Particle fluctuations in nonuniform and trapped Bose gases

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1. Trapped Bose atoms

Trapped gases of Bose atoms constitute an important class of nonuniform systems. Thermodynamics and dynamics of trapped atoms have been studied in many details. For review, see the book [1] and review articles [2–5]. One of the topics that have met a great deal of controversy is the problem of particle fluctuations in the systems with Bose-Einstein condensate. There have appeared a number of publications claiming the occurrence of thermodynamically anomalous condensate fluctuations everywhere below the condensation temperature, for both uniform as well as trapped systems. Thermodynamically anomalous fluctuations correspond to the particle dispersion proportional to $\frac{N^4}{3}$, instead of $N$ for the normal fluctuations. As has been explained in the review papers [3,5], the occurrence of these thermodynamically anomalous fluctuations implies thermodynamic instability. Hence, the systems with such anomalous fluctuations simply cannot exist. For the case of uniform systems, it has been shown [6–8] that the thermodynamically anomalous fluctuations are due to incorrect calculations, while the correct calculational procedure yields thermodynamically normal particle fluctuations.

In the present paper, this result is generalized to the case of arbitrary nonuniform systems, including the case of trapped atoms. It will be shown that for any Bose-condensed system, whether uniform or nonuniform, particle fluctuations are always thermodynamically normal. The notion of thermodynamically normal fluctuations is related to that of thermodynamic limit. For a uniform system of $N$ atoms in volume $V$, the thermodynamic limit is commonly defined as

$$N \to \infty, \quad V \to \infty, \quad \frac{N}{V} \to \text{const}. \tag{1}$$

For an arbitrary nonuniform system, the thermodynamic limit can be defined [9] as the limit

$$N \to \infty, \quad \langle \hat{A} \rangle \to \infty, \quad \frac{\langle \hat{A} \rangle}{N} \to \text{const}, \tag{2}$$

valid for the statistical average $\langle \hat{A} \rangle$ of any extensive observable $\hat{A}$.

Atoms are often trapped by means of a power-law confining potential

$$U(r) = \sum_{\alpha=1}^{d} \frac{\omega_\alpha}{2} \frac{r_\alpha}{l_\alpha}^{n_\alpha},$$

where $d$ is space dimensionality, $n_\alpha > 0$, and the potential parameters are related by the equations

$$\omega_\alpha = \frac{1}{m l_\alpha^2}, \quad l_\alpha = \frac{1}{\sqrt{m \omega_\alpha}}. \tag{4}$$
It is convenient to introduce the effective frequency and the effective localization length, respectively,
\[ \omega_0 \equiv \left( \prod_{\alpha=1}^{d} \omega_\alpha \right)^{1/d}, \quad l_0 \equiv \left( \prod_{\alpha=1}^{d} l_\alpha \right)^{1/d}, \]
which are connected by the relations
\[ \omega_0 = \frac{1}{ml_0^2}, \quad l_0 = \frac{1}{\sqrt{ml_0}}. \]

For this type of the confining potentials, the thermodynamic limit (2) reduces [9] to the limit
\[ N \to \infty, \quad \omega_0 \to 0, \quad N\omega_0^2 \to \text{const}, \]
or, equivalently, to
\[ N \to \infty, \quad l_0 \to \infty, \quad \frac{N}{l_0^2} \to \text{const}, \]
where the notation of the confining strength
\[ s \equiv \frac{d}{2} + \sum_{\alpha=1}^{d} \frac{1}{n_\alpha} \]
is introduced.

The passage to the uniform system corresponds to \( n_\alpha \to \infty \), when \( s \to d/2 \) and \( l_0 \to L/2 \), with \( L \) being the system length, such that \( L^d = V \).

The comparison of Eq. (1) and Eq. (7) tells us that, for a confined system, the effective volume can be defined [1,9] as \( V \equiv \text{const} \cdot l_0^d \). This definition seems to be not unique, since the proportionality constant here is not yet prescribed. However, we can remember that real trapped systems are always finite, being bounded by the trap volume \( V \). The power-law confining potential (3) is just a model for the real trapping potential. For sufficiently large traps, this is a good model, which does not contradict the fact that the real trap has a finite volume \( V \). Therefore, the relation \( V \equiv \text{const} \cdot l_0^d \) can be treated as defining the proportionality coefficient.

