinity. Generally, the coherence time depends on spatial location.

Depending on the coherence radius (in the case of isotropic systems), it is possible to distinguish three cases of first-order coherence:

$$r_{coh} \ll a \quad (\text{spatial chaos}),$$

$$a \ll r_{coh} \ll L \quad (\text{local coherence}),$$

$$r_{coh} \sim L \quad (\text{global coherence}).$$

Here \(a\) is the mean interparticle distance and \(L\) is the system linear size.

In the case of a Bose-condensed system, accomplishing the Bogolubov shift \(\psi(r, t) \rightarrow \eta(r, t) + \psi(r, t)\), we have

$$\rho(r, t, r', t') = \langle \eta(r, t) \eta^*(r', t') \rangle + \rho_0(r, t, r', t').$$

Then, in equilibrium, the coherence radius is of the system length, \(r_{coh} \sim L\), and the coherence time is of order of the observation time, \(t_{coh} \sim t_{obs}\) provided that \(\eta(r, t) \neq 0\).

The second-order coherence is characterized by the pair correlation function
\[
g(r, r') = \frac{\rho_2(r, r', r, r')}{\rho(r) \rho(r')}, \tag{364}
\]
in which
\[
\rho_2(r, r', r, r') = \langle \psi(r') \psi (r) \psi (r) \psi(r') \rangle
\]
is the second-order density matrix. For compactness, time \( t \) is not explicitly written.

Assuming that the interaction potential is integrable, it is possible to distinguish two opposite limiting situations. One case corresponds to a purely coherent system, when
\[
\rho(r) \rightarrow |\eta(r)|^2 = \rho_0(r), \quad \rho_2(r, r', r, r') \rightarrow \rho_0(r) \rho_0(r').
\]
Then \( g(r, r') \rightarrow 1 \) exhibiting global coherence.

Let us stress that the assumption of the interaction-potential integrability is crucial, since if it is not integrable, then \( g(r, r) = 0 \).

The opposite situation is when there are no correlations in the system, so that the Hartree–Fock approximation is valid,
\[
\rho_2(r, r', t, t') = \rho_0(r) \rho_1(r') + |\rho_1(r, r')|^2,
\]
with only noncondensed particles being present, \( \rho_1(r) = \rho(r) \). Then
\[
g(r, r') \rightarrow 1 + \frac{|\rho_1(r, r')|^2}{\rho_0(r) \rho_0(r')},
\]
and \( g(r, r) \rightarrow 2 \), since \( \rho_0(r, r) = \rho_0(r) \).

Summarizing, these opposite cases of second-order coherence are characterized by the conditions
\[
g(r, r) = \begin{cases} 1, & \text{coherence} \\ 2, & \text{chaos}. \end{cases} \tag{365}
\]

For example, the Hartree–Fock–Bogolubov approximation for a uniform Bose-condensed system gives
\[
g(r, r) = 1 + \frac{2 \rho_0}{\rho^2} (\rho_1 + \sigma_1).
\]
Then there is global second-order coherence, if \( \rho = \rho_0 \) and \( \rho_1 = \sigma_1 = 0 \), since \( g(r, r) = 1 \). But, generally, there occurs partial second-order coherence, when \( 1 < g(r, r) < 2 \).

We stress it again that an integrable interaction potential is assumed. Otherwise, \( g(r, r) \) would always be zero.

5.2. Interference effects

In the presence of several coherent parts of the whole system, there arise interference effects between these coherent parts. Thus, let the condensate function be composed of two parts, called coherent modes, so that
\[
\eta(r, t) = \eta_1(r, t) + \eta_2(r, t).
\]
The interference density
\[
\rho_{int}(r, t) \equiv |\eta(r, t)|^2 - \sum_n |\eta_n(r, t)|^2
\]
describes interference fringes arising as a result of the mode interference. As is clear,
\[
\rho_{int}(r, t) = 2 \text{Re} \eta_1^*(r, t) \eta_2(r, t).
\]
Assume that
\[
\eta_n(r, t) = \eta_0(t) e^{i k_n \cdot r},
\]
with real \( \eta_0(t) = \eta_0(t) \). Such expressions can arise in the process of expansion of two Bose condensates from different traps or from one trap separated in two parts. Then
\[
\rho_{int}(r, t) = 2 \rho_1(t) \cos(k_{12} \cdot r),
\]
where \( \rho_1(t) \equiv \eta(t) \eta(t) \) and \( k_{12} \equiv k_1 - k_2 \).

The other characteristic, describing interference effects, is the interference current
\[
j_{int}(r, t) \equiv j(r, t) - \sum_n j_n(r, t),
\]
in which the total current \( j(r, t) \) and partial currents \( j_n(r, t) \), respectively, are
\[
j(r, t) \equiv -\frac{i}{2m} \left[ \eta_1'(r, t) \nabla \eta_1(r, t) - \eta_2(r, t) \nabla \eta_2(r, t) \right],
\]
\[
j_n(r, t) \equiv -\frac{i}{2m} \left[ \eta_n'(r, t) \nabla \eta_n(r, t) - \eta_n(r, t) \nabla \eta_n(r, t) \right].
\]
The interference current writes
\[
j_{int}(r, t) = 2 \text{Re} j_{12}(r, t),
\]
where
\[
j_{12}(r, t) \equiv -\frac{i}{2m} \left[ \eta_1'(r, t) \nabla \eta_2(r, t) - \eta_2(r, t) \nabla \eta_1(r, t) \right].
\]
If the coherent modes depend on time as
\[
\eta_n(r, t) = \eta_0(r) e^{-ik_n t},
\]
with real \( \eta_0(r) = \eta_0(r) \), the interference current takes the form
\[
j_{int}(r, t) = 2 j_{12}(r) \sin(\omega_{12} t),
\]
in which \( \omega_{12} \equiv \omega_1 - \omega_2 \) and
\[
j_{12}(r) \equiv \frac{1}{2m} \left[ \eta_1(r) \nabla \eta_2(r) - \eta_2(r) \nabla \eta_1(r) \right].
\]
The interference current \( j_{int}(r, t) \) is called the Josephson current. Such currents appear, e.g., when Bose–Einstein condensate is separated into the wells of a double-well trap, or when several coherent modes are excited in a single trap [23, 24].

5.3. Coherent field

As has been explained above, a Bose-condensed system is described in the Fock space \( \mathcal{F}(\psi) \) generated by the field operators \( \psi \). The vacuum state of this space is the state \( |\eta\rangle \), such that \( \psi |\eta\rangle = 0 \). At the same time, we know that a coherent state is an eigenstate of a field operator [1, 87]. In the present case, the coherent state is the eigenstate of the field operator \( \psi = \eta + \psi_1 \). Here \( \eta \) is the condensate function, while \( \psi_1 \) is the field operator of uncondensed atoms. The condensate-function equation, as defined in (171), is
\[
\frac{i}{\partial t} \eta_0(r, t) = \left\langle \frac{\delta H[\eta, \psi]}{\delta \eta^*(r, t)} \right\rangle.
\]

If we assume that all the system is in the vacuum state and average over this state \(|\eta\rangle\), then we obtain the coherent-field equation (188) or, for a dilute gas, equation (189). Thus, the coherent-field equation is a particular case of the equation for the condensate wave function, when all the system is assumed to be in the vacuum state.

The assumption that the whole system is in its vacuum state is equivalent to the supposition that all particles are in the condensate, so that \(N_0 \approx N\). The physical situation, when the system is practically completely condensed, corresponds to the case of asymptotically weakly interacting gas at very low temperature. The related conditions are:

- Weak interaction: \(|\rho|a_s|^{1/3} \ll 1\).
- Low temperature: \(|\rho|^{1/3} \gg 1\).

Here \(\lambda_T \equiv \sqrt{2\pi \hbar m T}\).

A dilute gas interacts through the local potential \(\Phi(r) = \Phi_0 \phi(r)\), where \(\Phi_0 = 4\pi a_s m\), with \(a_s\) being scattering length. In the case of repulsion, \(a_s > 0\), and for attraction, \(a_s < 0\).

If the whole system is in a coherent state, being completely Bose-condensed, it is described by the Hamiltonian

\[
H^{(0)} = \int \eta^*(r) \left(-\frac{\nabla^2}{2m} + U - \mu_0\right) \eta(r) dr + \frac{1}{2} J_0 \int |\eta(r)|^4 dr.
\]

And the coherent-field is defined by the equation

\[
i \frac{\partial}{\partial t} \eta(r, t) = \frac{\delta H^{(0)}}{\delta \eta^*(r, t)} \left( \int |\eta(r, t)|^2 dr = N_0 \right).
\]

This leads to the Nonlinear Schrödinger (NLS) equation

\[
i \frac{\partial}{\partial t} \eta(r, t) = H[\eta]\eta(r, t),
\]

with the nonlinear Schrödinger Hamiltonian

\[
H[\eta] = -\frac{\nabla^2}{2m} + U(r, t) + \Phi_0 |\eta|^2 - \mu_0.
\]

In equilibrium, \(\eta(r, t) = \eta(r)\), and one gets the eigenproblem

\[
-\frac{\nabla^2}{2m} + U(r) + \Phi_0 |\eta(r)|^2 = \mu_0 |\eta(r)|
\]

in the form of a stationary NLS equation.

In this way, the correct meaning of the NLS equation for a Bose system is that this equation describes the coherent field corresponding to the vacuum state of a system that is assumed to be completely Bose-condensed. This equation is widely used for Bose systems with very weak interactions at zero temperature.

### 5.4. Hydrodynamic equations

The NLS equation is often employed for describing weakly interacting superfluids at zero temperature, since coherent systems are superfluid. If all the system is assumed to be coherent, it is superfluid as a whole. This follows from the definition of the superfluid fraction

\[
n_s = 1 - \frac{\beta}{3mN} \text{var}(\hat{P}), \quad \text{var}(\hat{P}) \equiv \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2.
\]

If the whole system is coherent, then its operator of momentum is

\[
\hat{P} = \int \eta^*(r)(-i\nabla)\eta(r) dr.
\]

From this, we have \(\text{var}(\hat{P}) = 0\). Therefore \(n_s = 1\). Hence the total system is superfluid.

One employs the Madelung representation

\[
\eta(r, t) = \sqrt{\rho_0(r, t)} e^{i\varphi(r, t)}, \quad \rho_0(r, t) = |\eta(r, t)|^2.
\]

Introducing the density of current

\[
\mathbf{j}_0(r, t) = -\frac{i}{2m} (\eta^* \nabla \eta - \eta \nabla \eta^*) = \rho_0(r, t) \mathbf{v}(r, t)
\]

and the velocity field

\[
\mathbf{v}(r, t) \equiv \frac{1}{m} \nabla S(r, t),
\]

and substituting them into the NLS equation, one derives the continuity equation and the velocity-field equation

\[
\frac{\partial \rho_0}{\partial t} + \nabla \cdot \mathbf{j}_0 = 0,
\]

\[
\frac{m}{2} \frac{\partial \mathbf{v}}{\partial t} + \nabla \left( U + \rho_0 \Phi_0 + \frac{mv^2}{2} + U_b \right) = 0,
\]

with the notation for the quantum potential

\[
U_b \equiv \frac{\sqrt{\rho}}{2m \sqrt{|\rho_0|}}.
\]

If there is no strong nonuniformity in the system, so that there are no sharp gradients, one neglects the quantum potential \(U_b\), retaining only first-order derivatives. This results in the hydrodynamic equations for a superfluid

\[
\frac{\partial \rho_0}{\partial t} + \nabla \cdot (\rho_0 \mathbf{v}) = 0, \quad \frac{m}{2} \frac{\partial \mathbf{v}}{\partial t} + \nabla \left( \mu_{\text{eff}} + \frac{mv^2}{2} \right) = 0,
\]

with the effective chemical potential

\[
\mu_{\text{eff}}(r, t) \equiv U(r, t) + \rho_0(r, t) \Phi_0.
\]

Recall that these hydrodynamic equations are valid only at zero temperature and very weak interactions, since uncondensed atoms are not taken into account.

