Bose-condensed atomic systems with nonlocal interaction potentials

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Received 18 January 2016
Accepted for publication 25 February 2016
Published 8 March 2016

Abstract
The general approach for describing systems with a Bose–Einstein condensate, where atoms interact through nonlocal pair potentials, is presented. Special attention is paid to nonintegrable potentials, such as the dipolar interaction potential. The potentials that are not absolutely integrable can have not well-defined Fourier transforms. Using formally these not defined Fourier transforms leads to unphysical conclusions. To make the Fourier transform well defined, the interaction potential has to be regularised. This is illustrated by the example of dipolar interactions.

Keywords: Bose–Einstein condensate, nonlocal interaction potentials, dipolar interactions, regularisation, screening, spectrum anisotropy

(Some figures may appear in colour only in the online journal)

1. Introduction

Atomic systems exhibiting Bose–Einstein condensation are widely studied both theoretically and experimentally, as can be inferred from the books [1–3] and review articles [4–13]. Trapped dilute atomic gases are often characterised by local interaction potentials of the delta-function type. But recently, trapped atoms interacting through dipolar forces have been condensed (see reviews [14–16]). Dipolar interactions are nonlocal and long range, and their theoretical description is more complicated than that of locally interacting atoms, because of which one usually considers only the Bogolubov approximation, which is valid at temperatures close to zero and asymptotically weak interactions.

Moreover, the dipolar interaction potential does not possess a well-defined Fourier transform. Formally taking this transform and using it leads to unphysical consequences.

The aim of the present paper is to suggest a self-consistent approach for atomic systems with nonlocal interaction potentials, valid for finite temperatures and for interactions of any strength. Special attention is paid to nonintegrable potentials, whose Fourier transforms are not well defined. As a typical example of this kind, dipolar interactions are treated. We show that such interactions need to be regularised in order to get a correct description of atomic systems. This regularisation is necessary for atoms of any statistics, whether Bose or Fermi. For the sake of concreteness, we consider here the atomic systems of Bose–Einstein statistics.

Throughout the paper, we use the notation where the Planck and Boltzmann constants are set to unity, $\hbar = 1$, $k_B = 1$.

2. Self-consistent approach

A self-consistent approach for describing Bose-condensed systems was developed in [17–19]. This approach resolves the Hohenberg–Martin dilemma [20] of conserving versus gapless theories and provides a theory that is conserving as well as gapless.

The general form of the energy Hamiltonian is

$$\hat{H} = \int \psi^\dagger(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U \right) \psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}',$$

(1)
where the field operators satisfy the Bose commutation relations, \( U = U(\mathbf{r}) \) is an external potential, if any, and \( \Phi(\mathbf{r}) \) is a nonlocal interaction potential. The field operators depend on time \( t \), which, for simplicity, is not explicitly shown.

For the occurrence of Bose–Einstein condensation, the necessary and sufficient condition is the global gauge symmetry breaking [1, 12, 13, 21]. A convenient way of breaking the gauge symmetry is by employing the Bogolubov shift [22, 23] representing the field operators as

\[
\hat{\psi}(\mathbf{r}) = \eta(\mathbf{r}) + \psi_1(\mathbf{r}),
\]

where \( \eta(\mathbf{r}) \) is the condensate function and \( \psi_1(\mathbf{r}) \) is the operator of uncondensed atoms.

Note that the Bogolubov shift is an exact canonical transformation, but not an approximation, as one sometimes writes.

To avoid double counting, the condensate function and the field operator of uncondensed atoms are assumed to be orthogonal,

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

The condensate function plays the role of the functional order parameter, such that

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

The latter implies that

\[
\langle \psi_1(\mathbf{r}) \rangle = 0.
\]

The condensate function is normalised to the number of condensed atoms

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

While the number of uncondensed atoms is the statistical average

\[
N_1 = \langle \hat{N}_1 \rangle
\]

of the operator

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

The evolution equation for the condensate function can be written as

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

The equation of motion for the operator of uncondensed atoms reads

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

The grand Hamiltonian generating these equations is

\[
\hat{H} = \hat{\Lambda} - \mu_0 N_0 - \mu_1 \hat{N}_1 - \hat{\Lambda},
\]

where the first term is the energy operator (1), the Lagrange multipliers \( \mu_0 \) and \( \mu_1 \) guarantees the validity of the normalisation conditions (6) and (7), while the last term, having the form

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

preserves the validity of condition (5). It has been proven [13, 24] that the variational equation (9) is equivalent to the Heisenberg equation of motion.

In systems with broken gauge symmetry, in addition to the single-particle density matrix

\[
\rho_\eta(\mathbf{r}, \mathbf{r}') = \langle \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') \rangle,
\]

there exists the anomalous matrix

\[
\sigma_\eta(\mathbf{r}, \mathbf{r}') = \langle \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') \rangle.
\]

The condensate function defines the density of condensed atoms

\[
\rho_\eta(\mathbf{r}) = |\eta(\mathbf{r})|^2.
\]

The diagonal elements of the single-particle density matrix give the density of uncondensed atoms

\[
\rho_0(\mathbf{r}) = \rho_\eta(\mathbf{r}, \mathbf{r}) = |\psi_1(\mathbf{r})|^2.
\]

The diagonal elements of the anomalous matrix define the density

\[
|\sigma_\eta(\mathbf{r})| = |\langle \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \rangle| = |\langle \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \rangle|.
\]

of pair-correlated atoms. The total atomic density is the sum

\[
\rho(\mathbf{r}) = \rho_\eta(\mathbf{r}) + \rho_0(\mathbf{r})
\]

yielding the total number of atoms

\[
N = \int \rho(\mathbf{r}) \, d\mathbf{r} = N_0 + N_1.
\]

The partial atomic ratios give the fractions of condensed, \( n_0 \), and uncondensed, \( n_1 \) atoms, respectively,

\[
n_0 = \frac{N_0}{N}, \quad n_1 = \frac{N_1}{N}, \quad (n_0 + n_1 = 1).
\]

For an equilibrium system, the statistical operator has the form

\[
\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} \quad (Z = Tr e^{-\beta \hat{H}}),
\]

with \( \beta = 1/kT \) being the inverse temperature, and with the same grand Hamiltonian (10).