If \( H \) is the system grand Hamiltonian, then the grand thermodynamic potential is
\[ \Omega = -PV = -T \ln \text{Tr} \exp(-\beta H), \]
where \( T \) is temperature and \( \beta \equiv 1/T \). This defines the system pressure
\[ P = \frac{T}{V} \rho \ln \text{Tr} \exp(-\beta H), \]
in which \( \rho \equiv N/V \) is the average density of atoms. Thus, remembering that any trap has a finite volume \( V \) allows us to use, for trapped atoms, the same thermodynamic relations as for uniform systems.

Particle fluctuations are characterized by the dispersion
\[ \Delta^2(\hat{N}) \equiv \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \]
of the number-of-particle operator \( \hat{N} \). This dispersion is straightforwardly connected with the isothermal compressibility
\[ \kappa_T \equiv -\frac{1}{V} \left( \frac{\partial P}{\partial V} \right)^{-1} = \frac{\Delta^2(\hat{N})}{\rho TN}, \]
and the hydrodynamic sound velocity
\[ s_T \equiv \frac{1}{m} \left( \frac{\partial P}{\partial \rho} \right) = \frac{1}{m\rho c_T} = \frac{NT}{m\Delta^2(N)}, \]
where \( m \) is atomic mass, and with the central structure factor
\[ S(0) = T\rho c_T = \frac{T}{m\kappa_T} = \frac{\Delta^2(\hat{N})}{N}. \]

Equations (12), (13), and (14) are exact, being valid for any nonuniform system. In order that these measurable quantities would have sense, it is necessary and sufficient that the particle fluctuations be thermodynamically normal, such that
\[ \frac{\Delta^2(\hat{N})}{N} \to \text{const} \quad (N \to \infty). \]

If the particle fluctuations would be thermodynamically anomalous, being proportional to \( N^{4/3} \), as is claimed by some authors, the compressibility (12) would be divergent, sound velocity (13) would be zero, while the structure factor (14) would be infinite. Such a thermodynamically anomalous behavior would mean that the considered system is thermodynamically unstable.

2. Nonuniform Bose systems

An arbitrary nonuniform Bose system is characterized by the energy Hamiltonian
\[ \hat{H} = \int \hat{\psi}^\dagger(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} + \]
\[ + \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r'}) \phi(\mathbf{r} - \mathbf{r'}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r'}) \, d\mathbf{r} \, d\mathbf{r'}, \]
in which \( \hat{\psi} \) is the Bose field operator, \( U(\mathbf{r}) \) is an external potential, such as the trapping potential, and \( \phi(\mathbf{r}) \) is an integrable symmetric interaction potential. Here and in what follows, the units are used where \( \hbar = 1, \kappa_B = 1 \).

The appearance of the Bose-Einstein condensate is the necessary and sufficient condition for the global gauge symmetry breaking [10]. The latter is conveniently realized by means of the Bogolubov shift [11,12] for the field operator
\[ \hat{\psi}(\mathbf{r}) = \eta(\mathbf{r}) + \psi_1(\mathbf{r}). \]
Here \( \eta(\mathbf{r}) \) is the condensate wave function and \( \psi_1(\mathbf{r}) \) is the Bose field operator of uncondensed atoms. To exclude
the double counting, these variables are to be orthogonal to each other:

\[ \int \eta^*(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r} = 0. \]  

(18)

The condensate wave function is normalized to the number of condensed atoms

\[ N_0 = \int \rho_0(\mathbf{r}) \, d\mathbf{r}, \quad \rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2. \]  

(19)

And the number of uncondensed atoms is given by the average

\[ N_1 = \langle \hat{N}_1 \rangle, \quad \hat{N}_1 \equiv \int \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r}. \]  

(20)

The total number of atoms in the system is

\[ N = N_0 + N_1 = \langle \hat{N} \rangle , \quad \hat{N} = N_0 + \hat{N}_1. \]  

(21)

The condensate wave function plays the role of the order parameter characterizing the gauge symmetry breaking:

\[ \eta(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle, \quad \langle \psi_1(\mathbf{r}) \rangle = 0. \]  

(22)

This means that the Hamiltonian should not contain the terms linear in the field operators of uncondensed atoms [13]. The latter condition can be realized by complimenting the Hamiltonian with a counterterm

\[ \hat{A} = \int \left[ \lambda(\mathbf{r})\psi_1^*(\mathbf{r}) + \lambda^*(\mathbf{r})\psi_1(\mathbf{r}) \right] d\mathbf{r}, \]  

(23)

for which

\[ \langle \hat{A} \rangle = 0, \]  

(24)

and the Lagrange multipliers \( \lambda(\mathbf{r}) \) are chosen so that to kill the terms linear in \( \psi_1(\mathbf{r}) \).