#### 5.5. Thomas–Fermi limit

In section 4.14, the Thomas–Fermi approximation has been introduced for the condensate-function equation. Now we shall analyze this approximation for the coherent-field equation (370) that is a stationary NLS equation.
Let us consider an isotropic harmonic trap, for which 
\[ \omega_0 \equiv \omega_x = \omega_y = \omega_z, \] so that the trapping potential is
\[ U(r) = \frac{m}{2} \omega_0^2 r^2 \quad (r \ll |r|). \]
In spherical coordinates \( r = (r, \vartheta, \varphi), \) we have
\[ \nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \sin \vartheta \frac{\partial}{\partial \vartheta} + \frac{1}{r^2 \sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}. \]

It is convenient to pass to dimensionless quantities by scaling the spatial coordinate in units of the oscillator length, 
\[ r \longrightarrow r/l_0, \quad \left( l_0 \equiv \frac{1}{\sqrt{m \omega_0}} \right), \]
and defining the dimensionless energy
\[ E \equiv \frac{\mu_0}{\omega_0}, \quad \text{Eq. (376)} \]
Keeping this scaling in mind, we treat below the variable \( r \) as being dimensionless. To return back to the dimensional spatial variable, we have to make the substitution \( r \longrightarrow r/l_0. \)

The ground-state solution to equation (370) does not depend on the spherical angles, which allows us to look for a solution in the form
\[ \eta(r) = \sqrt{N_0} \chi(r) \] \( r, \)
respecting the normalization conditions
\[ \int |\eta(r)|^2 dr = N_0, \quad \int_0^\infty |\chi(r)|^2 dr = 1. \]
By introducing the dimensionless coupling parameter
\[ g \equiv \frac{\Phi_0 N_0}{\omega_0 l_0^3} \equiv \frac{4 \pi l_0^3}{N_0}, \quad \text{Eq. (377)} \]
equation (370) reduces to
\[ -\frac{1}{2} \frac{d^2 \chi}{dr^2} + \frac{r^2}{2} \chi + \frac{g}{4 \pi r^2} \chi^3 = E \chi, \quad \text{Eq. (378)} \]
with the boundary condition \( \chi(0) = 0. \)

From the above equation, it is straightforward to find the asymptotic behavior of the solution at short and large distance,
\[ \chi(r) \simeq c r + c r^3 + c r^5 \quad (r \rightarrow 0), \]
\[ \chi(r) \propto r \exp \left( -\frac{r^2}{2} \right) \quad (r \rightarrow \infty). \]

The Thomas–Fermi limit corresponds to the strong-coupling limit \( g \rightarrow \infty, \) when the interaction term is much larger then the kinetic-energy term. Then one can neglect the kinetic term, coming to the equation
\[ \frac{r^2 \chi + g}{4 \pi r^2} \chi^3 = E_{TF}. \]
This results of the Thomas–Fermi approximate solution
\[ \chi_{TF}(r) \simeq \Phi(r_{TF} - r) \sqrt{\frac{2 \pi}{g}} (r_{TF}^2 - r^2), \quad \text{Eq. (380)} \]
where the Thomas–Fermi radius is
\[ r_{TF} \equiv \sqrt{2 E_{TF}}, \quad \text{Eq. (381)} \]
and \( \Phi(x) \) is the unit-step function
\[ \Phi(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \]

From the normalization integral, we get the expression for the energy
\[ E_{TF} = \frac{1}{2} \left( \frac{15}{4 \pi} g \right)^{2/5} = 0.536 \, 689 \, g^{2/5}, \quad \text{Eq. (382)} \]
that is valid for large \( g \rightarrow \infty. \)
Thus the condensate density becomes
\[ \rho_0(r) = |\eta(r)|^2 = \frac{N_0}{2 g l_0^3} \Phi(r_{TF} - r)(r_{TF}^2 - r^2), \quad \text{Eq. (383)} \]
with the Thomas–Fermi radius
\[ r_{TF} \equiv \left( \frac{15}{4 \pi} g \right)^{1/5} \gg 1, \quad \text{Eq. (384)} \]
In the center of the trap, the central density is
\[ \rho_0(0) = \left( \frac{15}{4 \pi} g \right)^{2/5} \frac{N_0}{2 g^{3/5} l_0^3}. \]
For the average kinetic energy, we have
\[ \mathcal{K} \equiv \frac{1}{2 N_0} \int \eta^2(r) \left( -\frac{\nabla^2}{2m} \right) \eta(r) dr = -\frac{1}{2m l_0^2} \int_0^\infty \chi^2 \frac{d^2 \chi}{dr^2} dr = \frac{\omega_0}{2} \int_0^\infty \frac{d \chi}{dr} \left| \frac{d \chi}{dr} \right|^2 dr. \]
Using here the expression
\[ \frac{d \chi}{dr} \left| \frac{d \chi}{dr} \right|^2 = \frac{2 \pi}{g} \frac{r_{TF}^2}{r_{TF}^2 - r^2} \frac{4 r^2}{r_{TF}^2} \Phi(r_{TF} - r), \]
and taking the integral
\[ \int_0^\infty \frac{dx}{1 - x^2} = \frac{1}{2} \ln \frac{1 + x}{1 - x}, \]
we see that \( \mathcal{K} \) diverges.
In order to correct the result for the average kinetic energy, one considers a boundary layer of thickness \( \delta, \) such that \( \delta/r_{TF} \ll 1. \) Then the integral
\[ \int_0^{r_{TF} - \delta} \frac{d \chi}{dr} \left| \frac{d \chi}{dr} \right|^2 dr \approx \frac{\pi}{g} \frac{r_{TF}^3}{3} \left( \ln \frac{r_{TF}^2}{\delta} - \frac{8}{3} \right) \]
is finite. The second term here can be neglected for small \( \delta, \) which yields
\[
K \approx \frac{\pi \omega_0^3}{2 g} r_{TF}^2 \ln \frac{2 r_{TF}}{\delta}.
\]

Taking the boundary-layer width \( \delta \sim r_{TF}^{1/3} \) and neglecting \( \ln 2 \), as compared to \( \ln(r_{TF}/\delta) \), we find
\[
\frac{K}{\omega_0} \approx \frac{2 \pi}{3g} r_{TF}^2 \ln r_{TF} \approx \frac{5}{2} r_{TF}^2, \tag{385}
\]
with the dimensionless coupling parameter
\[
\gamma = \frac{4 \pi}{15} r_{TF}.
\]

The Thomas–Fermi approximation is connected to the effective thermodynamic limit, when \( N \to \infty \) and \( \omega_0 \to 0 \), so that \( N \omega_0^3 \to \text{const.} \). Really, in this limit \( \omega_0^3 N^{-1/3} \) and \( I_0 \propto N^{1/6} \). Since \( N_0 \approx N \), we have \( g \propto N^{5/6} \) and \( \rho_0(0) \propto \text{const.} \). The Thomas–Fermi radius \( r_{TF} \propto g^{1/5} \propto N^{1/6} \), hence \( r_{TF} I_0 \propto N^{1/3} \). Therefore the energy \( E_{TF} \propto g^{2/5} \propto N^{1/3} \). And the total energy per atom is finite, \( E_{TF} \propto \text{const.} \).

The average kinetic energy per atom is
\[
\frac{K}{\omega_0} \propto \frac{\ln N}{N^{2/3}} \to 0 \quad (N \to \infty),
\]
which gives
\[
K \propto \frac{\ln N}{N^{2/3}} \to 0 \quad (N \to \infty).
\]

This behaviour shows that the Thomas–Fermi limit is the same as the strong-coupling limit, or thermodynamic limit.

### 5.6. Optimized approximants

If the coupling parameter \( g \) is not necessarily large, which can occur for a small scattering length or a small number of atoms, then a more delicate procedure for evaluating the observable quantities, e.g. energy, is required. To find accurate approximations for observable quantities in the whole range of the coupling parameter \( g \in [0, \infty) \), one can resort to optimized perturbation theory [88–91].

Suppose we are looking for a real function \( E(g) \) of a real variable \( g \). For concreteness, we can keep in mind the energy as a function of the coupling parameter. But the theory is applicable to any other function of a real variable. Complicated problems are rarely solved exactly. The standard situation is when the problem can be treated only by perturbation theory, yielding a sequence of perturbative approximants \( E_i(g) \), with the index \( i = 0, 1, 2, \ldots \) enumerating the approximation order. Practically in all realistic cases, the sequence \{\( E_i(g) \)\} diverges for any finite value of \( g \). How then one could extract information from a divergent sequence?

This can be done by resorting to optimized perturbation theory, whose main idea is the introduction of control functions \( u_i = u_i(g) \) that would transform the divergent sequence into a convergent one. This can be realized by including a set of parameters \( u_i \) either through initial approximations or by means of a sequence transformation, so that, instead of \( E_i(g) \), we would get \( E_i(g, u_i) \). The next step is the definition of the control functions \( u_i = u_i(g) \) leading to the optimized approximants
\[
\tilde{E}_i(g) \equiv E_i(g, u_i(g)).
\]

The role of the control functions \( u_i(g) \) is to control the convergence of the optimized sequence \{\( \tilde{E}_i(g) \)\}.

Since, by their meaning, control functions have to produce convergence, they should be related to a convergence criterion. Thus the Cauchy criterion of uniform convergence states that the sequence \{\( \tilde{E}_i(g) \)\} converges if and only if for each \( \varepsilon \), there exists \( N_\varepsilon \), such that
\[
|\tilde{E}_i(g) - \tilde{E}_j(g)| < \varepsilon, \quad (\forall i > N_\varepsilon, \ j \geq 1).
\]

It is clear that the fastest convergence would occur when the control functions could provide the minimum
\[
\min_{u_i} \left| E_{i+1}(g, u_{i+1}) - E_i(g, u_i) \right|,
\]
however, this expression contains two control functions. We need to simplify the Cauchy criterion to be able to get solvable equations defining optimal control functions. For this purpose, we represent the above minimum in the form
\[
\min_{u_i} \left| E_{i+1}(g, u_{i+1}) - E_i(g, u_i) + (u_{i+1} - u_i) \frac{\partial}{\partial u_i} E_i(g, u_i) \right|,
\]
Taking into account the change of the approximation order plus the variation of the control function. Then we use the inequality
\[
\left| E_{i+1} - E_i + (u_{i+1} - u_i) \frac{\partial}{\partial u_i} E_i \right| \leq |E_{i+1} - E_i|
\]
where \( E_i = E_i(g, u_i) \). An approximate minimum of the right-hand side can be found from one of the following optimization conditions.