The superfluid fraction is given by the expression

\[
n_s = 1 - \frac{\text{var}(\hat{P})}{mTNd},
\]

where \( d \) is the real-space dimensionality, the operator of momentum is

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

and the variance of an arbitrary operator \( \hat{A} \) is defined as

\[
\text{var}(\hat{A}) = \frac{1}{2} \langle \hat{A}^2 \hat{A} + \hat{A}\hat{A}^2 \rangle - \langle \hat{A} \rangle^2.
\]

For a self-adjoint operator, this yields

\[
\text{var}(\hat{A}) = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2.
\]
In equilibrium, the average momentum is zero,
\[ \langle \hat{P} \rangle = 0, \]
which, for dimensionality \( d = 3 \), leads to
\[ n_z = 1 - \frac{\langle \hat{P}_z \rangle}{3mTN}. \]

### 3. Uniform systems

When there is no external potential, \( U = 0 \), or when the trap is sufficiently large, the system can be treated as uniform. Then it is possible to Fourier transform the field operators,
\[ \psi_\mathbf{r}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{k=0} a_k e^{i \mathbf{k} \cdot \mathbf{r}}, \quad a_k = \frac{1}{\sqrt{V}} \int \psi_\mathbf{r}(\mathbf{r}) e^{-i \mathbf{k} \cdot \mathbf{r}} d\mathbf{r}. \]

Usually, one assumes that the interaction potential also enjoys the Fourier transformation
\[ \Phi_\mathbf{r}(\mathbf{r}) = \frac{1}{V} \sum_k \Phi_k e^{i \mathbf{k} \cdot \mathbf{r}}, \quad \Phi_k = \int \Phi_\mathbf{r}(\mathbf{r}) e^{-i \mathbf{k} \cdot \mathbf{r}} d\mathbf{r}. \]

If the Fourier transform is well defined, there exists the limit
\[ \Phi_0 = \lim \Phi_k = \int \Phi_\mathbf{r}(\mathbf{r}) d\mathbf{r}. \]

Note that if the trapping potential \( U \) is not zero, but sufficiently smooth, it is possible to resort to the local-density approximation, for which the similar Fourier transforms are also assumed.

The single-particle density matrix becomes
\[ \rho_\mathbf{r}(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{k=0} n_k e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} , \]
with the momentum distribution
\[ n_k = \langle a_k^\dagger a_k \rangle. \]

The anomalous average is
\[ \sigma_\mathbf{r}(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{k=0} \sigma_k e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} , \]
with
\[ \sigma_k = \langle a_k a_{-k} \rangle. \]

The condensate function and atomic densities do not depend on the spatial variable. The total average density reads
\[ \rho = \rho_0 + \rho_1 , \]
with the condensate density
\[ \rho_0 = |\eta|^2 \]
and the density of uncondensed atoms
\[ \rho_1 = \frac{1}{V} \sum_{k=0} n_k . \]

The diagonal anomalous average becomes
\[ \sigma_i = \frac{1}{V} \sum_{k=0} \sigma_k . \]

In the Hartree–Fock–Bogolubov approximation, we obtain [12, 13] the momentum distribution
\[ n_k = \frac{\omega_k}{2\varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right) - \frac{1}{2} , \]
and the anomalous average (27) reads
\[ \sigma_k = - \frac{\Delta_k}{2\varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right) . \]

Here we use the notations
\[ \omega_k = \frac{k^2}{2m} + \rho_0 \Phi_k + \frac{1}{V} \sum_{p=0} n_p \Phi_{k+p} - \mu_1 \]
and
\[ \Delta_k = \rho_0 \Phi_k + \frac{1}{V} \sum_{p=0} \sigma_p \Phi_{k+p} \]
defining the spectrum of collective excitations
\[ \varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2} . \]

In equilibrium,
\[ i \frac{\partial \eta}{\partial t} = \left\langle \frac{\delta H}{\delta \eta^*} \right\rangle = 0 , \]
which is equivalent to the variational condition
\[ \left\langle \frac{\delta H}{\delta \rho_0} \right\rangle = 0 . \]

From the latter, we get the condensate chemical potential
\[ \mu_0 = \rho_0 \Phi_0 + \frac{1}{V} \sum_{k=0} (n_k + \sigma_k) \Phi_k . \]

The condition of the condensate existence [12, 13]
\[ \lim_{k=0} \frac{1}{n_k} = 0 \]
requires a gapless spectrum, such that
\[ \lim_{k=0} \varepsilon_k = 0 , \]
in agreement with the Bogolubov [22, 23] and Hugenholtz–Pines [25] theorems. Condition (41) yields the chemical potential of uncondensed atoms
\[ \mu_1 = \rho_0 \Phi_0 + \frac{1}{V} \sum_{k=0} (n_k - \sigma_k) \Phi_k . \]

Then expression (34) takes the form
\[ \omega_k = \frac{k^2}{2m} + \rho_0 \Phi_k + \frac{1}{V} \sum_{p=0} (n_p \Phi_{k+p} - n_p \Phi_p + \sigma_p \Phi_p) . \]

In this way, for the spectrum of collective excitations (36) we find
\[ \varepsilon_k^2 = \left[ \frac{k^2}{2m} + \frac{1}{V} \sum_{p=0} \left( (\rho_p - \sigma)_p (\Phi_{k+p} - \Phi_p) \right) \right] \times \left[ \frac{k^2}{2m} + 2\rho_0\Phi_k + \frac{1}{V} \sum_{p=0} \left( (\rho_p + \sigma)_p \Phi_{k+p} - (\rho_p - \sigma)_p \Phi_p \right) \right]. \]

In order to simplify the formulas, we notice that expressions (32) and (33) strongly increase as \( k \to 0 \). Therefore, the main contribution in the summations, containing \( n_p \) and \( \sigma_p \), comes from the region of small \( p \). This suggests the possibility of using the approximations

\[ \sum_{p=0} \rho_p \Phi_{k+2} \approx \Phi_k \sum_{p=0} \rho_p, \quad \sum_{p=0} \sigma_p \Phi_{k+p} \approx \Phi_k \sum_{p=0} \sigma_p. \]

Then the chemical potentials (39) and (42) become

\[ \mu_0 = (\rho + \rho_1 - \sigma_1)\Phi_0 \]

and, respectively,

\[ \mu_1 = (\rho + \rho_1 - \sigma_1)\Phi_0. \]

Equation (43) reduces to

\[ \omega_k = \frac{k^2}{2m} + \rho \Phi_k - (\rho_1 - \sigma_1)\Phi_0, \]

while expression (35) becomes

\[ \Delta_k = (\rho_1 + \sigma)\Phi_k. \]

The collective spectrum (44) takes the form

\[ \varepsilon_k^2 = \left[ \frac{k^2}{2m} + (\rho_1 - \sigma_1) (\Phi_k - \Phi_0) \right] \times \left[ \frac{k^2}{2m} + (\rho + \rho_0 + \sigma) \Phi_k - (\rho_1 - \sigma_1)\Phi_0 \right]. \]

4. Thermodynamic characteristics

Having spectrum (50), it is possible to calculate the grand potential

\[ \Omega = E_B + T\sum_k \ln(1 - e^{-\beta \varepsilon_k}), \]

where

\[ E_B = -\frac{1}{2} N \rho \Phi_0 - \rho_0 \sum_p \frac{1}{p} (n_p + \sigma_p) \Phi_p \]

\[ -\frac{1}{2} V \sum_{k \rho} (n_k n_p + \sigma_k \sigma_p) \Phi_{k+p} + \frac{1}{2} \sum_k (\varepsilon_k - \omega_k). \]

With approximation (45), we have

\[ E_B = -\frac{1}{2} V \Phi_0 \left[ \rho^2 + 2\rho_0(\rho_1 + \sigma_1) + \rho_1^2 + \sigma_1^2 \right] + \frac{1}{2} \sum_k (\varepsilon_k - \omega_k). \]

Using here the fractions of condensed and uncondensed atoms

\[ n_0 = \frac{\rho_0}{\rho}, \quad n_1 = \frac{\rho_1}{\rho}, \]

and the notation

\[ \sigma = \frac{\sigma_1}{\rho} \]

we get

\[ E_B = -\frac{1}{2} N \rho \Phi_0 \left[ 1 + 2n_0(1 + \sigma) + n_1^2 + \sigma^2 \right] + \frac{1}{2} \sum (\varepsilon_k - \omega_k). \]

The average of the grand Hamiltonian can be represented as

\[ \langle H \rangle = \langle \tilde{H} \rangle - \mu N, \]

which defines the system chemical potential

\[ \mu = \mu_0 \rho_0 + \mu_1 \rho_1. \]

For the latter, we find

\[ \mu = \rho \Phi_0 + \frac{1}{V} \sum_k (n_k + (n_0 - n_1) \sigma_k) \Phi_k \]

which, in approximation (45), reads

\[ \mu = \rho \Phi_0 \left[ 1 + n_1(1 - \sigma) + n_0 \sigma \right]. \]

With the given grand potential, it is straightforward to calculate any required thermodynamic characteristics.