Taking into account the statistical constraints (19), (20), and (24) defines the grand Hamiltonian

\[ H[\eta, \psi_1] = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 - \hat{A}, \]  

(25)

which is a functional of the field variables \( \eta \) and \( \psi_1 \). The quantities \( \mu_0 \) and \( \mu_1 \) are the Lagrange multipliers guaranteeing the validity of the normalization conditions (19) and (20). With the Bogolubov shift (17), Hamiltonian (25) is the sum

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

(26)

of the terms labelled according to the entering powers of the operators \( \psi_1 \). The zero-order term

\[ H^{(0)} = \int \eta^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}')|\eta(\mathbf{r})|^2|\eta(\mathbf{r}')|^2 \, d\mathbf{r} \, d\mathbf{r}' \]  

(27)

does not contain the field operators of uncondensed atoms. The first-order term \( H^{(1)} = 0 \), being eliminated by the linear killer (23). The second-order term is

\[ H^{(2)} = \int \psi_1^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) \, d\mathbf{r} + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ |\eta(\mathbf{r})|^2 \psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}') + \eta^*(\mathbf{r})\eta(\mathbf{r}')\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}) + \frac{1}{2} \eta^*(\mathbf{r})\eta(\mathbf{r})\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}) \right] \, d\mathbf{r} \, d\mathbf{r}'. \]  

(28)

Respectively, the third-order term is

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

and for the fourth-order term, one has

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

(30)

The evolution equations for the variables \( \eta \) and \( \psi_1 \) can be represented by the variational forms

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

(31)

and

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

(32)

Let us introduce the normal density matrix

\[ \rho_1(\mathbf{r}, \mathbf{r}') \equiv \left\langle \psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}) \right\rangle \]  

(33)

and the so-called anomalous density matrix

\[ \sigma_1(\mathbf{r}, \mathbf{r}') \equiv \left\langle \psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}) \right\rangle. \]  

(34)

Their diagonal elements define the density of uncondensed atoms and the anomalous average, respectively:

\[ \rho_1(\mathbf{r}) = \left\langle \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) \right\rangle, \quad \sigma_1(\mathbf{r}) = \left\langle \psi_1(\mathbf{r})\psi_1(\mathbf{r}) \right\rangle. \]  

(35)

The local density of atoms is the sum

\[ \rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}). \]  

(36)

We shall also need the triple correlator

\[ \xi(\mathbf{r}, \mathbf{r}') \equiv \left\langle \psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})\psi_1(\mathbf{r}) \right\rangle. \]  

(37)

With these notations, Eq. (31) results in the evolution equation for the condensate wave function

\[ i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}')|\eta(\mathbf{r})|^2 \eta(\mathbf{r}') \, d\mathbf{r}'. \]  

(38)
\[ + \int \phi(r - r') \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta(r') + + \sigma_1(r, r') \eta^*(r') + \xi(r, r') \right] \, dr', \]

while Eq. (32) yields the equation of motion for the operator of uncondensed atoms

\[ i \frac{\partial}{\partial t} \psi_1(r) = - \left( - \frac{\nabla^2}{2m} + U - \mu \right) \psi_1(r) + + \int \phi(r - r') \left[ \eta(r') \right]^2 \psi_1(r) + + \eta^*(r') \psi_1(r') + \eta(r') \eta(r) \psi_1^1(r') + + \hat{X}(r, r') \, dr', \]

in which

\[ \hat{X}(r, r') \equiv \psi_1^1(r') \psi_1(r') \eta(r) + \psi_1^1(r') \eta(r') \psi_1(r) + + \eta^*(r') \psi_1(r') + \psi_1^1(r') \psi_1(r') \psi_1(r). \]

For an equilibrium system, one has

\[ \frac{\partial}{\partial t} \eta(r) = 0 \quad \text{(equilibrium)}. \]

Then Eq. (38) reduces to the eigenvalue problem

\[ \mu_0 \eta(r) = \left( - \frac{\nabla^2}{2m} + U \right) \eta(r) + + \int \phi(r - r') \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta(r') + + \sigma_1(r, r') \eta^*(r') + \xi(r, r') \right] \, dr', \]

defining the condensate wave function and the Lagrange multiplier \( \mu_0 \).

