Elementary Excitations in Trapped BEC and Zero Mode Problem

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Abstract

We propose a natural expansion of the atomic field operator in studying elementary excitations in trapped Bose-Einstein Condensation (BEC) system near T=0K. Based on this expansion, a system of coupled equations for elementary excitations, which is equivalent to the standard linearized GP equation, is given to describe the collective excitation of BEC in a natural way. Applications of the new formalism to the homogeneous case emphasize on the zero mode and its relevant ground state of BEC.

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1 Introduction

Since the realization of Bose-Einstein Condensation (BEC) in trapped alkali atomic vapors in 1995[1], much attentions have been attracted from both viewpoints of theories and experiments[2]. Among all the recent developments, the study of collective excitations occupies an important position in studying the properties of trapped BEC. When the temperature approaches the critical temperature, the theoretical description of collective excitation is still proceeding at present[3]. For the case that the temperature becomes near zero, the linearized GP equations[7, 8] can give correct numerical predictions in agreement with the experiments[12]. However, the linearized GP equations are difficult to be solved analytically, and they include confused zero mode problem[3]. In order to give some new light on this problem, we develop an equivalent formalism to the linearized GP equations based on a natural expansion of the atomic field operator.
Our study follows discussions in ref. [3] by Lewenstein and You, and the main difference is that we adopt specific eigenfunctions to expand the atomic field. It is noticed that the advantages of our expansion lie in the following facts: (1) The problem in solving the elementary excitation becomes the problem in diagonalizing the standard quadratic Hamiltonian of Boson operators, which has been completely solved in principle before [4]. (2) Our formalism adopts a simpler form than those formulated by other expansion of the atomic field operator. (3) Since only the several lowest excitations dominate the behavior of trapped BEC system near zero temperature, the limited-level approximation (which is explained in details in Sec. 2) is rational in most cases.

This paper is organized as the following: A general formalism for elementary excitations is present in Sec. 2, and then in Sec. 3 it is applied to the homogeneous case, which is interest since it can be used to be a good example to demonstrate the appearance and the physical meaning of the zero mode clearly. In Sec. 4, a conclusion will be made and some possible application of our special expansion will be discussed.

2 General Formalism

The Hamiltonian of trapped BEC system is

\[ \hat{H} = \int d^3\vec{r} [\hat{\psi}^\dagger(\vec{r})(-\frac{\hbar^2\nabla^2}{2M} + V_{tr}(\vec{r}) - \mu_0)\hat{\psi}(\vec{r}) + \frac{1}{2}g \hat{\psi}^\dagger(\vec{r})\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})\hat{\psi}(\vec{r})], \] (1)

where \( \mu_0 \) is the chemical potential, \( g = \frac{4\pi\hbar^2a_s}{M} \), \( a_s \) the s-wave scattering length of the interatomic potential, \( M \) the atomic mass, \( V_{tr}(\vec{r}) \) the external potential, and \( \hat{\psi}(\vec{r}) (\hat{\psi}^\dagger(\vec{r})) \) the atomic annihilation (creation) field operator.

Near \( T = 0K \), since almost all the atoms occupy the same one-particle quantum state \( \Phi_0(\vec{r}) \), it is convenient to separate out the special mode for the ground state of BEC from the atomic field operator

\[ \hat{\psi}(\vec{r}) = \sqrt{N_0}\Phi_0(\vec{r}) + \delta\hat{\psi}(\vec{r}). \] (2)

where \( \delta\hat{\psi}(\vec{r}) \) represents the quantum fluctuation of \( \hat{\psi}(\vec{r}) \) relative to \( \sqrt{N_0}\Phi_0(\vec{r}) \). Notice that, at present \( \int d^3\vec{r} \langle \delta\hat{\psi}^\dagger(\vec{r})\delta\hat{\psi}(\vec{r}) \rangle_{ensemble} \ll N_0 \), i.e. the thermal component atoms is negligible. Hence the Hamiltonian can be properly expanded in \( \delta\hat{\psi}(\vec{r}) \) series while substituting formula (2) into formula (1). (Only
the lower order of $\delta \hat{\psi}(\vec{r})$ is important, so up to two orders of $\delta \hat{\psi}(\vec{r})$ is main-
tained in our consideration.) From the above Hamiltonian, $\Phi_0(\vec{r})$ can be de-
termined in zero order of $\delta \hat{\psi}(\vec{r})$ by making use of variation methods, which
satisfy the time-independent GP equation\[6, 7\]
\[(-\frac{\hbar^2 \nabla^2}{2M} + V_{tr}(\vec{r}) + gN_0 \Phi_0^*(\vec{r})\Phi_0(\vec{r}))\Phi_0(\vec{r}) = \mu_0 \Phi_0(\vec{r}).\] (3)