It is necessary to note that all thermodynamic characteristics depend on the quantity \( \Phi_0 \), which, hence, has to be well defined. Even in the simplest Bogolubov approximation, when

\[ \frac{\rho_1}{\rho_0} \ll 1, \quad \frac{\sigma}{\rho_0} \ll 1, \]

so that it is admissible to neglect \( \rho_1 \) and \( \sigma_1 \), as compared to the condensate density \( \rho_0 \), we have

\[ \mu = \mu_0 = \mu_1 = \rho \Phi_0 \]

and

\[ E_B = -\frac{1}{2} N \rho \Phi_0 + \frac{1}{2} \sum_k (\varepsilon_k - \omega_k). \]

Anyway, the thermodynamic characteristics depend on \( \Phi_0 \).

Thus, the limit \( \Phi_0 \) has to be well defined. It must be a scalar in order that the thermodynamic characteristics be scalar quantities. This implies that the Fourier transform of the interaction potential has to be correctly defined, giving an unambiguous limit (23).

5. Fourier transform

It is useful to remember the conditions when Fourier transforms can be correctly defined, since not every function enjoys a well-defined Fourier transform. For this purpose, let us recall some known mathematical facts. For simplicity, we recall these facts for the case of one variable. The generalisation to several variables is straightforward.

Definition of bounded variation. A function \( f(x) \), with \( x \in (-\infty, \infty) \), is of bounded variation in a finite interval if in that interval it has only a finite number of extrema and a finite number of finite discontinuities.
Dirichlet theorem. If a function \( f(x) \) is of bounded variation in any finite interval and is absolutely integrable, such that
\[
\int_{-\infty}^{\infty} |f(x)| \, dx < \infty,
\]
then its Fourier transform
\[
F(k) = \int_{-\infty}^{\infty} f(x)e^{-ikx} \, dx
\]
eexists and the inverse Fourier transform gives
\[
\int_{-\infty}^{\infty} F(k)e^{ikx} \, dk = \frac{1}{2\pi} [f(x - 0) + f(x + 0)].
\]
The details can be found in [26].

For the case of several variables, the sufficient condition for the existence of Fourier transform of a potential \( \Phi(r) \) is its absolute integrability:
\[
\int |\Phi(r)| \, dr < \infty.
\]
We may also note that the correct definition of the limit (23) requires the validity of interchanging the limit and integration.

Lebesgue theorem. A sufficient condition for the interchange of a limiting procedure and integration is the absolute integrability of the considered function.

For the case of the interaction potential, the limit (23) exists, so that the change of the orders
\[
\lim_{k \to 0} \int \Phi(r)e^{-ik \cdot r} \, dr = \int \lim_{k \to 0} \Phi(r)e^{-ik \cdot r} \, dr
\]
is valid, provided that the interaction potential is absolutely integrable, according to condition (61).

A good illustration of nonlocal potentials is the potential of dipole–dipole interactions. Dipoles can be electric, with the dipolar moment \( \mathbf{d}_i \), or magnetic, with the magnetic moment \( \mu_i \), where the index \( i \) enumerates particles. We shall consider dipoles with the moment \( \mathbf{d}_i \), keeping in mind that the same problems concern dipoles with the moment \( \mu_i \). Dipolar interactions are widespread for different kinds of condensed matter [27], for polymers [28], biological systems [29, 30], and for many magnetic nanoclusters and nanomolecules [31, 32].

Two dipoles at the distance \( r \) from each other interact through the dipolar potential
\[
D(r) = \frac{1}{r^3} \left[ (\mathbf{d}_1 \cdot \mathbf{d}_2) - 3(\mathbf{d}_1 \cdot \mathbf{n})(\mathbf{d}_2 \cdot \mathbf{n}) \right],
\]
where
\[
r \equiv |r|, \quad \mathbf{n} \equiv \frac{\mathbf{r}}{r}, \quad \mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2.
\]
One often considers polarised dipoles, all directed along the same unit vector \( \mathbf{e}_i \), so that
\[
\mathbf{d}_i = d_0 \mathbf{e}_i \quad (d_0 \equiv |\mathbf{d}_i|).
\]
Then the dipolar potential reduces to
\[
D(r) = \frac{d_0^2}{r^3} (1 - \cos^2 \vartheta),
\]
where \( \vartheta \) is the angle between the direction of a dipole and the spatial vector \( \mathbf{n} = \mathbf{r}/r \),
\[
\cos \vartheta = (\mathbf{e}_i \cdot \mathbf{n}).
\]
If the dipoles are directed along the \( z \)-axis, then \( \cos \vartheta = z/r \).

One formally defines the Fourier transform
\[
D_k = \int D(r)e^{-ik \cdot r} \, dr.
\]
Then in the general case (62), one gets
\[
D_k = \frac{4\pi}{3} \left[ 3(d_i \cdot \mathbf{k})(d_j \cdot \mathbf{k}) - (\mathbf{d}_i \cdot \mathbf{d}_j) \right],
\]
with \( k = |\mathbf{k}|. \) And for the case of polarised dipoles, one has
\[
D_k = \frac{4\pi}{3} d_0^2 (3 \cos^2 \vartheta_k - 1),
\]
with \( \vartheta_k \) being the angle between the dipole direction and the vector \( \mathbf{k} \),
\[
\cos \vartheta_k = \frac{(\mathbf{k} \cdot \mathbf{e}_i)}{k}.
\]
If the dipole direction is along the \( z \)-axis, then \( \vartheta_k = k/z \).

However, there are problems with the dipolar interaction potential. Thus, it is easy to see that the integral
\[
D_0 \equiv \int D(r) \, dr
\]
is not well defined. For an infinite system, it has to be understood as an improper integral
\[
\int D(r) \, dr = \lim_{V \to \infty} \int_V D(r) \, dr.
\]
But if one integrates first over spherical angles, one gets zero. Whereas, if one integrates first over the radius, one gets infinity. Hence
\[
\lim_{k \to 0} D_k \neq D_0,
\]
contrary to condition (23).