Note that the Lagrange multipliers \( \mu_0 \) and \( \mu_1 \) do not need to coincide with each other. Their relation to the system chemical potential \( \mu \) is given \([13-15]\) by the equality

\[ \mu = \mu_0 n_0 + \mu_1 n_1, \]

in which the atomic fractions of condensed and uncondensed atoms, respectively, are

\[ n_0 \equiv \frac{N_0}{N}, \quad n_1 \equiv \frac{N_1}{N}. \]

The formalism of this section provides the basis for the self-consistent theory of arbitrary nonuniform Bose-condensed systems \([8,13-15]\).

\[ 3. \text{Hartree-Fock-Bogolubov approximation} \]

To proceed further, let us resort to the Hartree-Fock-Bogolubov (HFB) approximation, following the way of \([13-15]\). Then Hamiltonian (26) in the HFB approximation becomes

\[ H_{HFB} = E_{HFB} + + \int \psi_1^1(r) \left( - \frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(r) \, dr + + \int \phi(r - r') \times \left[ \rho(r') \psi_1^1(r) \psi_1(r) + \rho(r', r) \psi_1^1(r') \psi_1(r) + + \frac{1}{2} \sigma(r, r') \psi_1^1(r') \psi_1(r) \psi_1(r) \right] \, dr \, dr', \]

where

\[ E_{HFB} = H^{(0)} - \frac{1}{2} \int \phi(r - r') \times \left[ \rho_1(r, r') \right]^2 + \left| \sigma_1(r, r') \right|^2 \, dr \, dr', \]

and the notation is introduced for the total normal density matrix

\[ \rho(r, r') \equiv \eta(r) \eta^*(r') + \rho_1(r, r'), \]

and for the total anomalous density matrix

\[ \sigma(r, r') \equiv \eta(r) \eta^*(r') + \sigma_1(r, r'). \]

In the HFB approximation, the condensate-function equation (38) takes the form

\[ i \frac{\partial}{\partial t} \psi_1(r) = \left( - \frac{\nabla^2}{2m} + U - \mu_0 \right) \psi_1(r) + + \int \phi(r - r') \times \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta^*(r') + + \sigma_1(r, r') \eta^*(r') \right] \, dr'. \]

And Eq. (39) for the field operator of uncondensed atoms reduces to

\[ i \frac{\partial}{\partial t} \psi_1(r) = \left( - \frac{\nabla^2}{2m} + U - \mu \right) \psi_1(r) + + \int \phi(r - r') \times \left[ \rho(r') \psi_1(r) + \rho(r, r') \psi_1(r') + + \sigma(r, r') \psi_1^1(r') \right] \, dr'. \]

For an equilibrium system, the eigenvalue problem (40) becomes

\[ \mu_0 \eta(r) = \left( - \frac{\nabla^2}{2m} + U \right) \eta(r) + + \int \phi(r - r') \times \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta(r') + + \sigma_1(r, r') \eta^*(r') \right] \, dr'. \]

The HFB Hamiltonian (41) can be diagonalized by means of the general Bogolubov canonical transformations \([16]\) that, in the used notation, read as

\[ \psi_1(r) = \sum_k \left[ b_k u_k(r) + b_k^* v_k(r) \right], \]

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\[ \psi_1(r) = \sum_k \left[ b_k u_k(r) + b_k^* v_k(r) \right], \]
With the diagonal Hamiltonian (54), it is straightforward to calculate the required averages. Thus, for the distribution of excitations, one gets

\[ \pi_k \equiv \langle b_k^\dagger b_k \rangle = \left[ \exp(\beta \varepsilon_k) - 1 \right]^{-1}. \]

The normal density matrix (33) is

\[ \rho_1(r, r') = \sum_k \left[ \pi_k u_k^*(r) u_k^*(r') + (1 + \pi_k) v_k^*(r) u_k(r') \right]. \]

And the anomalous density matrix (34) becomes

\[ \sigma_1(r, r') = \sum_k \left[ \pi_k u_k^*(r) u_k^*(r') + (1 + \pi_k) v_k^*(r) u_k(r') \right]. \]

For the diagonal elements of Eq. (57) and Eq. (58), we obtain

\[ \rho_1(r) = \sum_k \left[ \pi_k |u_k(r)|^2 + (1 + \pi_k) |v_k(r)|^2 \right] \]

and, respectively,

\[ \sigma_1(r) = \sum_k \left( 1 + 2\pi_k \right) u_k(r) v_k^*(r). \]

### 4. Local-density approximation

When the spatial variation of the external nonuniform potential is sufficiently slow and the trap is sufficiently large, one can employ the local-density approximation [1,2,17], which is also called the semi-classical approximation and is widely used for describing trapped atoms [9,18,19].