It is possible to set
\[
E_{i+1}(g, u_{i+1}) = E_i(g, u_i), \quad u_i = u_i(g).
\]
If this equation has either multiple or no solution, control functions can be found from the minimum
\[
\min_{u_i} \left| E_{i+1}(g, u_{i+1}) - E_i(g, u_i) \right|.
\]

The other admissible optimization condition can be
\[
(u_{i+1} - u_i) \frac{\partial}{\partial u_i} E_i(g, u_i) = 0.
\]
If there are either multiple or there is no solution, control functions can be defined either setting \( u_i = u_{i-1} \) or from the minimum
\[
\min_{u_i} \left| (u_{i+1} - u_i) \frac{\partial}{\partial u_i} E_i(g, u_i) \right|.
\]
The simplest form of an optimization condition is
\[ \frac{\partial}{\partial u_i} E_i(g, u_i) = 0. \]
If this equation gives no solution, then it is possible to look for the minimum
\[ \min_{u_i} \left| \frac{\partial}{\partial u_i} E_i(g, u_i) \right|. \]
The existence of the latter minimum requires the condition
\[ \frac{\partial^2}{\partial u_i^2} E_i(g, u_i) = 0, \]
defining the control function as an inflection point.
In practical applications, one can use any of the above conditions, since, strictly speaking, they are similar to each other. It is reasonable to try first the simplest of these conditions.

5.7. Coherent modes

To illustrate the optimized perturbation theory, let us find the eigenvalues of the stationary NLS equation, whose eigenfunctions are called coherent modes [79, 92]. The eigenvalues describe collective energy levels of trapped atoms in the coherent state. The coherent modes can also be termed topological coherent modes, since the related density distributions differ from each other by different numbers of zeros.

We consider a cylindrical trap, with a transverse, or radial, frequency \( \omega_z \equiv \omega_k = \omega_r \) and a longitudinal, or axial, frequency \( \omega_r \). The trap anisotropy is characterized by the anisotropy parameter,
\[ \lambda \equiv \frac{\omega_z}{\omega_r}. \]

It is natural to use the cylindrical coordinates
\[ r = \{r_x, \varphi, r_z\}, \quad r_\perp = \sqrt{r_x^2 + r_y^2}, \quad \varphi = \arctan \left( \frac{r_y}{r_x} \right) \]
The dimensionless coupling parameter is defined as
\[ g \equiv 4\pi \frac{\omega_k}{l_\perp} N_0 \left( l_\perp \equiv \frac{1}{\sqrt{\rho_0}} \right). \]

It is convenient to pass to the dimensionless spatial variables
\[ r \equiv \frac{r_x}{l_\perp}, \quad z \equiv \frac{r_z}{l_\perp}, \]
with \( r \in [0, \infty), \varphi \in [0, 2\pi) \), and \( z \in (-\infty, +\infty) \). The dimensionless condensate function is introduced through the relation
\[ \eta(r) = \sqrt{\frac{N_0}{l_\perp^2}} \psi(r, \varphi, z), \quad \int |\psi(r, \varphi, z)|^2 r \, dr \, d\varphi \, dz = 1. \]

Finally, the dimensionless energy is given by the expression
\[ E \equiv \frac{\varepsilon}{\omega_r}. \]

In these variables, the stationary NLS equation takes the form
\[ \hat{H}_{\text{NLS}} \psi = E \psi, \quad (389) \]
with the nonlinear Schrödinger Hamiltonian
\[ \hat{H}_{\text{NLS}} \equiv -\frac{\nabla^2}{2} + \frac{1}{2} (r^2 + \lambda^2 z^2) + g |\psi|^2, \]
in which
\[ \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}. \]
The eigenproblem (389) defines the spectrum of eigenvalues, the lowest of which corresponds to the chemical potential \( \mu_0 = (\min E) \omega_r \).

The control parameters \( u \) and \( v \), playing the role of effective radial and axial frequencies, are included in the initial approximation of the Hamiltonian
\[ \hat{H}_0 = -\frac{\nabla^2}{2} + \frac{1}{2} (u^2 r^2 + \lambda^2 v^2 z^2), \]
whose eigenvalues are
\[ E_{\text{n}mkn}^{(0)} = (2n + |m| + 1) u + \left( k + \frac{1}{2} \right) \lambda v. \]

Here \( n = 0, 1, 2, \ldots \) is radial quantum number, \( m = 0, \pm 1, \pm 2, \ldots \) is azimuthal quantum number, and \( k = 0, 1, 2, \ldots \) is axial quantum number. The eigenfunction, corresponding to the zero-order Hamiltonian, reads as
\[ \psi_{\text{n}mkn}(r, \varphi, z) = \left[ \frac{2n! |u|^{m+1}}{(n+|m|)!} \right]^{1/2} r^{|m|} \exp \left( -\frac{u}{2} r^2 \right) L_n^{|m|}(ur^2) \frac{e^{im\varphi}}{\sqrt{2\pi}} \times \frac{1}{\sqrt{2^k k!}} \left( \frac{\lambda v}{\pi} \right)^{1/4} \exp \left( -\frac{\lambda}{2} v z^2 \right) H_k(\sqrt{\lambda} v z). \]

The notations are used for the associated Laguerre polynomial
\[ L_n^m(x) = \frac{e^{x-m} \frac{d^n}{dx^n} (e^{-x} x^n)^m}{n! \frac{d^n}{dx^n} (e^{-x} x^n)^{n+m}} = \sum_{k=0}^n (-1)^k \frac{(n+m)!}{(n-k)! (m+k)!} k! x^k \]
and Hermite polynomial
\[ H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2} = n! \sum_{k=0}^{[n/2]} (-1)^k \frac{(2x)^{n-2k}}{k!(n-2k)!}. \]

The Rayleigh-Schrödinger perturbation theory gives the first-order approximation
\[ E_{\text{n}mkn}^{(1)} = (\psi_{\text{n}mkn}, \hat{H}_{\text{NLS}} \psi_{\text{n}mkn}) = E_{\text{n}mkn}^{(0)}(g, \lambda, u, v), \]
where
\[ p \equiv 2n + |m| + 1, \quad q \equiv (2k + 1) \lambda. \]

Accomplishing integration, we meet the integral
\[ I_{\text{mk}} = \frac{1}{u \sqrt{\lambda v}} \int |\psi_{\text{mk}}(r, \varphi, z)|^4 r dr d\varphi dz \]

\[ = \frac{2}{\pi^3} \sqrt{n!} (n + |m|)!^2 k! \int_0^\infty x^{2|m|} e^{-x^2} [L_n^{|m|}(x)]^4 \, dx \times \int_0^\infty e^{-2z^2} H_n^1(t) \, dt. \]

Then we obtain

\[ E_{\text{mk}}^{(1)} = \frac{p}{2} \left( u + \frac{1}{u} \right) + \frac{q}{4} \left( v + \frac{1}{v} \right) + \frac{1}{2} u \sqrt{v} x, \quad (395) \]

where we introduce the notation for the effective coupling parameter

\[ x \equiv 2g \sqrt{\lambda I_{\text{mk}}}. \quad (396) \]

The optimization conditions

\[ \frac{\partial}{\partial u} E_{\text{mk}}^{(1)} = 0, \quad \frac{\partial}{\partial v} E_{\text{mk}}^{(1)} = 0 \quad (397) \]

result in the equations

\[ 1 - \frac{1}{u^2} + \frac{\sqrt{v} x}{u} = 0, \quad 1 - \frac{1}{v^2} + \frac{u x}{\sqrt{v} v} = 0, \]

defining the control functions \( u = u_{\text{mk}}(g, \lambda) \) and \( v = v_{\text{mk}}(g, \lambda) \).

From the optimization conditions, it follows that the control functions are such that \( 0 \leq u \leq 1 \) and \( 0 \leq v \leq 1 \) for \( x \geq 0 \), while \( u \geq 1 \) and \( v \geq 1 \) for \( x \leq 0 \). The marginal case of an ideal gas is recovered in the limit

\[ \lim_{x \to 0} u = \lim_{x \to 0} v = 1. \]

Thus we come to the optimized approximant

\[ \tilde{E} \equiv E_{\text{mk}}^{(1)}(g, \lambda, u_{\text{mk}}(g, \lambda), v_{\text{mk}}(g, \lambda)) \]

\[ = \frac{p}{u} + \frac{q}{4} \left( v + \frac{1}{v} \right). \quad (398) \]

This approximant describes well the energy levels of atoms in a trap for the whole region of the effective coupling parameter \( x \in [0, \infty) \). In the limit of weak coupling \( x \to \pm 0 \), the control functions are

\[ u \simeq 1 - \frac{1}{2p} x + \frac{p + 3q}{8p^2 q} x^2 - \frac{3p^2 + 16pq + 20q^2}{64p^2 q^2} x^3, \]

\[ v \simeq 1 - \frac{1}{2q} x + \frac{p + q}{4pq^2} x^2 - \frac{7p^2 + 20pq + 12q^2}{64p^2 q^3} x^3. \]

In the limit \( x \to \pm 0 \) they tend to one, approaching the case of noninteracting atoms in a harmonic trap, as it should be.

Under strong coupling \( x \to +\infty \), the control functions behave as

\[ u \simeq \left( \frac{p}{q} \right)^{2/5} x^{-2/5} + \frac{q^2 - 3p^2}{5(pq^2)^{1/5}} x^{-6/5} + \frac{3p^2 - p^2 q^2 - q^4}{5pq} x^{-2}, \]

\[ v \simeq \left( \frac{q^2 - 3p^2}{p} \right)^{2/5} x^{-2/5} + \frac{2(p^2 - 2q^2)}{5} \left( \frac{q}{p^3} \right)^{2/5} x^{-6/5} + \frac{6q^4 - 4p^2 q^2 - p^4}{5p^2} x^{-2}. \]

Note that there are no real solutions for \( x \to -\infty \), since strongly attractive atomic interactions make the system unstable.