Moreover, the limit \( k \to 0 \) for \( D_k \) is not defined at all, as can be seen from the above forms of \( D_k \). Such a limit explicitly depends on the angle (68). Usually, one alleges that this anisotropy is appropriate for a system with dipolar interactions. However, this is absolutely wrong. The quantity \( D_0 \), similar to \( \Phi_0 \), enters many thermodynamic characteristics, as is explained in section 4. The thermodynamic quantities, such as the chemical potential, energy and grand potential, by their meaning are scalars and principally cannot be anisotropic. Since the limit \( D_0 \) is not defined, then all thermodynamic characteristics are not defined, which makes no sense.

This problem arises because the dipolar potential (62) or (63) is not absolutely integrable. Really, since
\[
\int_0^\pi |1 - 3 \cos^2 \vartheta| \sin \vartheta \, d\vartheta = \frac{8}{3\sqrt{3}},
\]
we have
\[
\int |D(r)| \, dr = \lim_{R \to \infty \ b \to 0} \frac{16\pi}{3\sqrt{3}} d_0^2 \ln \frac{R}{b} \to \infty.
\]
This integral tends to infinity for any of the limits, either \( R \to \infty \), or \( b \to 0 \). Therefore, the Fourier transform for an absolutely nonintegrable function may not exist, which is the case for the dipolar potential whose Fourier transform is defined neither for \( k \to 0 \) nor for \( k \to \infty \). The problem arises not due to the anisotropy of the dipolar potential, but due to its nonintegrability, which makes the formally introduced Fourier transform senseless.

6. Cutoff regularisation

Actually, the difficulties with the dipolar interaction potential are well known in physics of condensed matter [27] and have been discussed in many publications. Thus, the divergence of the dipolar potential at a short distance, resulting in infinite molecular polarisability, has been called the polarisation catastrophe [33, 34]. The way out of this catastrophe is physically transparent, requiring to consider dipolar particles not as point-like objects, but as finite-size particles described by spatial distributions. This way leads to the smearing of dipolar interactions at short distances, which can be characterised by different smearing functions [35–40]. The simplest is the short-range cutoff regularisation removing the \( 1/r^3 \) singularity. This implies the use of the short-range regularised potential

\[
D(r, b) = \Theta(r - b) D(r),
\]

(71)

where \( \Theta(r) \) is a unit-step function and \( b \) is the sum of two atomic radii. In the case of identical atoms, \( b \) is the effective atomic diameter.

For the Fourier transform

\[
D_k(b) = \int D(r, b) e^{-i k \cdot r} \, dr
\]

of potential (71), we have

\[
D_k(b) = \int_{b}^{\infty} r^2 \, dr \int_{0}^{\pi} \sin \vartheta \, d\vartheta \int_{0}^{2\pi} d\varphi \, D(r) e^{-i k \cdot r}.
\]

(72)

Considering the polarised potential (63), directing the \( z \)-axis along the wave vector \( \mathbf{k} \), integrating out the angle \( \varphi \), and using the notation

\[
x \equiv \cos \vartheta = \frac{\mathbf{k} \cdot \mathbf{r}}{kr} = \frac{\mathbf{k} \cdot \mathbf{n}}{k},
\]

we get

\[
D_k(b) = \frac{3}{4} D_k \int_{b}^{\infty} \frac{dr}{r} \int_{-1}^{1} dx \left(1 - 3x^2\right) e^{-ikrx}.
\]

(73)

Integrating over \( x \) gives

\[
D_k(b) = D_k I_k(b),
\]

(74)

with

\[
I_k(b) = 9 \int_{kb}^{\infty} \left( \sin y - \cos y \frac{y}{y^2} - \frac{\sin y}{3y^2} \right) e^{-y/kb} \, dy,
\]

(75)

where \( y = kr \). Taking the last integral results in

\[
I_k(b) = \frac{3}{(kb)^2} \left[ \sin(kb) - kb \cos(kb) \right].
\]

(76)

Integral (73) has the property

\[
\lim_{k \to 0} I_k(b) = \lim_{b \to 0} I_k(b) = 1.
\]

The presence of the short-range cutoff makes it possible to define the short-wave limit, that is, the large-\( k \) limit,

\[
D_k(b) \simeq -3D_k \frac{\cos(kb)}{(kb)^2} (k \to \infty).
\]

(77)

Recall that without the short-range cutoff regularisation the large-\( k \) limit is not defined, as is clear from equation (67). Respectively, in the limiting expression (74), it is impossible to set \( b \) to zero.

However, the long-wave limit, when \( k \to 0 \), is not defined, since

\[
D_k(b) \simeq D_k \quad (k \to 0),
\]

(78)

and we return to the problem discussed in the previous section. This is connected to the fact that potential (71) is not absolutely integrable, being divergent at large \( r \).

7. Screening regularisation

When one considers separate molecules or clusters, such finite small systems require only short-range regularisation. But for large systems, a long-range regularisation, taking into account long-range correlations, is also necessary. The necessity of regularising the dipolar potential by long-range screening was emphasised by Jonscher [41–43]. This screening is usually described by an exponential function [39, 41–45].

The dipolar potential that is regularised both for short-range as well as for long-range interactions can be written in the form

\[
D(r, b, \kappa) = \Theta(r - b) D(r) e^{-\kappa r},
\]

(79)

where \( \kappa \) is a screening wave vector, hence \( 1/\kappa \) is a screening radius. This potential is absolutely integrable, so that it enjoys a well-defined Fourier transform

\[
D_k(b, \kappa) = \int D(r, b, \kappa) e^{-i k \cdot r} \, dr.
\]

(80)

For the case of polarised dipoles, we have

\[
D_k(b, \kappa) = D_k I_k(b, \kappa),
\]

(81)

with the integral

\[
I_k(b, \kappa) \equiv 9 \int_{kb}^{\infty} \left( \sin y - \cos y \frac{y}{y^2} - \frac{\sin y}{3y^2} \right) e^{-y/kb} \, dy,
\]

(82)

in which \( y = kr \). With the change of the variable \( x = rb \), giving \( y = kbx \), we get

\[
I_k(b, \kappa) = 9kb \int_{1}^{\infty} \left[ \sin(kbx) - \cos(kbx) \frac{kbx}{(kbx)^2} - \frac{\sin(kbx)}{3(kbx)^2} \right] e^{-kbx} \, dx.
\]

(83)

Removing the screening returns us back to the case of the previous section,

\[
\lim_{\kappa \to 0} I_k(b, \kappa) = I_k(b),
\]

(84)
with a not well-defined Fourier transform. It is clear that the limits $b \to 0$ and $\kappa \to 0$ do not commute with the limit $k \to 0$,

$$
\lim_{b \to 0} \lim_{\kappa \to 0} I_k(b, \kappa) = 1 \quad (k > 0),
\lim_{k \to 0} I_k(b, \kappa) = 0 \quad (b > 0, \kappa > 0). \quad (80)
$$

It is possible to notice that integral (79) depends, actually, on two variables

$$
q \equiv kb, \quad c \equiv \kappa b.
$$

Therefore, integral (79) can be represented as

$$
I_k(b, \kappa) = I_k(c),
$$

with the integral

$$
J_k(c) = 9q \int_1^{\infty} \left[ \frac{\sin(qx)}{(qx)^2} - \frac{\cos(qx)}{(qx)^2} - \frac{\sin(qx)}{3(qx)^2} \right] e^{-cx} \, dx.
$$