In this approximation, one looks for the Bogolubov functions represented as the products

\[ u_k(r) \equiv v(k, r) \varphi_k^0(r), \quad v_k(r) \equiv v(k, r) \varphi_k^0(r) \]

factorized with the plane waves

\[ \varphi_k^0(r) \equiv \frac{1}{\sqrt{V}} \exp(i k \cdot r). \]

The amplitudes \( v(k, r) \) and \( v(k, r) \) are assumed to be slowly varying in space, as compared to the spatial variation of the plane wave,

\[ \frac{\nabla v(k, r)}{|v(k, r)|} \ll \frac{\nabla \varphi_k^0(r)}{|\varphi_k^0(r)|}. \]

In the Bogolubov equations (51), one makes the replacements

\[ \int \omega(r, r') u_k^*(r') \, dr' \cong \omega(k, r) u_k^0(r), \]

\[ \int \omega(r, r') v_k^*(r') \, dr' \cong \omega(k, r) v_k^0(r), \]

and

\[ \Delta(r, r') \cong \Delta(k, r) u_k^0(r), \]

\[ \Delta(r, r') \cong \Delta(k, r) v_k^0(r), \]

where the form

\[ \omega(k, r) \equiv \frac{k^2}{2m} + U(r) + 2\Phi_0 \rho(r) - \mu_1(r). \]
is used, instead of Eq. (52), and the quantity
\[ \Delta(r) \equiv [\rho_0(r) + \sigma_1(r)] \Phi_0 \] is used instead of Eq. (53), with the notation
\[ \Phi_0 \equiv \int \Phi(r) \, dr . \] In what follows, we assume that \( \Phi_0 > 0 \). Then the Bogolubov equations (51) reduce to the eigenproblem
\[ \left[ \omega(k, r) - \epsilon(k, r) \right] u(k, r) + \Delta(r) v(k, r) = 0 , \] \[ \Delta^*(r) u(k, r) + \left[ \omega^*(k, r) + \epsilon(k, r) \right] v(k, r) = 0 . \] (69)
The amplitudes \( u(k, r) \) and \( v(k, r) \) can be taken to be real and, in view of Eqs. (49), satisfying the relation
\[ u^2(k, r) - v^2(k, r) = 1 . \] Solving eigenproblem (69) yields the Bogolubov spectrum of collective excitations
\[ \epsilon(k, r) = \sqrt{\omega^2(k, r) - \Delta^2(k, r)} . \] And for the amplitudes, we find
\[ u^2(k, r) = \frac{\omega(k, r) + \epsilon(k, r)}{2 \epsilon(k, r)} , \] \[ v^2(k, r) = \frac{\omega(k, r) - \epsilon(k, r)}{2 \epsilon(k, r)} , \] \[ u(k, r)v(k, r) = -\frac{\Delta(r)}{2 \epsilon(k, r)} . \] The necessary condition for the condensate existence [5], equivalent to the Hugenholtz-Pines theorem [20], requires that
\[ \lim_{k \to 0} \epsilon(k, r) = 0 , \quad \epsilon(k, r) \geq 0 . \] (72)
This gives the Lagrange multiplier
\[ \mu_1(r) = U(r) + \left[ \rho_0(r) + 2 \rho_1(r) - \sigma_1(r) \right] \Phi_0 . \] (73)
Introducing the local sound velocity \( c(r) \) by the equation
\[ mc^2(r) \equiv [\rho_0(r) + \sigma_1(r)] \Phi_0 \] transforms Eq. (66) to
\[ \omega(k, r) = \frac{k^2}{2m} + mc^2(r) , \] while Eq. (67) becomes
\[ \Delta(r) = mc^2(r) . \] (76)
For the Bogolubov spectrum (70), we obtain the familiar expression
\[ \epsilon(k, r) = \sqrt{c^2(r) k^2 + \left( \frac{k^2}{2m} \right)^2} , \] (77)
built with the local sound velocity.
Instead of distribution (56) for excitations, we have
\[ \pi(k, r) = \{ \exp[\beta \epsilon(k, r)] - 1 \}^{-1} , \] (78)
with the symmetry properties
\[ \pi(-k, r) = \pi(k, r) , \quad \epsilon(-k, r) = \epsilon(k, r) . \] (79)
Using Eqs. (71), we find the normal density matrix (57) as
\[ \rho_1(r, r') = \sum_k n(k, r) \varphi_k(r) \varphi_k^*(r') , \] (80)
with the distribution of atoms
\[ n(k, r) = \frac{\omega(k, r)}{2 \epsilon(k, r)} \coth \left[ \frac{\epsilon(k, r)}{2T} \right] - \frac{1}{2} . \] (81)
For the anomalous density matrix (58), we get
\[ \sigma_1(r, r') = \sum_k \sigma(k, r) \varphi_k(r) \varphi_k^*(r') , \] (82)
where
\[ \sigma(k, r) = mc^2(r) \coth \left[ \frac{\epsilon(k, r)}{2T} \right] . \] (83)
The diagonal elements of Eq. (80) and Eq. (82) give the density of uncondensed atoms and the anomalous average, respectively:
\[ \rho_1(r) = \frac{1}{V} \sum_k n(k, r) , \quad \sigma_1(r) = \frac{1}{V} \sum_k \sigma(k, r) . \] (84)
The grand thermodynamic potential (9) becomes
\[ \Omega = E_B + T \int \ln \left[ 1 - \exp \left\{ - \beta \epsilon(k, r) \right\} \right] \frac{dk}{(2\pi)^3} \] (85)
Employing the above formulas, one can calculate all thermodynamic characteristics.