The weak-coupling expansion for the energy levels reads as

\[ \tilde{E} \simeq a_0 + a_1 x + a_2 x^2 + a_3 x^3 \quad (x \to \pm 0), \]

with the coefficients

\[ a_0 = p + \frac{q}{2}, \quad a_1 = \frac{1}{2}, \quad a_2 = -\frac{p + 2q}{16pq}, \quad a_3 = \left( \frac{p + 2q}{8pq} \right)^2. \]

In the strong coupling limit \( x \to +\infty \), the energy becomes

\[ \tilde{E} \simeq b_0 x^{2/5} + b_1 x^{-2/5} + b_2 x^{-6/5} + b_3 x^{-2}, \]

where

\[ b_0 = \frac{5}{4} (p^2 q)^{1/5}, \quad b_1 = \frac{2p^2 + q^2}{4(p^2 q)^{1/5}}, \]

\[ b_2 = -\frac{3p^4 - 2p^2 q^2 + 2q^4}{20(p^2 q)^{1/5}}, \]

\[ b_3 = \frac{2p^6 - p^3 q^2 - 2p^2 q^4 + 2q^6}{20p^2 q}. \]

The shape of the atomic cloud in the trap is characterized by the mean-square radius and the mean-square length defined by the expressions

\[ r_0^2 \equiv \langle \psi_{\text{mk}}^2 r^2 \psi_{\text{mk}} \rangle, \quad z_0^2 \equiv \langle \psi_{\text{mk}}^2 z^2 \psi_{\text{mk}} \rangle, \quad (399) \]

for which we obtain

\[ r_0^2 = \frac{p}{u} \quad z_0^2 = \frac{2k + 1}{2\lambda v}. \quad (400) \]

For weak coupling, it follows

\[ r_0^2 \simeq p \left( 1 + \frac{x}{2p} \right), \quad z_0^2 \simeq \frac{2k + 1}{2\lambda v} \left[ 1 + \frac{x}{2(2k + 1)\lambda} \right] \quad (x \to 0). \]

And when the coupling is strong, then

\[ r_0^2 \simeq (p^2 q)^{1/5} x^{2/5}, \quad z_0^2 \simeq \left( \frac{(p^2 q)^{1/5}}{2\lambda} \right) x^{2/5} \quad (x \to +\infty). \]

The ratio of the mean-square radius to the mean-square length defines the aspect ratio

\[ \frac{r_0^2}{z_0^2} = \frac{2p\lambda v}{(2k + 1)u}. \]

63
In the weak and strong coupling limits, respectively,
\[
\frac{r_0^2}{z_0} \approx \frac{2 \rho \lambda}{2k + 1} \quad (x \to \pm 0), \quad \frac{r_0^2}{z_0} \approx 2 \lambda^2 \quad (x \to +\infty).
\]

Of special interest is the ground-state energy, with \( n = m = k = 0, p = 1, \) and \( q = \lambda. \) At low temperature, atoms pile down to this lowest energy level. For the ground state, we have
\[
x = \frac{2g \sqrt{\lambda}}{(2\pi)^{3/2}}, \quad I_{00} = (2\pi)^{-3/2}.
\]

The ground-state energy follows from expression (398),
\[\tilde{E} = \frac{1}{u} + \frac{\lambda}{4}(v + \frac{1}{v})\]

with control functions given by the solutions to the optimization equations
\[1 - \frac{1}{u^2} + \sqrt{v}x = 0, \quad 1 - \frac{1}{v^2} + \frac{ux}{\lambda \sqrt{v}} = 0.
\]

In the weak-coupling limit \( x \to 0, \) the energy behaves as
\[\tilde{E} \approx a_0 + ax + ax^2 + ax^3,
\]

with the coefficients
\[a_0 = 1 + \frac{\lambda}{2}, \quad a_1 = \frac{1}{2}, \quad a_2 = -\frac{1 + 2\lambda}{16\lambda},
\]
\[a_3 = \left(1 + \frac{3\lambda}{8\lambda}\right)^2.
\]

In terms of the coupling parameter \( g, \) this is equivalent to
\[\tilde{E} \approx 1 + \frac{\lambda}{2} + \frac{g \sqrt{\lambda}}{(2\pi)^{3/2}} \quad (g \to 0).
\]

And in the strong-coupling limit, we find
\[\tilde{E} \approx 0.547 \, 538 (g \lambda)^{3/4} \quad (g \to \infty).
\]

This result is only 2\% different from the Thomas–Fermi limit.

Thus, optimized perturbation theory allows us to derive, for any quantity of interest, rather accurate approximations valid in the whole region of parameters.

5.8. Attractive interactions

As is mentioned in the previous section, the energy levels of trapped atoms may not exist at sufficiently strong coupling, when the coupling parameter (387) is negative. A negative coupling parameter corresponds to attractive atomic interactions, having a negative scattering length \( a_0 < 0, \) hence the coupling parameter \( g < 0, \) and the effective coupling parameter (396) is also negative, \( x < 0. \) The eigenproblem (389) does not have real solutions for the ground-state energy, if \( x < x_c < 0. \) This means that there is a critical line \( x_c = x_c(\lambda) \) separating the values of \( x > x_c, \) for which real eigenvalues exist, from the values \( x < x_c, \) where there are no real solutions. Respectively, there should exist a critical value \( g_c(\lambda), \) giving the related critical line
\[g_c(\lambda) = \frac{(2\pi)^{3/2}}{2\sqrt{\lambda}} x_c(\lambda).
\]

According to definition (387), the coupling parameter is connected with the number of atoms. Therefore, there exists a critical number of atoms \( N_c, \) above which the system of trapped atoms becomes unstable, while it is stable for \( N < N_c. \)

The critical number \( N_c \) depends on \( \lambda \) and characteristic trap lengths \( l_1, l_2 \) or \( l_0, \) that is, on trap frequencies. The trap lengths and frequencies are connected through the relations
\[l_0 \equiv \frac{1}{\sqrt{m \omega_0}} = l_1 = \lambda^{1/3} l_2,
\]
\[\omega_0 \equiv (\omega_0 \lambda \gamma)^{1/3} = \lambda^{1/3} \omega_1 = \frac{\omega}{\lambda^{1/3}}.
\]

Varying the trap lengths, it is possible to find the maximal critical number of atoms, below which the system is stable. Depending on which of the trap lengths is assumed to be varied, it is possible to present the critical number \( N_c \) in three forms:
\[N_c = \alpha_v(\lambda) \frac{l_1}{a_s} = \alpha_x(\lambda) \frac{l_2}{a_s} = \alpha_0(\lambda) \frac{l_0}{a_s},
\]

where
\[\alpha_v(\lambda) \equiv \frac{g_c(\lambda)}{4\pi} \frac{x_c(\lambda)}{\sqrt{\lambda}} = \frac{1}{2} \frac{x_c(\lambda)}{2\sqrt{\lambda}}.
\]
\[\alpha_x(\lambda) \equiv \frac{g_c(\lambda)}{4\pi} \sqrt{\lambda} = \frac{x_c(\lambda)}{2}.
\]
\[\alpha_0(\lambda) \equiv \frac{g_c(\lambda)}{4\pi} \lambda^{1/3} = \frac{x_c(\lambda)}{2\lambda^{1/3}}.
\]

The critical value \( x_c \) can be found by resorting to optimized perturbation theory analyzed in the previous section [92]. As an example, let us consider a spherical trap, where \( \lambda = 1 \) and \( u = v. \) Then the optimization equation for the control function \( u \) reads
\[x u^{3/2} + u^2 - 1 = 0.
\]

This equation possesses real solutions only for \( x > x_c, \) where
\[x_c = -\frac{4}{5^{3/4}} = -0.534 \, 992, \]

hence
\[g_c = \frac{(2\pi)^{3/2}}{2} x_c = -4.21296.
\]

For \( x < x_c, \) there are no real solutions. In the general case, when \( \lambda \neq 1, \) it is necessary to study the general form of the optimization equations presented in the previous section. This study can be done numerically. In order to obtain analytic expressions, we involve self-similar approximation theory [70–72], as is explained in [92]. This yields the effective critical coupling.
\[ x_\text{c}(\lambda) = \frac{-2\lambda}{1 + 2\lambda}, \quad (402) \]

with \(|x_\text{c}| \leq 1 \), and the critical coupling parameter

\[ g_\text{c}(\lambda) = -(2\pi)^{3/2} \frac{\sqrt{\lambda}}{1 + 2\lambda}. \quad (403) \]

From these expressions, we have

\[ \alpha_\ell(\lambda) = \left[ \frac{\pi}{2} \left( \frac{\sqrt{\lambda}}{1 + 2\lambda} \right) \right]^{1/\ell}, \quad \alpha_\ell(\lambda) = \left[ \frac{\pi}{2} \left( \frac{\lambda}{1 + 2\lambda} \right) \right]^{1/\ell}, \]

The trap shape is characterized by the value of \( \lambda \). The trap has a cigar shape, if \( \lambda < 1 \), a disk shape, when \( \lambda > 1 \), and it is spherical, for \( \lambda = 1 \). In the limit of \( \lambda \to 0 \) or \( \lambda \to \infty \), we get

\[ \alpha_\ell(\lambda) \approx \begin{cases} 1.253 \lambda^{1/2} & (\lambda \to 0) \\ 0.627\lambda^{-1/2} & (\lambda \to \infty), \end{cases} \]

and the cigar-shape trap is optimal, with \( \lambda = 0.5 \).

When \( l_z \) is fixed, then

\[ \max_\lambda \alpha_\ell(\lambda) = 0.443 \quad (\lambda = 0.5), \]

and the cigar-shape trap is optimal, with \( \lambda = 0.5 \).

Finally, when \( l_0 \) is fixed, then

\[ \max_\lambda \alpha_\ell(\lambda) = 0.627 \quad (\lambda \to \infty), \]

and the disk-shape trap is optimal, with \( \lambda \to \infty \).

Hence the spherical trap is optimal, when \( \lambda = 1 \).

In the general situation, the critical number of atoms can be represented [92] in the form

\[ N_\text{c} = \frac{\pi}{2} \left( \frac{l_1 l_2}{l_0} \right)^{1/3}. \quad (404) \]

This can be rewritten as

\[ \frac{|\alpha_\ell|}{l_0} N_\text{c} = \frac{\pi}{2} \left( \frac{l_0^{3/2}}{l_1^{3/2} + l_2^{3/2}} \right)^{1/3}. \quad (405) \]

where \( l_0 \equiv (l_1, l_2, l_3)^{1/3} \). In terms of the trap frequencies, the latter reduces to

\[ \frac{|\alpha_\ell|}{l_0} N_\text{c} = \frac{\pi}{2} \left( \frac{1}{\omega_x} + \frac{1}{\omega_y} + \frac{1}{\omega_z} \right)^{-1}. \]

The accuracy of the approximate analytical expressions (404) and (405) has been estimated for the case of a spherical trap and compared with the numerically found value of \( N_\text{c} \). The difference of the analytical and numerical values is only about 10%.

### 5.9. Collective excitations

The stationary NLS equation (389) gives the spectrum of coherent modes that are the stationary solutions corresponding to the coherent field. Around each of the stationary solutions, there can exist small nonequilibrium oscillations describing collective excitations.

To study collective excitations, arising around a coherent mode, it is necessary to consider the time-dependent NLS equation

\[ \frac{i}{\hbar} \frac{\partial \eta(r, t)}{\partial t} = H[\eta(r, t)] \eta(r, t), \quad (406) \]

with the nonlinear Schrödinger Hamiltonian

\[ H[\eta] \equiv -\frac{\nabla^2}{2m} + U(r) + \Phi_0 |\eta|^2 - \varepsilon. \]

Again, we write here \( \varepsilon \), instead of \( \mu_\Phi \), keeping in mind that there can exist the whole variety of coherent modes with the related energy spectrum. The lowest of these energies gives \( \mu_\Phi \).