The latter integral can be expressed through the exponential integral function

$$
\text{Ei}(z) = -\int_{-z}^{\infty} \frac{e^{-t}}{t} \, dt \quad (|\arg(z)| < \pi),
$$

in which the integral is defined in the sense of the principal value, with a branch cut along the negative real axis [46]. Then we find

$$
J_k(c) = -\frac{3\pi c}{2q} \left[ \frac{q^2 + c^2}{2q^2} \right] \left[ (1 - c^2) \sin q - (2 - c)q \cos q \right]
$$

$$
- \left(2 - c\right)q \cos q + \frac{3ic}{4} \left[ (q^2 + c^2) \text{Ei}(-c - i) \right.
$$

$$
- \text{Ei}(-c + i)]. \quad (84)
$$

To show that this expression is real valued, we can employ the series representation for the exponential integral function

$$
\text{Ei}(z) = \gamma + \ln z + \sum_{n=1}^{\infty} \frac{z^n}{n n!},
$$

where $\gamma = 0.57721$ is the Euler–Mascheroni constant. Using the relation

$$
\text{Ei}(-c - i) - \text{Ei}(-c + i) = 2i(\alpha - \pi) + 2i \sum_{n=1}^{\infty} \frac{(q^2 + c^2)^{n/2}}{n n!} \sin[n(\alpha - \pi)],
$$

in which

$$
\alpha = \arctan \frac{q}{c},
$$

we obtain

$$
J_k(c) = -\frac{3\pi c}{2q} \left[ (1 - c^2) \sin q - (2 - c)q \cos q \right]
$$

$$
- \frac{3}{2q^2} \left( \alpha + \sum_{n=1}^{\infty} \frac{(q^2 + c^2)^{n/2}}{n n!} \sin[n(\alpha - \pi)] \right).
$$

Function (84) possesses the following properties. When $q \to 0$, under a finite $c$, we have

$$
J_k(c) \simeq \frac{(1 + c)e^{-c}}{5c^2} q^2 - \frac{(6 + 6c + 3c^2 + c^3)e^{-c}}{70c^2} q^4 \quad (q \to 0). \quad (86)
$$

This defines the long-wave limit of the Fourier transform (77) in the form

$$
D_k(b, \kappa) \simeq \frac{(1 + \kappa b)e^{-\kappa b}}{5\kappa^2} k^2 \quad (k \to 0). \quad (87)
$$

Note that this limit is principally dependent on a finite value of the screening parameter $\kappa$ that cannot be set to zero. Thus, in the long-wave limit, we get

$$
D_k(b, \kappa) \equiv \lim_{k \to 0} D_k(b, \kappa) = 0, \quad (88)
$$

that agrees with the integral

$$
\int D(r, b, \kappa) \, dr = 0, \quad (89)
$$

and which is in agreement with condition (23).

In the short-wave limit, when $k \to \infty$, and $c$ being finite, we get

$$
J_k(c) \simeq -\frac{3e^{-c}}{2q} \left[ \frac{\cos q}{q^2} - \frac{1 - c}{q^2} \sin q - \frac{c(1 + c)}{q^4} \cos q \right],
$$

which gives for the Fourier transform

$$
D_k(b, \kappa) \simeq -3D_k e^{-\kappa b} \left( \frac{\cos(bk)}{(bk)^2} \right) \quad (k \to \infty). \quad (91)
$$

Here the finiteness of the short-range cutoff $b$ is important.

In the limit of a small screening parameter, under finite $q$, we find

$$
J_k(c) \simeq a_0(q) + a_1(q)c + a_2(q)c^2 \quad (c \to 0), \quad (92)
$$

where the coefficient functions are

$$
a_0(q) = \frac{3}{q^3} (\sin q - q \cos q),
$$

$$
a_1(q) = \frac{9}{2q^3} (q \cos q - q \sin q) + \frac{1}{2q} \left[ \text{Si}(q) - \frac{\pi}{2} \right], \quad a_2(q)
$$

$$
= \frac{3}{2q^3} (3 \sin q - q \cos q),
$$

and the notation for the sine integral

$$
\text{Si}(q) = \int_0^{\infty} \frac{\sin(t)}{t} \, dt
$$

is used. When $q \to 0$, we get

$$
a_0(q) \simeq 1, \quad a_1(q) \simeq \frac{3\pi}{2q}, \quad a_2(q) \simeq \frac{3}{q^2} \quad (q \to 0). \quad (93)
$$

If we try to find here the long-wave limit, we get the Fourier transform

$$
D_k(b, \kappa) \simeq D_k \left( 1 - \frac{3\pi \kappa}{4k} + \frac{3\kappa^2}{k^2} \right) \quad (\kappa \to 0, \, k \to 0). \quad (93)
$$
This expression is divergent at \( k \to 0 \), demonstrating that the expansion in powers of the screening parameter \( c \to 0 \) is not defined. The function \( J_q(c) \) is not analytical at \( c = 0 \), hence, the Fourier transform \( D_k(b, \kappa) \) is not analytical at \( \kappa = 0 \).

For a very large screening parameter, we have

\[
J_q(c) \simeq e^{-c} \left[ \frac{d_1(q)}{c^2} + \frac{d_2(q)}{c^2} \right] \quad (c \to \infty),
\]

with

\[
d_1(q) = \frac{3}{q^4} \left[ (3 - q^2) \sin q - 3q \cos q \right],
\]

\[
d_2(q) = \frac{3}{q^4} \left[ (12 - q^2)q \cos q + (5q^2 - 12) \sin q \right].
\]

Here, the long-wave limit of the Fourier transform is defined, yielding

\[
D_k(b, \kappa) \simeq D_k \frac{b e^{-kb}}{5\kappa} k^2 \quad (b \to \infty, \; k \to 0).
\]

In this way, in order that the dipolar interaction potential would enjoy a well-defined Fourier transform, it is necessary to regularise this potential both for short-range as well as for long-range interactions. The behaviour of the function \( J_q(c) \), defining the Fourier transform of the dipolar potential, is illustrated in figure 1.

The regularised dipolar potential is an effective potential taking into account short-range and long-range particle correlations. One may ask whether the use of an effective potential, instead of the bare interaction potential, is admissible. The answer is yes. The study of any many-particle system can be started with a self-consistent mean-field approximation, containing an effective potential, which is called the **correlated mean-field approximation** [47]. The higher approximations, beyond the correlated mean-field approximation, can be obtained by means of an iterative procedure for Green functions [48–50].

### 8. Excitation spectrum

After the interaction potential is properly regularised, so that it enjoys a well-defined Fourier transform, it is possible to study the properties of the system. It is necessary to emphasise that without the regularisation the formal investigation of the system properties in a mean-field approximation is not correct and would lead to wrong conclusions. It is admissible to deal with a singular bare interaction potential only in higher-order approximations, taking into account particle correlations smearing the singularities in the bare potential. However, in a simple mean-field approximation, the use of a bare potential having no well-defined Fourier transform is inadmissible. But a correlated mean-field approximation involving an effective regularised potential is justified.