5. Particle fluctuations and stability

Particle fluctuations are defined by the number-of-particle operator dispersion (11). The latter is proportional to the isothermal compressibility (12) which is to be thermodynamically normal for the stability of the system.

In the grand canonical ensemble, used here, the compressibility is
\[ \kappa_T = \frac{\Delta^2(\hat{N})}{\rho TN} , \quad \rho \equiv \frac{1}{V} \int \rho(r) \, dr . \] (86)
In the canonical ensemble, the number of particles is fixed. However, it would be incorrect to conclude that the compressibility then is zero. Expression (86) is not defined for the canonical ensemble. Instead, one should use the formula
\[ \kappa_T = \frac{1}{V} \left( \frac{\partial^2 F}{\partial N^2} \right)^{-1}_{TN} , \] where
\[ F = \frac{1}{V} \int \rho(r) \ln \rho(r) \, dr . \]
where $F$ is the canonical free energy.

In the same way, it would be principally wrong to state that, fixing the number of atoms $N$ and setting the particle dispersion (11) to zero, would result in the equality $\Delta^2(\hat{N}_0) = \Delta^2(\hat{N}_1)$ that would define the condensate fluctuations $\Delta^2(\hat{N}_0)$ in the canonical ensemble by calculating the dispersion $\Delta^2(\hat{N}_1)$ of uncondensed atoms. This way of reasoning is wrong because the particle dispersion (11) is not defined for the canonical ensemble. In addition, calculating $\Delta^2(\hat{N}_1)$ in the Fock space has nothing to do with the canonical ensemble, as far as in the Fock space, the number of particles is not fixed.

In the Fock space, the correct conclusion [10] for the particle fluctuations, after using the Bogolubov shift (17), is that the condensate fluctuations are zero,

$$\Delta^2(\hat{N}_0) = 0,$$

and that the particle fluctuations are completely due to those of uncondensed atoms,

$$\Delta^2(\hat{N}) = \Delta^2(\hat{N}_1).$$

Expressions (87) and (88), for large particle numbers $N$ are asymptotically exact [10].

It is also important that the fluctuations of the total number of particles are thermodynamically normal if and only if the fluctuations of both the condensate fraction as well as of uncondensed atoms are thermodynamically normal. And, vice versa, the fluctuations of the total number of particles are thermodynamically anomalous if and only if at least one of the fractions produces thermodynamically anomalous fluctuations. The corresponding theorem has been rigorously proved in [6–8].