Elementary collective excitations are described by a linearized equation, with respect to small deviations from a given coherent mode,

\[ \eta(r, t) = \eta(r) + \delta \eta(r, t). \]

Small deviations from a stationary solution \( \eta(r) \) correspond to small oscillations of the coherent mode defined by the stationary NLS equation

\[ \left[ -\frac{\nabla^2}{2m} + U(r) + \Phi_0 |\eta(r)|^2 \right] \eta(r) = \varepsilon \eta(r). \]

Linearizing with respect to \( \delta \eta(r, t) \), and representing the latter as

\[ \delta \eta(r, t) = u(r)e^{-i\omega t} + v^*(r)e^{i\omega t}, \quad (407) \]

implies the linearization with respect to \( u(r) \) and \( v(r) \). This linearization results in the Bogolubov equations

\[ \{ \omega - H[\eta(r)] - \Phi_0 |\eta(r)|^2 \} m(r) - \Phi_0 \eta^2(r)v(r) = 0, \]

\[ \{ \omega + H[\eta(r)] + \Phi_0 |\eta(r)|^2 \} v(r) + \Phi_0 |\eta(r)|^2 u(r) = 0. \]

These equations are appropriate for describing small deviations from any coherent topological mode.
If one is interested in the excitations of the ground-state coherent field, the latter can be taken real, \( \eta(r) = \eta^*(r) \). For a slowly varying trapping potential \( U(r) \), one can use the local-density approximation, assuming that the condensate density \( \rho_0(r) \equiv |\eta(r)|^2 \) is also slowly varying. Considering a dilute gas and employing the Thomas–Fermi approximation, that is, neglecting the kinetic term in the stationary NLS equation, yields

\[
\varepsilon \equiv U(r) + \rho_0(r) \Phi_0,
\]

which results in the condensate density

\[
\rho_0(r) \simeq \frac{\varepsilon - U(r)}{\Phi_0}; \quad (U(r) \ll \varepsilon).
\]

The Bogolubov equations reduce to

\[
\begin{align*}
\left( \omega + \frac{V^2}{2m} - \rho_0 \Phi_0 \right) u(r) - \rho_0 \Phi_0 v(r) &= 0, \\
\left( \omega - \frac{V^2}{2m} + \rho_0 \Phi_0 \right) v(r) + \rho_0 \Phi_0 u(r) &= 0,
\end{align*}
\]

where \( \rho_0 = \rho_0(r) \) is a slowly varying function of \( r \).

Following the local-density approximation, one sets

\[
u(r) = \nu_0 e^{ik \cdot r}, \quad v(r) = \nu_0 e^{ik \cdot r},
\]

where \( u_0 = u_0(r) \) and \( v_0 = v_0(r) \) are slowly varying functions. Then the Bogolubov equations transform into

\[
\begin{align*}
\left( \omega - \frac{k^2}{2m} - \rho_0 \Phi_0 \right) u_0 - \rho_0 \Phi_0 v_0 &= 0, \\
\rho_0 \Phi_0 u_0 + \left( \omega + \frac{k^2}{2m} + \rho_0 \Phi_0 \right) v_0 &= 0.
\end{align*}
\]

The existence of nontrivial solutions requires that the determinant of the system of equations be zero. This gives the local Bogolubov spectrum

\[
\varepsilon(k, r) = \sqrt{c^2(r)k^2 + \left( \frac{k^2}{2m} \right)^2},
\]

with the local sound velocity

\[
\frac{c(r)}{m} \equiv \sqrt{\frac{\rho_0(r)}{m} \Phi_0}.
\]

In the long-wave limit, the spectrum is of phonon type,

\[
\varepsilon(k, r) \simeq c(r)k \quad (k \to 0).
\]

And for large \( k \), one gets the spectrum

\[
\varepsilon(k, r) \simeq \frac{k^2}{2m} \quad (k \to \infty)
\]

of the single-particle type.

The obtained spectrum of collective excitations, for a purely coherent system, looks similar to spectrum (358) derived in the local-density approximation, but here the sound velocity has the Bogolubov form (410), since in a purely coherent system, there are no uncondensed atoms and the anomalous average is zero.

### 5.10. Moving superfluid

Recall that a totally coherent system is superfluid, with the superfluid fraction \( n_s = 1 \). For a moving system, with a constant superfluid velocity \( v \), the coherent field, in the laboratory frame, is denoted by \( \eta_c(r, t) \). The time-dependent NLS equation is

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \eta_c(r, t) = H[\eta_c(r, t)] \eta_c(r, t).
\]

This evolution equation is invariant under the Galilean transformation

\[
\eta_c(r, t) = \eta_c(r - vt, t) \exp \left\{ -i \left( \frac{mv \cdot r - mv^2 t}{2} \right) \right\}.
\]

To find the spectrum of collective excitations, we consider a small deviation from the function \( \eta_c(r - vt) \), looking for a solution in the form

\[
\eta_c(r - vt, t) = \eta_c(r - vt) + u_c(r)e^{-i\omega t} + v_c(r)e^{i\omega t}.
\]

Linearizing (411) with respect to \( u_c(r) \) and \( v_c(r) \), we use the equality

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \eta_c(r - vt) = v \cdot \hat{\mathbf{p}} \eta_c(r - vt),
\]

where \( \hat{\mathbf{p}} \equiv -i\nabla \) is the momentum operator. The linearization results in the Bogolubov equations

\[
\begin{align*}
\left[ \omega - v \cdot \hat{\mathbf{p}} - H[\eta_c(r - vt)] - \Phi_0 |\eta_c(r - vt)|^2 \right] u_c(r) \& - \Phi_0 \eta_c(r - vt) v_c(r) &= 0, \\
\left[ \omega - v \cdot \hat{\mathbf{p}} + H[\eta_c(r - vt)] + \Phi_0 |\eta_c(r - vt)|^2 \right] v_c(r) \& + \Phi_0 |\eta_c(r - vt)|^2 u_c(r) &= 0.
\end{align*}
\]

Considering excitations over the ground state, in the local-density approximation, we get the collective spectrum of a moving superfluid,

\[
\varepsilon_c(k, r - vt) = v \cdot k + \sqrt{c^2(r - vt)k^2 + \left( \frac{k^2}{2m} \right)^2},
\]

with the similar definition of the sound velocity \( c(r - vt) \), as for an immovable system, but with \( \rho_0 = \rho_0(r - vt) \). The spectrum can be rewritten as

\[
\varepsilon_c(k, r - vt) = \varepsilon(k, r - vt) + v \cdot k,
\]

with \( \varepsilon(k, r - vt) \) being the spectrum (409) in a system at rest.

Since excitations increase the system energy, the spectrum must be non-negative for all \( k \), so that \( \varepsilon_c(k, r - vt) \geq 0 \). Otherwise, the coherent mode would be unstable. In the long-wave limit, this implies that
\[ \varepsilon_i(k, \mathbf{r} - \mathbf{v}) \approx c(\mathbf{r} - \mathbf{v})k + \mathbf{v} \cdot \mathbf{k} \quad (k \to 0). \]

There always exists a vector \( \mathbf{k} \), such that \( \mathbf{v} \cdot \mathbf{k} = -vk \), where \( v \equiv |\mathbf{v}| \). Therefore, for the stability of motion, it is required that

\[ \min_k \frac{\varepsilon_i(k, \mathbf{r} - \mathbf{v})}{k} = c(\mathbf{r} - \mathbf{v}) - v > 0. \]

Hence the critical velocity of superfluid motion has to be smaller than the sound velocity,

\[ \min_k \frac{\varepsilon_i(k, \mathbf{r} - \mathbf{v})}{k} = c(\mathbf{r} - \mathbf{v}) > v, \]  

(414)

which is equivalent to the local Landau criterion. The motion is dynamically stable, provided that \( v < c(\mathbf{r} - \mathbf{v}) \). The stability criterion can be represented as the stability condition for a moving wave packet:

\[ \rho_0(\mathbf{r} - \mathbf{v}) > \frac{mv^2}{\Phi_{ij}} = \frac{(mv)^2}{4\pi a_i}. \]  

(415)

A wave packet, moving faster than the sound velocity, becomes unstable.

5.11. Coherent mixtures

It is possible to create mixtures of several coherent components. To remain coherent, the components have to consist of atoms with weak interactions between all components enumerated by \( i = 1, 2, \ldots, \) so that

\[ \sqrt{\rho_i a_i^3} \ll 1 \quad \left( \rho_i \equiv \frac{N_i}{V} \right). \]  

(416)

where \( \rho_i \) is the mean density of an \( i \)th component, \( N_i \) is the number of particles in a component, and \( a_i \) is a scattering length for scattering between an atom of the \( i \)th component and an atom of the \( j \)th component.

The system is dilute if all interactions are short-range, such that

\[ \sqrt{\rho_i a_i^3} \ll 1, \]  

(417)

where \( r_i \) is an effective interaction radius of interactions between atoms of the \( i \)th and \( j \)th species.

Temperature has to be low, satisfying the inequality

\[ \rho_i \lambda_i^3 \ll 1 \quad \left( \lambda_i \equiv \frac{2\pi}{m_i T} \right). \]  

(418)

\( m_i \) being atomic mass in the \( i \)th component.

Under these conditions, the dilute-gas approximation for the interaction potential is admissible. There are three local interaction potentials

\[ \Phi_0(\mathbf{r}) = \Phi_0(\delta(\mathbf{r})), \quad \Phi_{ij} \equiv \int \Phi_j(\mathbf{r})d\mathbf{r}, \]

\[ \Phi_j = 4\pi a_j \frac{m_j}{m_j}, \quad m_j \equiv \frac{2m_i m_j}{m_i + m_j}, \]  

(419)

with \( a_j = a_1 \) and \( m_j \) being reduced mass.

The Hamiltonian of a coherent mixture is

\[ H_{\text{mix}} = \sum_i \int \eta_i^*(\mathbf{r}, t) \left( -\frac{\nabla^2}{2m_i} + U_i - \varepsilon_i \right) \eta_i(\mathbf{r}, t) d\mathbf{r} + \frac{1}{2} \sum_j \Phi_{ij} \int |\eta_j(\mathbf{r}, t)|^2 |\eta_i(\mathbf{r}, t)|^2 d\mathbf{r}, \]  

(420)

where \( U_i = U_j(\mathbf{r}, t) \) are external trapping potentials. The quantities \( \varepsilon_i \) play the role of the species chemical potentials, guaranteeing the normalization conditions

\[ \int |\eta_i(\mathbf{r}, t)|^2 d\mathbf{r} = N_i. \]

Therefore not all different species can be uniformly mixed. However not all different species can be uniformly mixed.

In equilibrium, \( \eta_i(\mathbf{r}, t) = \eta_j(\mathbf{r}), \) and we get the stationary NLS equations

\[ \left[ -\frac{\nabla^2}{2m_i} + U_i(\mathbf{r}) + \sum_j \Phi_{ij} |\eta_j(\mathbf{r})|^2 \right] \eta_i(\mathbf{r}) = \varepsilon_i \eta_i(\mathbf{r}). \]  

(422)

of the partial species Hamiltonians, without interactions between the components.