Let us consider the excitation spectrum of a Bose-condensed system having the interaction potential consisting of two terms,
In the long-wave limit, the spectrum is of the phonon type, 
\[ \epsilon_k \simeq c_B k \quad (k \to 0), \] (103)
The sound velocity here is obtained by taking account of the properties of the function 
\[ J_k(c) \simeq A \left( \frac{k}{\kappa} \right)^2 \quad (q \to 0), \]
where 
\[ A \equiv \frac{1}{5} (1 + \kappa b) e^{-\kappa b}, \]
so that 
\[ f_k \simeq A D k \left( \frac{k}{\kappa} \right)^2 \quad (k \to 0). \]
Thus, for the sound velocity, we find 
\[ \epsilon_k^2 = \left( \rho_0 + \sigma_1 \right) \frac{\Phi_0}{m} \left[ 1 + 2m(\rho_1 - \sigma_1) \frac{A}{\kappa^2} D_k \right]. \] (104)
The sound velocity is anisotropic because of \( D_k \). Although it is necessary to stress that the anisotropy appears only if \( \rho_1 \) and \( \sigma_1 \) are not zero, but are defined by the expressions 
\[ \rho_1 = \int n_k \frac{d k}{(2\pi)^3}, \quad \sigma_1 = \int \sigma_k \frac{d k}{(2\pi)^3}, \] (105)
in which the functions \( n_k \) and \( \sigma_k \) are defined in equations (32) and (33). The condensate density \( \rho_0 = \rho - \rho_1 \) is expressed through the density of uncondensed atoms \( \rho_1 \).
The functions \( n_k \) and \( \sigma_k \) are connected to each other, 
\[ \sigma_k = - \frac{\Delta_k}{\omega_k} \left( n_k + \frac{1}{2} \right). \]
It is important to emphasise that the anomalous average \( \sigma_1 \) is of order or even larger than \( \rho_1 \). Because of this, they are to be taken into account together or both omitted. But neglecting the anomalous average \( \sigma_1 \), while keeping the normal density \( \rho_1 \), is principally wrong [12, 13, 51].

9. Bogolubov approximation

The Bogolubov approximation is applicable for temperature close to zero and asymptotically weak interactions, such that both \( \rho_1 \) and \( \sigma_1 \) are much smaller than the condensate density \( \rho_0 \rightarrow \rho \). Neglecting \( \rho_1 \) and \( \sigma_1 \) in spectrum (102) yields the Bogolubov spectrum 
\[ \epsilon_k = \sqrt{\frac{\rho_0}{m} \left( \Phi_0 + f_0 \right) k^2 + \left( \frac{k^2}{2m} \right)^2}. \] (106)
In the long-wave limit, the spectrum is of the phonon type, 
\[ \epsilon_k \simeq c_B k \quad (k \to 0), \] (107)
with the sound velocity 
\[ c_B \equiv \sqrt{\frac{\rho_0}{m} \Phi_0} = \frac{1}{m} \sqrt{4\pi \rho a_s}. \] (108)
As is evident, in the Bogolubov approximation, the sound velocity is isotropic. Anisotropy arises only in the higher-order approximation, as can be seen in the sound velocity (104).

But at finite \( k \), spectrum (106) is anisotropic. We can consider two opposite cases, the so-called parallel geometry, with \( \mathbf{k} \) parallel to the dipole direction, 
\[ \mathbf{k} \cdot \mathbf{e}_d = k \quad (\partial_k = 0), \] (109)
so that 
\[ D_k = \frac{8\pi}{3} d_0^2 \quad (\partial_k = 0), \] (110)
and the perpendicular geometry, when 
\[ \mathbf{k} \cdot \mathbf{e}_d = 0 \quad \left( \partial_k = \frac{\pi}{2} \right). \] (111)
so that 
\[ D_k = - \frac{4\pi}{3} d_0^2 \quad \left( \partial_k = \frac{\pi}{2} \right). \] (112)
It is convenient to introduce the dimensionless spectrum 
\[ \epsilon(q) \equiv \frac{b}{c_B} \epsilon_k \quad (q = kb). \] (113)
Also, we define the correlation length 
\[ \xi_c \equiv \frac{1}{mc_B} = \frac{1}{\sqrt{4\pi \rho a_s}}. \] (114)
Then spectrum (106) leads to the expression 
\[ \epsilon^2(q) = \left[ 1 + D_q J_q(c) \right] q^2 + \left( \frac{\xi_c}{2b} q \right)^2. \] (115)
Let us denote the spectrum for the parallel geometry as 
\[ \epsilon_\parallel(q) = \epsilon(q) \quad (\partial_k = 0), \] (116)
and for the perpendicular geometry, as 
\[ \epsilon_\perp(q) = \epsilon(q) \quad \left( \partial_k = \frac{\pi}{2} \right). \] (117)
The quantity 
\[ a_D \equiv m d_0^2 \] (118)
is called the dipolar length, and the ratio 
\[ \alpha \equiv \frac{4\pi d_0^2}{\Phi_0} = \frac{a_D}{3a_s} \] (119)
characterises the relative strength of the dipolar interactions with respect to the local interactions. With these notations, for spectrum (116) we get 
\[ \epsilon_\parallel^2(q) = \left[ 1 + 2\alpha J_q(c) \right] q^2 + \left( \frac{\xi_c}{2b} q \right)^2. \] (120)
Spectrum (117) becomes 
\[ \epsilon_\perp^2(q) = \left[ 1 - \alpha J_q(c) \right] q^2 + \left( \frac{\xi_c}{2b} q \right)^2. \] (121)
Assuming that the screening parameter is inversely proportional to the correlation length, we have

\[ c \equiv \kappa b = \frac{b}{\xi_c} \left( \kappa = \frac{1}{\xi_c} \right). \] (122)

Then, for spectra (120) and (121), we obtain

\[ \epsilon_{||}(q) = q \sqrt{1 + 2\alpha J_q(c) + \frac{q^2}{4c^2}}, \] (123)

and, respectively,

\[ \epsilon_{\perp}(q) = q \sqrt{1 - \alpha J_q(c) + \frac{q^2}{4c^2}}. \] (124)

One also considers the relative difference between the parallel and perpendicular geometries, defined by the quantity

\[ \Delta(q) \equiv 2 \frac{\epsilon_{||}(q) - \epsilon_{\perp}(q)}{\epsilon_{||}(q) + \epsilon_{\perp}(q)}. \] (125)

As examples of atoms with magnetic dipoles [14–16], it is possible to mention \(^{52}\)Cr, with the magnetic dipole \(\mu_0 = 6\mu_B\) and the dipolar length \(a_D = 2.4 \times 10^{-7}\) cm, \(^{166}\)Er, with \(\mu_0 = 7\mu_B\) and \(a_D = 1.05 \times 10^{-6}\) cm, and \(^{164}\)Dy, with \(\mu_0 = 10\mu_B\) and \(a_D = 2.09 \times 10^{-6}\) cm. Some molecules can have the dipolar lengths as large as \(a_D \sim 10^{-5}\) cm.