When the HFB approximation is involved, Eq. (88) is not convenient to use, since the HFB approximation is an effective second-order approximation with regard to the powers of the field operators of uncondensed atoms $\psi_1$. In that second-order approximation, the quantity $N^2$ is not defined, being of the fourth order with respect to $\psi_1$. But we can employ another way of calculating the particle dispersion (11). We may notice that the latter can be expressed through the density-density correlation function

$$D(\mathbf{r}, \mathbf{r}’) \equiv \left\langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}’)\hat{\psi}(\mathbf{r}’)\right\rangle$$

as

$$\Delta^2(\hat{N}) = \int [D(\mathbf{r}, \mathbf{r}’) - \rho(\mathbf{r})\rho(\mathbf{r}’)] \, d\mathbf{r} \, d\mathbf{r}’.$$  (90)

The density-density correlation function (89) is related to the diagonal correlation function

$$C(\mathbf{r}, \mathbf{r}’) \equiv \left\langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}’)\hat{\psi}(\mathbf{r}’)\right\rangle$$

by the equality

$$D(\mathbf{r}, \mathbf{r}’) = \rho(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}’) + C(\mathbf{r}, \mathbf{r}’).$$

In turn, the diagonal correlation function (91) is connected with the pair correlation function

$$g(\mathbf{r}, \mathbf{r}’) \equiv \frac{\left\langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}’)\hat{\psi}^\dagger(\mathbf{r}’)\right\rangle}{\rho(\mathbf{r})\rho(\mathbf{r}’)}$$

through the relation

$$C(\mathbf{r}, \mathbf{r}’) = \rho(\mathbf{r})\rho(\mathbf{r}’)g(\mathbf{r}, \mathbf{r}’).$$  (94)

Therefore the particle dispersion (90) can be represented as

$$\Delta^2(\hat{N}) = N + \int \rho(\mathbf{r})\rho(\mathbf{r}’) \left\{ g(\mathbf{r}, \mathbf{r}’) - 1 \right\} \, d\mathbf{r} \, d\mathbf{r}’ =$$

$$= N + \int \left\{ C(\mathbf{r}, \mathbf{r}’) - \rho(\mathbf{r})\rho(\mathbf{r}’) \right\} \, d\mathbf{r}’.$$  (95)

This formula is valid for arbitrary nonuniform systems.

Accomplishing the Bogolubov shift (17) in Eq. (91) yields

$$C(\mathbf{r}, \mathbf{r}’) = \rho(\mathbf{r})\rho(\mathbf{r}’) + \rho(\mathbf{r})\rho(\mathbf{r}’)+$$

$$+ 2\Re \left\{ \eta^*(\mathbf{r})\eta^*(\mathbf{r})\rho_1(\mathbf{r}, \mathbf{r}’)+ \eta^*(\mathbf{r})\eta^*(\mathbf{r})\sigma_1(\mathbf{r}, \mathbf{r}’)+$$

$$+ \eta^*(\mathbf{r})\xi(\mathbf{r}, \mathbf{r}’)+ \eta^*(\mathbf{r})\xi(\mathbf{r}, \mathbf{r}’)+ C_1(\mathbf{r}, \mathbf{r}’),$$

where

$$C_1(\mathbf{r}, \mathbf{r}’) \equiv \left\langle \psi_1^\dagger(\mathbf{r})\psi_1^\dagger(\mathbf{r}’)\psi_1(\mathbf{r})\psi_1(\mathbf{r}’)\right\rangle.$$  (97)

In the HFB approximation, the triple correlator (37) is zero, while the correlation function (97) becomes

$$C_1(\mathbf{r}, \mathbf{r}’) = \rho_1(\mathbf{r})\rho_1(\mathbf{r}’) + |\rho_1(\mathbf{r}, \mathbf{r}’)|^2 + |\sigma_1(\mathbf{r}, \mathbf{r}’)|^2.$$  (98)

Then the correlation function (96) reduces to

$$C(\mathbf{r}, \mathbf{r}’) = \rho(\mathbf{r})\rho(\mathbf{r}’) + 2\Re \left\{ \eta^*(\mathbf{r})\eta^*(\mathbf{r})\rho_1(\mathbf{r}, \mathbf{r}’)+$$

$$+ \eta^*(\mathbf{r})\xi(\mathbf{r}, \mathbf{r}’)+ \sigma_1(\mathbf{r}, \mathbf{r}’)+ \rho_1(\mathbf{r}, \mathbf{r}’)+$$

$$+ |\sigma_1(\mathbf{r}, \mathbf{r}’)|^2.$$  (99)