The mixture does not stratify, if mixture stability conditions are valid. Thus thermodynamic stability condition requires that the mixture free energy be smaller than the free energy of the stratified system. At zero temperature, this reduces to the stability condition for the internal energies

\[ E_{\text{mix}} < E_{\text{sep}}, \]  

(424)

where

\[ E_{\text{mix}} = H_{\text{mix}} + \sum_i \varepsilon_i N_i, \quad E_{\text{sep}} = H_{\text{sep}} + \sum_i \varepsilon_i N_i. \]

Assuming that the components are in their ground states, one can resort to the local-density approximation, where the
are slowly varying in space. Then in all equations, one can consider the densities as almost constant. The internal energy of the mixture can be written in the form

\[ E_{\text{mix}} = \frac{1}{2} \sum_{ij} \Phi_{ij} \frac{N_i N_j}{V} + \sum_i U_i N_i, \]

where \( U_i \) includes all single-particle energy terms. Separating here the sum into two terms, as

\[ \sum_{ij} \rightarrow \sum_{i=j} + \sum_{i \neq j}, \]

we get

\[ E_{\text{mix}} = \frac{1}{2} \sum_i \Phi_i \frac{N_i^2}{V} + \frac{1}{2} \sum_{i \neq j} \Phi_{ij} \frac{N_i N_j}{V} + \sum_i U_i N_i. \]  

(425)

While the stratified system has the internal energy

\[ E_{\text{sep}} = \frac{1}{2} \sum_i \Phi_i \frac{N_i^2}{V} + \sum_i U_i N_i. \]  

(426)

The separated species are assumed to be in equilibrium with each other. The condition of mechanical equilibrium requires that the pressures in each of the component be equal

\[ P_i = -\frac{\partial E_{\text{sep}}}{\partial V_i} = P_j = -\frac{\partial E_{\text{sep}}}{\partial V_j}. \]  

(427)

The pressure in an \( i \)th component is

\[ P_i = \frac{1}{2} \Phi_i \left( \frac{N_i^2}{V_i} \right). \]

Thence condition (427) yields

\[ \frac{P_i}{P_j} = \frac{\Phi_j}{\Phi_i} \left( \frac{N_i}{N_j} \right)^2 = 1, \]

from which it follows

\[ \frac{V_j}{V_i} = \frac{N_j}{N_i} \sqrt{\frac{\Phi_i}{\Phi_j}}. \]

Using the equality

\[ \frac{V}{V_i} = 1 + \sum_{j(i)} \frac{V_j}{V_i}, \]

we get

\[ \frac{V}{V_i} = 1 + \sum_{j(i)} \frac{N_j}{N_i} \sqrt{\frac{\Phi_i}{\Phi_j}}. \]

The energy of a stratified system (426) becomes

\[ E_{\text{sep}} = \frac{1}{2} \sum_i \Phi_i \frac{N_i^2}{V} + \frac{1}{2} \sum_{i \neq j} \Phi_{ij} \frac{N_i N_j}{V} + \sum_i U_i N_i. \]  

(428)

In this way, the stability condition (424) reduces to

\[ \sum_{i \neq j} N_i N_j \left( \Phi_{ij} - \sqrt{\Phi_i \Phi_j} \right) < 0. \]

Requiring that this condition be satisfied for any \( N_i \) and \( N_j \) leads to the conclusion that it is necessary and sufficient that condition

\[ \Phi_{ij} < \sqrt{\Phi_i \Phi_j} \quad (i \neq j) \]  

(429)

be valid.

Generalizing the mixture stability condition to nonzero temperatures, leads [93] to the inequality

\[ \Phi_{ij} < \sqrt{\Phi_i \Phi_j} + \frac{TV}{N_i N_j} \Delta S_{\text{mix}}, \]  

(430)

with \( i \neq j \) and the entropy of mixing

\[ \Delta S_{\text{mix}} = -N_i \ln \frac{N_i}{N} - N_j \ln \frac{N_j}{N}. \]

Hence finite temperature facilitates the mixture stability.

5.12. Spectrum branching

The stability of a mixture can also be investigated by studying the spectra of collective excitations [94–96]. For this purpose, we consider the dynamical equations (421), looking for small deviations from stationary solutions,

\[ \eta_j(r, t) = \eta_j(r) + \delta \eta_j(r, t), \]

with

\[ \delta \eta_j(r, t) = u_j(r)e^{i\omega t} + v_j(r)e^{i\omega t}. \]

Linearizing with respect to \( u_j(r) \) and \( v_j(r) \), we obtain the equations

\[ (\omega - H_j[\eta])u_j(r) - \eta_j(r) \sum_i \Phi_{ij} [\eta_i(r)u_i(r) + \eta_i(r)v_i(r)] = 0, \]

\[ (\omega + H_j[\eta])v_j(r) + \eta_j(r) \sum_i \Phi_{ij} [\eta_i(r)v_i(r) + \eta_i(r)u_i(r)] = 0. \]

Here the Hamiltonian \( H_j[\eta] \) is expressed through stationary solutions \( \eta_j(r) \). In what follows, we consider \( \eta_j(r) \) as ground states. Then in the local-density approximation, we have

\[ \left( \omega + \frac{\nabla^2}{2m_j} \right) u_j(r) - \sum_i \sqrt{\rho_i \rho_j} \Phi_{ij} [u_i(r) + v_i(r)] = 0, \]

\[ \left( \omega - \frac{\nabla^2}{2m_j} \right) v_j(r) + \sum_i \sqrt{\rho_i \rho_j} \Phi_{ij} [v_i(r) + u_i(r)] = 0. \]

Substituting here

\[ u_j(r) = u_j e^{ik \cdot r}, \quad v_j(r) = v_j e^{ik \cdot r}, \]

we get an algebraic system of linear equations with respect to \( u_j \) and \( v_j \).

Note that in the local-density approximation, \( u_i \) and \( v_i \) are treated as slow functions of spatial variable \( r \) depending on the latter through the local densities and the slowly varying external potentials. Respectively, the spectra of collective excitations depend on \( k \) as well as on \( r \). In order to simplify notations, we omit below the dependence of the spectra on the
spatial variable \( r \). This dependence can be restored by taking into account the local densities \( \rho_i = |\eta_i(r)|^2 \).

The existence of nontrivial solutions of a system of linear equations implies their zero determinant. In what follows, we consider a binary mixture \((j = 1, 2)\). And the following notations will be used:

\[
\epsilon_j(k) \equiv \sqrt{c_j^2 k^2 + \left( \frac{k^2}{2m_j} \right)^2}, \quad \epsilon_{\pm}(k) \equiv \sqrt{\rho_j \phi_j},
\]

\[
\epsilon_{12}(k) \equiv c_{12} k, \quad \epsilon_{c21}^2 \equiv \sqrt{\rho_{\text{mix}} \phi_{\text{mix}}}, \quad \epsilon_{12}^2 \equiv \sqrt{\rho_{\text{mix}} \phi_{\text{mix}}},
\]

The requirement of zero determinant results in the equation

\[
[\omega^2 - \epsilon_1^2(k)] \omega^2 - \epsilon_2^2(k) = \epsilon_{12}^2(k),
\]

where \( \omega \) is the wave number. Solving the latter with respect to \( \omega \) yields the spectrum

\[
\epsilon_{\pm}(k) = \sqrt{c_1^2 k^2 + \left( \frac{k^2}{2m_1} \right)^2 + 4\epsilon_{12}^4(k)},
\]

(433)

The spectrum \( \epsilon_{\pm}(k) \) describes the density wave that is common for both species. While the spectrum \( \epsilon_{\pm}(k) \) corresponds to the oscillations of the components with respect to each other.

In the long-wave limit, both these spectra are of phonon type

\[
\epsilon_{\pm}(k) \approx c_{\pm} k \quad (k \to 0),
\]

(434)

with the sound velocities

\[
c_{\pm}^2 \equiv \frac{1}{2} \left[ c_1^2 + c_2^2 \pm \sqrt{(c_1^2 - c_2^2)^2 + 4\epsilon_{12}^4} \right].
\]

(435)

But neither of \( c_{\pm} \) is the hydrodynamic sound velocity

\[
s^2 \equiv \left( \frac{\partial P}{\partial \rho_m} \right)_{TN},
\]

(436)

where \( \rho_m \) is the mass density \( \rho_m = \sum_i m_i \rho_i \). The pressure in this mixture is

\[
P_{\text{mix}} = -\frac{\partial E_{\text{mix}}}{\partial V} = \frac{1}{2} \sum_y \phi_y \rho_y \rho_y \left( \rho_i \equiv \frac{N_i}{V} \right).
\]

Using the approximate relation \( \partial \rho_i / \partial \rho_m \approx \rho_i / \rho_m \) gives

\[
s^2 \approx \sum_y \phi_y \frac{\rho_y}{\rho_m} \rho_y
\]

Thus, for a binary mixture, the hydrodynamic sound velocity is

\[
s^2 = \frac{\phi_1 \rho_1^2 + \phi_2 \rho_2^2 + 2\phi_{12} \rho_1 \rho_2}{m_1 \rho_1 + m_2 \rho_2}.
\]

(437)

In the short-wave limit, the spectra are of the single-particle type,

\[
\epsilon_{\pm}(k) \approx \frac{k^2}{2m_1}, \quad \epsilon_{\pm}(k) \approx \frac{k^2}{2m_2} \quad (k \to \infty).
\]

The mixed system is dynamically stable, provided that the spectra of collective excitations are positive, \( \epsilon_{\pm}(k) > 0 \), except maybe zero \( k \). Therefore, in view of equation (433), it should be \( \epsilon_{12}^2(k) < \epsilon_{12}^2(k) \). In the long-wave limit, this gives

\[
c_2^2 < c_1 c_2 \quad (k \to 0).
\]

(438)

And using notations (431), we see that the dynamic stability condition (438) for an immovable mixture is the same as the thermodynamic stability condition \( \phi_{12} < \sqrt{\phi_{11} \phi_{22}} \).

When the components move with the velocities \( v_1 \) and \( v_2 \), respectively, then, instead of equation (432), we obtain

\[
[(\omega - v_1 \cdot k)^2 - \epsilon_1^2(k)] [(\omega - v_2 \cdot k)^2 - \epsilon_2^2(k)] = \epsilon_{12}^4(k).
\]

(439)

It is convenient to pass to the coordinate system describing the relative motion of the components, where \( v_1 = -v_2 \equiv v \).

Then the dynamical instability occurs when \( \omega \to 0 \) as \( |v| \to v \).

When \( \omega \to 0 \), equation (439) takes the form

\[
[y_1^2 k^2 - \epsilon_1^2(k)] [y_2^2 k^2 - \epsilon_2^2(k)] = \epsilon_{12}^4,
\]

in which

\[
y_\pm \equiv \frac{v \cdot k}{k} = v \cos \theta.
\]

At the same time, the solution to the above equation with respect to \( y_\pm \) is

\[
y_\pm^2 = \frac{\epsilon_{12}^2(k)}{k^2}.
\]

Therefore the critical velocity is defined as the minimal solution of the equation

\[
(v \cos \theta)^2 = \frac{\epsilon_{12}^2(k)}{k^2},
\]

understanding that \( v_\pm \) is to be minimal for all \( k \). Thus we need to maximize the left-hand side of the above equation, while minimizing its right-hand side. The maximum of the left-hand side corresponds to \( \cos \theta = 1 \). And, since \( \epsilon_{\pm}(k) \leq \epsilon_{\pm}(k) \), we find the critical velocity

\[
v = \min_k \frac{\epsilon_{\pm}(k)}{k} = c_{\pm}.
\]

(440)

When \( v = |v| \) reaches \( v \), the system stratifies. The condition for the stability of moving components is \( v \leq v_\pm = c_{\pm} \).