The typical behaviour of the excitation spectra (123) and (124) are shown in figures 2–4. Increasing the dipolar interactions leads to the appearance of a roton minimum and then to the roton instability. The relative difference (125) is shown in figures 5 and 6. The minimal relative interaction strength \(\alpha_{\text{min}}\) corresponds to the appearance of the roton minimum, which is defined as the occurrence of a zero derivative of the spectrum, with respect to the wave vector. The maximal \(\alpha_{\text{max}}\) is the relative dipolar strength at which the roton minimum touches zero, thus displaying the roton instability.

The origin of the roton minimum in systems with dipolar interactions is rather clear, being caused by the attractive part of these anisotropic interactions, which results in the appearance of the negative term in the spectrum (124). The possibility of the roton minimum in the spectrum of trapped Bose gases with dipolar forces has been theoretically considered for quasi-one-dimensional [52–55] and quasi-two-dimensional [56–58] cases. For sufficiently strong dipolar forces, Bose gas can become unstable [59–61], which also depends on the trap shape. This instability is due to the roton minimum touching zero [62].

The most intensive experimental studies have been done for \(^{52}\)Cr, whose Bose–Einstein condensation has been experimentally observed [63, 64]. The scattering length for these
10. Local-density approximation

The theory of the previous sections, developed for uniform systems, can be straightforwardly generalised to trapped atoms, when the trapping potential is sufficiently smooth, such that the local-density approximation is valid. Then the off-diagonal parts of correlation functions are treated as being fast, while their diagonal parts, as slow. As a result, the spatial dependence, induced by the trapping potential, enters only through the atomic densities and density distributions that are treated as slow functions of the spatial variables [13].

In the presence of an external trapping potential \( U(\mathbf{r}) \), using the local-density approximation, we have the following representation for the single-particle density matrix

\[
\rho_1(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{k=0} n_k(\mathbf{r}) e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}
\]

and for the anomalous average

\[
\sigma_1(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{k=0} n_k(\mathbf{r}) e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')},
\]

where \( V \) is a quantisation volume, needed only at the intermediate stage, and where

\[
n_k(\mathbf{r}) = \frac{\omega_k(\mathbf{r})}{2 \xi(\mathbf{r})} \coth \left( \frac{\xi(\mathbf{r})}{2T} \right) - \frac{1}{2},
\]

\[
\sigma_k(\mathbf{r}) = -\frac{\Delta_k(\mathbf{r})}{2 \xi(\mathbf{r})} \coth \left( \frac{\xi(\mathbf{r})}{2T} \right).
\]

Here, we use the notations

\[
\omega_k(\mathbf{r}) = \frac{k^2}{2m} + U(\mathbf{r}) + \rho(\mathbf{r}) \Phi_0 + \rho_0(\mathbf{r}) \Phi_k + \frac{1}{V} \sum_{p=0} n_p(\mathbf{r}) \Phi_{k+p} - \mu_1(\mathbf{r})
\]

and

\[
\Delta_k(\mathbf{r}) = \rho_0(\mathbf{r}) \Phi_k + \frac{1}{V} \sum_{p=0} \rho_p(\mathbf{r}) \Phi_{k+p},
\]

defining the local spectrum of collective excitations

\[
\xi(\mathbf{r}) = \sqrt{\omega_k^2(\mathbf{r}) - \Delta_k^2(\mathbf{r})}.
\]

The density of uncondensed atoms and the anomalous average become

\[
\rho_1(\mathbf{r}) = \frac{1}{V} \sum_{k=0} n_k(\mathbf{r}) = \int \eta(\mathbf{r}) \frac{d \mathbf{k}}{(2\pi)^3},
\]

\[
\sigma_1(\mathbf{r}) = \frac{1}{V} \sum_{k=0} \sigma_k(\mathbf{r}) = \int \eta(\mathbf{r}) \frac{d \mathbf{k}}{(2\pi)^3}.
\]

The total atomic density is

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

The condensate function, defined by condition (8), satisfies the equation

\[
- \frac{\nabla^2}{2m} + U(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}') \, d\mathbf{r}' \eta(\mathbf{r})
\]

\[
+ \int \Phi(\mathbf{r} - \mathbf{r}') [\rho_1(\mathbf{r}, \mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}')] \, d\mathbf{r}' = \mu_0 \eta(\mathbf{r}).
\]
In the Bogolubov approximation, when almost all the atoms are condensed, so that the quantities related to uncondensed atoms and the anomalous average can be neglected, the condensate-function equation (134) simplifies to the nonlinear Schrödinger equation
\[
\left[-\frac{\nabla^2}{2m} + U(r) + \int \Phi(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}') \, d\mathbf{r}'\right] \eta(\mathbf{r}) = \mu_0 \eta(\mathbf{r}). \tag{135}
\]