As is stressed above, the HFB approximation is of second order with respect to the operators of uncondensed atoms. The terms, containing higher orders are not defined in this approximation and have to be omitted. This concerns the last two terms in Eq. (99). At the same time, in the frame of this approximation for an equilibrium system, the function $\eta(\mathbf{r})$ in the second and third terms of Eq. (99) can be replaced by the real value $\sqrt{\rho(\mathbf{r})}$. As a result, for the particle dispersion (95), we obtain

$$\Delta^2(\hat{N}) =$$

$$= N + 2\int \sqrt{\rho(\mathbf{r})\rho(\mathbf{r}’)} \left\{ \rho_1(\mathbf{r}, \mathbf{r}’) + \sigma_1(\mathbf{r}, \mathbf{r}’) \right\} \, d\mathbf{r} \, d\mathbf{r}’.$$  (100)

In the spirit of the local-density approximation, the latter expression can be rewritten as

$$\Delta^2(\hat{N}) =$$

$$= N + 2\int \rho(\mathbf{r}) \left\{ \rho_1(\mathbf{r}, \mathbf{r}’) + \sigma_1(\mathbf{r}, \mathbf{r}’) \right\} \, d\mathbf{r} \, d\mathbf{r}’.$$  (101)

Invoking Eq. (80) and Eq. (82) gives

$$\int \rho_1(\mathbf{r}, \mathbf{r}’) \, d\mathbf{r}’ = \lim_{k \to 0} n(\mathbf{k}, \mathbf{r}),$$  (102)
\[
\int \sigma(r, r') \, dr' = \lim_{k \to 0} \sigma(k, r) .
\]

Hence dispersion (101) reads as

\[
\Delta^2(\hat{N}) = N + 2 \int \rho(r) \lim_{k \to 0} \left[ n(k, r) + \sigma(k, r) \right] \, dr . \tag{103}
\]

Using Eq. (81) and Eq. (83), we get

\[
\lim_{k \to 0} \left[ n(k, r) + \sigma(k, r) \right] = \frac{1}{2} \left[ T \frac{mc^2(r)}{m^2c^2(r)} - 1 \right] .
\]

It is worth emphasizing that both Eq. (81), as well as Eq. (83), diverge in the long-wave limit \( k \to 0 \). But their divergences, being of opposite signs, cancel each other. This means that taking into account the anomalous average (83) is of principal importance. Without it, the dispersion (103) would diverge, and the compressibility (86) would be infinite, which implies the system instability.

In that way, the particle fluctuations are described by the dispersion

\[
\Delta^2(\hat{N}) = \int \frac{T \rho(r)}{mc^2(r)} \, dr . \tag{104}
\]

Therefore, the compressibility (86) is

\[
\kappa_T = \frac{1}{m \rho N} \int \frac{\rho(r)}{c^2(r)} \, dr . \tag{105}
\]

These formulas show that particle fluctuations are thermodynamically normal and compressibility (105) is finite, even in the thermodynamic limit. At the critical temperature \( T_c \), where \( c(r) \) tends to zero, the compressibility diverges as \( T \to T_c \). This divergence is typical for the point of a second-order phase transition, where the system is unstable. However everywhere below \( T_c \), the compressibility is finite and fluctuations are thermodynamically normal. This conclusion does not depend on the statistical ensemble involved. Both canonical and grand canonical ensembles for Bose systems produce the results coinciding in the thermodynamic limit [21], provided all calculations are done correctly, by using the representative statistical ensembles [8,13–15,22].

The compressibility (105) is a directly observable quantity, being related to the structure factor (14). The latter can be measured by studying light scattering from ultracold atomic gases [23,24]. No one scattering experiment with Bose-condensed systems has ever showed a thermodynamically anomalous structural factor.

Thermodynamically anomalous fluctuations for a stable statistical system can arise solely because of incorrect calculations. For example, if in the HFB or Bogolubov approximation, one includes in calculations the fourth- or higher-order terms, which are not defined in the second-order approximation, then one can get any kind of thermodynamic anomalies. However, such anomalies are physically meaningless, being mathematically wrong. For correctly calculating the fourth-order terms, one has to use a fourth-order Hamiltonian.

Nonperturbative thermodynamics of an interacting Bose gas, for all temperatures below \( T_c \), has recently been studied by Floerchinger and Wetterich [25] by using renormalization-group techniques, which effectively take into account all orders of field operators. Their results confirm that the compressibility is finite everywhere below \( T_c \), hence, all particle fluctuations are thermodynamically normal.

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