The effect of the dynamical stratification cannot be treated by the thermodynamic stability condition, in which kinetic energy enters additively.

Note that in the laboratory frame, the velocities \( v_1 \) and \( v_2 \) can be directed arbitrarily. If they point in one direction, the arising instability can be directed arbitrarily. If they point in opposite directions, they point in opposite to each other. Hence it is always possible to call the resulting instability the counterflow instability or simply flow instability.
5.13. Quantum vortices

The NLS equation

\[ i \frac{\partial}{\partial t} \eta(r,t) = H[\eta] \eta(r,t), \]

with the NLS Hamiltonian

\[ H[\eta] = -\frac{\nabla^2}{2m} + U(r) + \Phi_0 |\eta|^2 - \varepsilon \left( \Phi_0 = 4\pi a_r/m \right), \]

describes various coherent topological modes. One of the most interesting modes is the quantum vortex filament.

To describe this mode, it is convenient to pass to cylindrical coordinates \( r = \{ r_L, \varphi, z \} = \{ r_L, \varphi \} \), where \( r_L = \{ r_L, \varphi \} \). Then

\[
\nabla^2 = \nabla^2_\perp + \partial^2_\varphi, \quad \nabla^2_\perp = \frac{\partial^2}{\partial r_L^2} + \frac{1}{r_L} \frac{\partial}{\partial r_L} + \frac{1}{r_L^2} \frac{\partial^2}{\partial \varphi^2}.
\]

The trapping harmonic potential reads as

\[ U(r) = \frac{m}{2} \left( \omega_L^2 r_L^2 + \omega_\varphi^2 \varphi^2 \right) \left( l_\varphi \equiv \frac{1}{\sqrt{m\omega_\varphi}}, \quad l_\varphi \equiv \frac{1}{\sqrt{m\omega_\varphi}} \right), \]

Let us consider a disk-shape trap, where \( l_\varphi \ll l_\varphi \), hence \( \omega_L \ll \omega_\varphi \). We assume that there is no scattering on the trap boundary and \( |\alpha| \ll l_\varphi \). We can look for the solution of the evolution equation by separating the variables,

\[ \eta(r,t) \propto \sqrt{N_0} \chi(r_L) e^{i\omega_\varphi \varphi(z)} e^{-iE_L t}, \]

with the normalization conditions

\[ \int \chi(r_L)^2 \, dr_L = 1 \quad (dr_L = 2\pi r_L \, dr_L), \]

\[ \int |\psi(z)|^2 \, dz = 1. \]

The quantum number \( \nu \) is called winding number, taking the values \( \nu = 0, \pm 1, \pm 2, \ldots \). Keeping in mind a cylindrical trap, we denote its radius and length by \( R \) and \( L \), respectively.

Assuming that the longitudinal part of the trapping potential is much larger than the interaction term, we get the longitudinal confinement characterized by the harmonic-oscillator equation

\[ \left( -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{m}{2} \omega_z^2 \right) \psi(z) = E_z \psi(z), \]

whose ground-state solution is

\[ \psi(z) = \frac{1}{\pi^{1/4} \sqrt{l_z}} \exp \left( -\frac{z^2}{2l_z^2} \right), \quad E_z = \frac{1}{2} \omega_z. \]

Introducing the effective length \( L_{\text{eff}} \) by the equation

\[ \int_{-L/2}^{L/2} |\psi(z)|^2 \, dz = \frac{1}{L_{\text{eff}}} \int_{-L/2}^{L/2} |\psi(z)|^2 \, dz, \]

for the harmonic oscillator, we get \( L_{\text{eff}} = \sqrt{2\pi} l_z \). In the uniform case, when \( \psi(z) \to 1/\sqrt{L} \), the effective length would be \( L_{\text{eff}} \to L \).

Substituting \( \eta(r,t) \) into the evolution equation, multiplying the latter by \( \psi^*(z) \), and integrating over \( z \), we come to the effective radial equation.

\[
\left[ -\frac{1}{2m} \left( \frac{d^2}{dr_L^2} + \frac{1}{r_L} \frac{d}{dr_L} \right) + \frac{\nu^2}{2r_L^2} + \frac{m}{2} \omega_z^2 r_L^2 \right] \psi(r_L) + \frac{\Phi_0}{L_{\text{eff}}} |\chi(r_L)|^2 - \varepsilon \chi(r_L) = 0. \tag{441}
\]

As is seen, the quantity

\[ \frac{\Phi_0}{L_{\text{eff}}} = \sqrt{8\pi} \frac{a_r}{ml_\varphi} \]

plays the role of an effective interaction strength. Here we assume that the interactions are repulsive, such that \( \Phi_0 > 0 \).

For what follows, we need to introduce the healing length

\[ \xi \equiv \frac{1}{\sqrt{2m\varepsilon}}. \tag{442} \]

which depends on the eigenvalue \( \varepsilon \). And we define the dimensionless real function

\[ f(r) \equiv \frac{\Phi_0 N_0}{\sqrt{\varepsilon L_{\text{eff}}}} \chi(r_L) \left( r \equiv \frac{r_L}{\xi} \right). \]

Then equation (441) reduces to

\[
\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{\nu^2}{r^2} + \frac{\xi^4}{L_{\text{eff}}^4} + 1 \right) f - f^3 = 0, \tag{443}
\]

with the normalization condition

\[ \frac{\pi L_{\text{eff}}}{m \Phi_0 N_0} \int_0^{R\xi} f^2(r) \, r \, dr = 1 \tag{444} \]

defining \( \varepsilon \). The boundary conditions are

\[ f_\nu(r) \propto r^{|\nu|} \quad (r \to 0), \]

\[ f_\nu(r) \propto r^\nu \exp \left( -\frac{\xi^2}{2L_{\text{eff}}^2} r^2 \right) \quad (r \to \infty). \]

The healing length is assumed to be much shorter than the trap characteristic transverse length \( l_\varphi \sim R \), so that \( \xi \ll l_\varphi \). Therefore, for \( l_\varphi \ll r \ll R/\xi \), it is possible to neglect the trapping term, thus, obtaining the equation

\[
\left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{\nu^2}{r^2} + 1 \right) f - f_\nu^3 = 0. \tag{445}
\]

This equation is invariant with respect to the sign change \( f_\nu \to -f_\nu \), because of which any sign can be chosen. Below we choose positive \( f(r) \). The boundary conditions can be presented in the form

\[ \lim_{r \to 0} f_\nu(r) = 0, \quad \lim_{r \to \infty} f_\nu(r) = 1, \tag{446} \]

keeping here in mind that \( r \to \infty \) implies \( r \gg 1 \).

When there are no vortices, hence \( \nu \gg 1 \), then \( f_\nu(r) = 1 \). The normalization condition (444) gives
\[ \varepsilon_0 = \rho_0 \Phi_0, \quad \rho_0 \equiv \frac{N_0}{\pi R^2 L_{\text{eff}}}. \]  

(447)

This yields the healing length
\[ \xi_0 \equiv \frac{1}{\sqrt{2m\varepsilon_0}} = \frac{1}{\sqrt{2mp_0 \Phi_0}} = \frac{1}{\sqrt{2m c}}. \]  

(448)

where \( c \) is the Bogolubov sound velocity
\[ c \equiv \sqrt{\frac{p_0}{m \Phi_0}}. \]

This healing length can be employed as an approximation for the healing length in the presence of a vortex.

The vortex with the winding number \( \nu = 1 \) is called basic. For this basic vortex there are the asymptotic expansions
\[ f_1(r) \propto r(1 + c_2 r^2 + c_4 r^4 + \cdots) \quad (r \to 0), \]
\[ f_1(r) \approx 1 - \frac{1}{2} r^2 - \frac{9}{8} r^4 - \frac{161}{16} r^6 \quad (1 \ll r \ll \frac{R}{\xi}). \]

(449)

Note that the Thomas–Fermi approximation is not applicable for solving equation (445), since neglecting the kinetic term would give
\[ f_{TF}(r) = \sqrt{1 - \frac{1}{r^2}} \quad (r \ll 1), \]
which is divergent at \( r \to 0 \).

Approximate analytic solution of equation (445), satisfying expansions (449) can be found by employing self-similar approximation theory that gives [97] the filament solution
\[ f_1(r) \approx \frac{r^2}{\sqrt{1 + r^2/4}}. \]

(450)

This is a rather good approximation, whose maximal residual for the related equation (445) is of order 0.1 at \( r \sim 1 \). It is possible to essentially improve the accuracy of solutions by using higher-order approximants of self-similar approximation theory. But here we limit ourselves by the simple expression (450). Recall that this simple expression is valid, if boundary effects are negligible.

The normalization condition (444) gives
\[ \frac{R^2}{4\xi^2} = \frac{mR^2}{2\varepsilon_0} + \ln\left(1 + \frac{R^2}{4\xi^2}\right) \quad \left(\xi^2 = \frac{1}{2m \varepsilon_0}\right). \]

Since \( \xi \ll R \), we can write
\[ \xi_1 = \varepsilon_0 + \frac{4}{mR^2} \ln\left(\frac{R}{2\xi}\right) \]  

(451)

The vortex energy per particle is defined as
\[ \varepsilon_{\text{vor}} \equiv \varepsilon_1 - \varepsilon_0. \]

(452)

This energy can be treated as small, compared to \( \varepsilon_0 \). Therefore it is possible to iterate \( \varepsilon_1 \) with \( \xi_{\text{vor}} \), given by expression (448), confirming that the ratio
\[ \frac{\varepsilon_{\text{vor}}}{\varepsilon_0} = \frac{8\varepsilon_0^2}{R^2} \ln\left(\frac{R}{2\xi_0}\right) \]

is small for \( \xi_0 \ll R \).

Thus for the vortex energy per particle, we have
\[ \varepsilon_{\text{vor}} = \frac{4}{m \rho_0 L_{\text{eff}}} \ln\left(\frac{R}{2\xi_0}\right). \]

(453)

The total vortex energy is
\[ N_0 \varepsilon_{\text{vor}} = \frac{4\pi}{m \rho_0 L_{\text{eff}}} \ln\left(\frac{R}{2\xi_0}\right). \]

The energy, required for producing a vortex, can be provided by rotation with the angular momentum \( \hat{L} \equiv -i [\mathbf{r} \times \nabla] \). In cylindrical coordinates, the \( z \)-th component of the angular momentum is \( \hat{L}_z = -i \partial / \partial \phi \). Rotation, with the angular velocity \( \Omega \) around the \( z \)-axis, is described by the operator of kinetic energy of rotation \( \hat{\Omega} \hat{L}_z \), which gives the kinetic energy \( r \hat{\Omega} \). The critical rotation frequency \( \Omega_0 \), necessary for creating a vortex with a winding number \( \nu \), is defined by the relation
\[ \nu \Omega_0 = \varepsilon_\nu - \varepsilon_0. \]

(454)

For the basic vortex this yields
\[ \Omega_1 = \frac{4}{m R^2} \ln\left(\frac{R}{2\xi_0}\right). \]

(455)

The energy of a vortex with a winding number \( \nu \) is proportional to \( \nu^2 \), while the orbital moment is proportional to \( \nu \). Therefore the energy of several basic vortices is lower than the energy of one large vortex with the same angular momentum.