The condition of the condensate existence (41), which now reads
\[
\lim_{k \to 0} \varepsilon_k(\mathbf{r}) = 0, \tag{136}
\]
yields
\[
\mu_1(\mathbf{r}) = U(\mathbf{r}) + \rho(\mathbf{r}) \Phi_0 + \frac{1}{V} \sum_{k=0} \left[ n_k(\mathbf{r}) - \sigma_k(\mathbf{r}) \right] \Phi_k. \tag{137}
\]
Substituting this into equation (129) gives
\[
\omega_1(\mathbf{r}) = \frac{k^2}{2m} + \rho(\mathbf{r}) \Phi_k + \frac{1}{V} \sum_{p=0} \left[ n_p(\mathbf{r}) \Phi_{kp} + \rho(\mathbf{r}) \Phi_p \right]. \tag{138}
\]
Then for the spectrum of collective excitations (131), we have the equation
\[
\varepsilon_k^2(\mathbf{r}) = \left\{ \frac{k^2}{2m} + \frac{1}{V} \sum_{p=0} \left[ n_p(\mathbf{r}) - \sigma_p(\mathbf{r}) \Phi_{kp} + \Phi_p \right] \right\}
	imes \left\{ \frac{k^2}{2m} + 2 \rho(\mathbf{r}) \Phi_k + \frac{1}{V} \sum_{p=0} \left[ n_p(\mathbf{r}) + \sigma_p(\mathbf{r}) \Phi_{kp} + \Phi_p \right] \right\} - \left[ n_p(\mathbf{r}) - \sigma_p(\mathbf{r}) \Phi_p \right]. \tag{139}
\]
Resorting to approximation (45), we get, instead of (137),
\[
\mu_1(\mathbf{r}) = U(\mathbf{r}) + \left[ \rho(\mathbf{r}) + \rho(\mathbf{r}) + \sigma_1(\mathbf{r}) \right] \Phi_0, \tag{140}
\]
instead of (138),
\[
\omega_1(\mathbf{r}) = \frac{k^2}{2m} + \rho(\mathbf{r}) \Phi_k - \rho_1(\mathbf{r}) - \sigma(\mathbf{r}) \Phi_0, \tag{141}
\]
and for expression (130), we have
\[
\Delta_1(\mathbf{r}) = \left[ \rho_1(\mathbf{r}) + \sigma(\mathbf{r}) \right] \Phi_k. \tag{142}
\]
The equation for the spectrum (139) becomes
\[
\varepsilon_k^2(\mathbf{r}) = \left\{ \frac{k^2}{2m} + \left[ \rho_1(\mathbf{r}) - \sigma(\mathbf{r}) \right] \Phi_k \right\}
	imes \left\{ \frac{k^2}{2m} + \left[ \rho_1(\mathbf{r}) + \rho_1(\mathbf{r}) + \sigma_1(\mathbf{r}) \right] \Phi_k \right\} - \left[ \rho_1(\mathbf{r}) - \sigma_1(\mathbf{r}) \Phi_0 \right]. \tag{143}
\]
Keeping in mind dipolar interactions, we use the Fourier transform (99), which gives the spectrum equation
\[
\varepsilon_k^2(\mathbf{r}) = \left\{ \frac{k^2}{2m} + \left[ \rho_1(\mathbf{r}) - \sigma(\mathbf{r}) \right] \Phi_k \right\}
	imes \left\{ \frac{k^2}{2m} + 2 \left[ \rho_1(\mathbf{r}) + \sigma_1(\mathbf{r}) \right] \Phi_k \right\} + \left[ 2 \rho_1(\mathbf{r}) + \rho_1(\mathbf{r}) + \sigma_1(\mathbf{r}) \right] \Phi_0. \tag{144}
\]
In the Bogolubov approximation, the spectrum equation reduces to the form
\[
\varepsilon_k^2(\mathbf{r}) = \frac{\rho(\mathbf{r})}{m} \left( \Phi_0 + f_k \right) k^2 + \left( \frac{k^2}{2m} \right)^2. \tag{145}
\]
In the long-wave limit, the spectrum is phononic,
\[
\varepsilon_k(\mathbf{r}) \simeq \frac{\rho(\mathbf{r}) k}{m} \quad (k \to 0), \tag{146}
\]
with the isotropic sound velocity
\[
c_0(\mathbf{r}) = \frac{\sqrt{\rho(\mathbf{r}) m}}{k}. \tag{147}
\]
A special case is when the scattering length can be varied by means of the Feshbach resonance [65, 66] and even made zero. In an isotropic harmonic trap, the Bose condensate of $^{52}\text{Cr}$ becomes unstable and collapses at $\alpha \approx 15 \sigma_0 = 0.794 \times 10^{-7} \text{ cm}$. This corresponds to $\alpha \approx 1$. When the scattering length is zero, $\alpha = 0$, hence $\Phi_0 = 0$, the spectrum in the Bogolubov approximation reads
\[
\varepsilon_k^2(\mathbf{r}) = 2 \frac{2 \rho(\mathbf{r}) f_k^2 + \frac{k^2}{2m}}{2m} \quad (\alpha = 0). \tag{148}
\]
In the long-wave limit, using the behaviour of $f_k$ from section 8, we find
\[
\varepsilon_k(\mathbf{r}) \simeq \frac{k^2}{2m} \sqrt{\frac{4m}{\kappa^2} \Lambda(\mathbf{r}) D_k} \quad (k \to 0). \tag{149}
\]
Although the roton instability here occurs when the inequality
\[
\frac{\alpha D}{\kappa^2} \rho(\mathbf{r}) \geq \frac{3}{16 \pi A}\]
is valid, but such a quadratic spectrum does not satisfy the Landau criterion for superfluidity, which means that the condensate is not stable at all. This is in agreement with the fact that in a uniform system, Bose condensate with purely dipolar forces is not stable. This is also true for a large isotropic trap. But if the trap is of a pancake shape, the condensate can be stabilised [65, 66]. However, for a strongly anisotropic trap, the local-density approximation cannot be appropriate.

Recall that at nonzero temperature and finite interactions, the condensate density does not coincide with the superfluid density, although superfluidity and condensation arise together at the Bose condensation point. In the self-consistent mean-field approach [12, 13, 17–19], the superfluid density writes
\[
\rho_f(\mathbf{r}) = \rho(\mathbf{r}) - \frac{2Q(\mathbf{r})}{3T}, \tag{149}
\]
with the dissipated heat
\[
Q(\mathbf{r}) = \oint \frac{k^2}{2m} \left[ n_k(\mathbf{r}) + n_k^2(\mathbf{r}) - \sigma_k^2(\mathbf{r}) \right] \frac{dk}{(2\pi)^3}. \tag{149}
\]
Employing the equality
\[
n_k(\mathbf{r}) + n_k^2(\mathbf{r}) - \sigma_k^2(\mathbf{r}) = \frac{1}{4 \sin^2 \{ \beta \xi(\mathbf{r}) \}}, \tag{149}
\]
where
\[
\beta = \frac{\kappa^2}{\kappa^2} \rho(\mathbf{r}). \tag{149}
\]
where $\beta = 1/T$, we find

$$Q(\mathbf{r}) = \int \frac{k^2}{8\pi \sinh^2(\beta \varepsilon_k(\mathbf{k}))} \frac{dk}{(2\pi)^3}, \quad (150)$$

11. Conclusion

The main message of this paper is that it is necessary to be cautious dealing with nonlocal long-range interactions. Such long-range interactions can exist in different finite quantum systems [68]. Before considering Fourier transforms of such long-range interactions, it is necessary to check whether the considered interaction potential is absolutely integrable. The absolute integrability is a sufficient condition for the existence of the corresponding Fourier transform. If the interaction potential is not absolutely integrable, it may have no well-defined Fourier transform. Then, formally calculating a Fourier transform of a nonintegrable potential, one can get an incorrect expression leading to senseless unphysical results. For instance, one can come to a conclusion that thermodynamic characteristics, such as chemical potentials and energies are not scalars, which certainly has no meaning.

The consideration is specified by the example of a Bose-condensed system with nonlocal interactions. The self-consistent mean-field approach is used [12, 13, 17–19]. This approach enjoys the unique properties, as compared to all other mean-field approximations: it is the sole mean-field theory guaranteeing the correct second order of the Bose–Einstein condensation transition [69]. Also, it is the sole mean-field approach yielding the values of the condensate fraction in very good agreement with Monte Carlo calculations for arbitrary interaction strength [70].

As a particular case, atoms with dipolar interactions are treated. The bare dipolar interaction potential, for a three-dimensional system, is not absolutely integrable, and does not have a correctly defined Fourier transform. A formally calculated Fourier transform is not well defined and leads to wrong conclusions. To get a correctly defined Fourier transform of the dipolar potential, it is necessary to regularise it, making it absolutely integrable. The correctly defined Fourier transform of the regularised potential yields results essentially differing from the ill-defined transform of the bare potential. Thus, all the thermodynamic characteristics are scalars, as they should be. The spectrum of collective excitations is anisotropic, but the sound velocity in the Bogolubov approximation is isotropic. The sound velocity becomes anisotropic only in higher approximations, e.g. in the Hartree–Fock–Bogolubov approximation taking into account the necessary self-consistency conditions [12, 13, 17–19].

The spectrum of collective excitations and the relative spectrum difference for the parallel and perpendicular geometries, at a small relative dipolar strength, are in qualitative agreement with those experimentally observed [67] for the atoms of $^{52}\text{Cr}$. However, a detailed comparison with particular experiments has not been the aim of the present paper. This requires a separate publication. The goal of this paper has been to suggest a general approach for describing systems with nonlocal long-range interactions and to explain the necessity of regularising the related interaction potentials before taking their Fourier transforms.

Acknowledgment

Financial support from RFBR (grant #14-02-00723) is appreciated.

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