5.14. Dark solitons

In the previous section, a disk-shape trap was considered, resulting in a quasi-two-dimensional radial equation. Now we shall consider an elongated pencil-shape trap leading to a quasi-one-dimensional equation.

An elongated trap is characterized by the inequality \( l_\perp \ll l_z \), hence \( \omega_\perp \ll \omega_z \). The scattering length is assumed to be such that \( |a| \ll l_z \), so that there are no geometric effects caused by the boundary. The solution to the evolution equation is presented in the variable-separated form
\[ \eta(r, t) = \sqrt{N_0} \chi(r_z) \psi(z, t) e^{-i E t}, \]
with the same normalizations for \( \chi(r_z) \) and \( \psi(z, t) \) as in the previous section. The transverse confinement is assumed to be strong, such that the oscillator term prevails over the interaction one. Hence the transverse equation is
\[ \left( -\frac{\nabla_{r_z}^2}{2m} + \frac{m \omega_\perp^2 r_z^2}{2} \right) \chi(r_z) = E \chi(r_z). \]

The solution for the transverse harmonic ground state is
\[ \chi(r_z) = \frac{1}{\sqrt{\pi \omega_{1}}} \exp\left(-\frac{r_z^2}{2 \omega_{1}^2}\right). \]

(447)
Let us define the effective area $A_{\text{eff}}$ by the equation
\[
\frac{1}{A_{\text{eff}}} \equiv 2\pi \int_0^R |\chi(r_\perp)|^2 r_\perp dr_\perp.
\]
In the uniform case, when $\chi(r_\perp) \to 1/\sqrt{\pi R^2}$, the effective area $A_{\text{eff}} \to \pi R^2$. While for the harmonic potential, the effective area becomes $A_{\text{eff}} = 2\pi R_\perp^2$.

Substituting $\eta(r_\perp, t)$ into the evolution equation, multiplying the latter by $\eta(r_\perp)$, and integrating over $r_\perp$ yields the effective axial equation
\[
\frac{1}{\partial_t} \psi(z, t) = \left[ -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{m}{2} \omega^2 z^2 + \frac{\Phi_0}{A_{\text{eff}}} |\psi(z, t)|^2 - \varepsilon \right] \psi(z, t).
\]

Here the expression
\[
\frac{\Phi_0}{A_{\text{eff}}} = \frac{2a_s}{mL^2}
\]
plays the role of an effective one-dimensional interaction strength. Again we assume that the interaction is repulsive, that is, $\Phi_0 > 0$.

If the trap is sufficiently long, such that $\xi \ll L \sim L$ and $\xi \ll L$, then, one can neglect the boundary effects, omitting the harmonic term and introducing the variable
\[
x \equiv \frac{z - vt}{\xi}, \quad \left( \xi = \frac{1}{\sqrt{2mc}} \right).
\]

It is convenient to pass to the dimensionless function
\[
f(x) \equiv \frac{\Phi_0 N_0}{\varepsilon A_{\text{eff}}} \psi(z, t),
\]
for which equation (456) reduces to
\[
\frac{d^2 f}{dx^2} + (1 - |f|^2)f = 2\gamma \frac{df}{dx} \left( \gamma \equiv \frac{mv^2}{2c} \right)
\]
(458)
The equation is invariant with respect to the sign inversion $f \to -f$. The boundary conditions can be written as
\[
\lim_{x \to -\infty} f(x) = -1, \quad \lim_{x \to +\infty} f(x) = 1.
\]
And the normalization condition reads as
\[
\frac{\varepsilon A_{\text{eff}}}{\Phi_0 N_0} \int_{-L/2}^{L/2} \left| f \left( \frac{z - vt}{\xi} \right) \right|^2 dz = 1,
\]
which defines $\varepsilon$.

The ground state has the form
\[
f_0(x) = \begin{cases} -1, & x < 0 \\ 1, & x > 0 \end{cases}
\]
defining the eigenvalue
\[
\varepsilon_0 = \rho_0 \Phi_0 = mc^2 \left( \rho_0 \equiv \frac{N_0}{A_{\text{eff}} L} \right),
\]
in which $c$ is the sound velocity, as in the previous section.

A nontrivial solution of equation (458), satisfying the boundary conditions (459), is the kink soliton
\[
f(x) = i\sqrt{2} \gamma + \sqrt{1 - 2\gamma^2} \tanh \left( \frac{x}{\sqrt{2}} \sqrt{1 - 2\gamma^2} \right).
\]
(462)
The corresponding density
\[
|f(x)|^2 = 2\gamma^2 + (1 - 2\gamma^2) \tanh^2 \left( \frac{x}{\sqrt{2}} \sqrt{1 - 2\gamma^2} \right)
\]
is minimal at $x = 0$, where
\[
\min_x |f(x)|^2 = 2\gamma^2,
\]
because of which this solution is named dark soliton.

The normalization condition (460) gives
\[
\varepsilon = \varepsilon_0 + \frac{2c}{L} \sqrt{1 - 2\gamma^2}.
\]
(463)

For large $L \gg \xi$, the second term is much smaller than $\varepsilon_0$.

The soliton energy per particle is
\[
\varepsilon_0 = \frac{\varepsilon - \varepsilon_0}{\varepsilon},
\]
which is small, as compared to $\varepsilon_0$ since
\[
\frac{\varepsilon_0}{\varepsilon_0} \propto \frac{\varepsilon}{\xi} \ll 1 \quad (\xi \ll L).
\]

Then the expression for the parameter $\gamma$ can be iterated with $\varepsilon_0$, resulting in
\[
\gamma \equiv \frac{mv^2}{2c} \varepsilon = \frac{v}{\sqrt{2c}}
\]
The healing length is
\[
\xi \approx \frac{1}{\sqrt{2mc_0}} = \frac{1}{\sqrt{2mc}}.
\]
In this way, for the soliton velocity, we find
\[
\varepsilon_0 = \frac{2c}{L} \sqrt{1 - \frac{v^2}{c^2}}.
\]
(465)
When $v$ increases, then $\varepsilon_0$ diminishes. The acceleration of the soliton velocity to $v \to c$ yields $\varepsilon_0 \to 0$.

5.15. Bright solitons

Let us consider the quasi-one-dimensional evolution equation (456) in the stationary case. And assume that in the longitudinal direction the trapping potential is essentially smaller than the interaction term. Then equation (456) reduces to the equation
\[
\left[ -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{\Phi_0}{A_{\text{eff}}} |\psi(z)|^2 - \varepsilon \right] \psi(z) = 0.
\]
(466)
Suppose that interactions are attractive, $\Phi_0 < 0$. Impose the boundary conditions
\[
\lim_{z \to \pm \infty} \psi(z) = 0.
\]
For $\Phi_0 < 0$, these conditions are satisfied only for negative energy, $\varepsilon = -|\varepsilon|$. Thus we come to the equation

$$\left( \frac{1}{2m} \frac{d^2}{dz^2} + \frac{\Phi_0}{A_{\text{eff}}} N_0 |\psi|^2 - |\varepsilon| \right) \psi = 0. \quad (467)$$

The dimensionless spatial variable is defined as

$$x \equiv \frac{z}{\xi} \quad \left( \xi \equiv \sqrt{\frac{\varepsilon}{m^2 |\varepsilon|}} \right). \quad (468)$$

And the dimensionless function is

$$f(x) \equiv \sqrt{\frac{\Phi_0}{\varepsilon} A_{\text{eff}} N_0} \psi(z).$$

Then equation (467) reduces to

$$\frac{d^2f}{dx^2} + (|f|^2 - 1)f = 0, \quad (469)$$

with the boundary condition

$$\lim_{x \to \pm \infty} f(x) = 0. \quad (470)$$

The equation is invariant with respect to the replacement $f \to -f$. Therefore it is possible to take $f$ as a positive or a negative solution. Below we define it as being positive. The normalization condition reads as

$$\int_{-L/2}^{L/2} \left( \frac{z}{\xi} \right)^2 dz = 1. \quad (471)$$

There is no uniform ground state satisfying the boundary conditions (470). The soliton solution is

$$f(x) = \frac{\sqrt{2}}{\cosh x}. \quad (472)$$

The normalization condition gives

$$\varepsilon = -\frac{m}{8}(\rho_0 \Phi_0 L)^2. \quad (473)$$

This defines the healing length

$$\xi = \frac{2}{\rho_0 m \Phi_0 L}. \quad (474)$$

The soliton is named bright, since it is of bell shape, with a maximum at $x = 0$.

The other situation, when a bright soliton arises, is the case of a gap soliton, when the effective mass is negative, $m = -|m|$, while the interactions are repulsive, $\Phi_0 > 0$. In that case, instead of equation (467), we get the equation

$$\left( \frac{1}{2|m|} \frac{d^2}{dz^2} + \frac{\Phi_0}{A_{\text{eff}}} N_0 |\psi|^2 - \varepsilon \right) \psi = 0. \quad (475)$$

The evolution equation for the condensate wave function is invariant under the Galilean transformation. Therefore it is straightforward to generalize the stationary solution to the nonstationary situation, obtaining a bright soliton moving with velocity $v$,

$$\psi(z, t) = \psi(z - vt) \exp \left\{ \left( \frac{mvz - \frac{mv^2}{2} t}{2} \right) \right\}. \quad (476)$$

In all soliton solutions, it is admissible to make the shift $z \to z - z_0$, with $z_0$ being the initial soliton location.

## 6. Conclusion

This tutorial is the continuation of the first part [1], where a general mathematical foundation of quantum statistics has been given for both Bose–Einstein and Fermi-Dirac statistics. In the present part, the properties of Bose systems are treated, with an emphasis on physics of systems with Bose–Einstein condensate. Specifics, related to trapped atoms, are emphasized.

Since this is a tutorial, the explanations are sufficiently detailed in order that the reader could follow the main steps of calculations. Of course, it is impossible to treat all so numerous topics related to Bose systems. Here only some of the topics are considered, which to the understanding of the author, are of principal interest for describing the basic properties of Bose-condensed systems. Many important problems are not touched here. For instance, those considering nonequilibrium Bose-condensed systems, including such a fascinated topic as quantum turbulence [98, 99]. The choice, to some extent, can be subjective. The selection of the material is done on the basis of lectures the author has given in the Free University of Berlin, Germany, and São Paulo State University, Brazil.

The methods described here for treating cold trapped atoms can be employed for considering other finite quantum systems [100].

For a tutorial, there has been no intention to give an extensive list of references, as it would be necessary for a review article. Only those papers are cited that are of historical interest or directly used.

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