Combining eqs. (1-3), and ignoring the terms of the third and fourth
order of $\delta \hat{\psi}(\vec{r})$ in eq.(1), the Hamiltonian can be simplified as,
\[
\hat{H} \simeq \frac{1}{2} gN_0^2 \int d^3 \vec{r} \hat{\Phi}_0^*(\vec{r})\hat{\Phi}_0(\vec{r})\Phi_0(\vec{r})
+ \int d^3 \vec{r} \delta \hat{\psi}^\dagger(\vec{r})(-\frac{\hbar^2 \nabla^2}{2M} + V_{tr}(\vec{r}) - \mu_0 + 2gN_0 \Phi_0^*(\vec{r})\Phi_0(\vec{r}))\delta \hat{\psi}(\vec{r})
+ \frac{1}{2} gN_0 \int d^3 \vec{r} \hat{\Phi}_0^*(\vec{r})\hat{\Phi}_0(\vec{r})\delta \hat{\psi}(\vec{r})\delta \hat{\psi}(\vec{r})
+ \frac{1}{2} gN_0 \int d^3 \vec{r} \hat{\Phi}_0^*(\vec{r})\hat{\Phi}_0(\vec{r})\Phi_0(\vec{r})\Phi_0(\vec{r}).\] (4)

In order to further simplify the Hamiltonian, we select a set of special
complete wave functions $\{\Phi_n(\vec{r})\}$ to expand the atomic field operator,
\[
\hat{\psi}(\vec{r}) = \sum_{n\neq 0} \hat{a}_n \Phi_n(\vec{r}) + \hat{A}_0 \Phi_0(\vec{r}),\] (5)
where $\{\Phi_n(\vec{r})\}$ satisfy the following equations\[11\]
\[(-\frac{\hbar^2 \nabla^2}{2M} + V_{tr}(\vec{r}) + gN_0 \Phi_0^*(\vec{r})\Phi_0(\vec{r}))\Phi_n(\vec{r}) = \mu_n \Phi_n(\vec{r}),\] (6)
\[\hat{a}_n\] is the annihilation boson operator of the single state $\Phi_n(\vec{r})$ ($n \neq 0$), $\hat{A}_0$
the annihilation boson operator of the single state $\Phi_0(\vec{r})$. Due to the fact
that $(-\frac{\hbar^2 \nabla^2}{2M} + V_{tr}(\vec{r}) + gN_0 \Phi_0^*(\vec{r})\Phi_0(\vec{r}))$ is Hermitian, its eigenstates $\Phi_n(\vec{r})$
($n = 0, 1, \cdots$) are orthogonals and complete
\[
\int d^3 \vec{r} \hat{\Phi}_m^*(\vec{r})\Phi_n(\vec{r}) = \delta_{mn}.\] (7)

In most cases, only the lower part of elementary excitations determines the
properties of the system near zero temperature, so it is a good approxima-
tion to hold only the lower f-level of eq.(1), i.e. $n = \{0, 1, \cdots, f - 1\}$. In
addition, when $f \rightarrow \infty$, the present treatment becomes rigorous in principle.
Substituting eq. (5) into eq. (2), we obtain
\[ \delta \hat{\psi}(\vec{r}) = \sum_{n=0}^{f-1} \hat{a}_n \Phi_n(\vec{r}), \] (8)
where
\[ \hat{a}_0 = \hat{A}_0 - \sqrt{N_0}. \] (9)
In terms of eqs. (8,6), the Hamiltonian (4) can be reexpressed as
\[ \hat{H} \simeq -\frac{B_{00}}{2} N_0 + \sum_{m,n} A_{mn} \hat{a}_m^\dagger \hat{a}_n \]
\[ + \frac{1}{2} \sum_{m,n} (B_{mn}^* \hat{a}_m \hat{a}_n + B_{mn} \hat{a}_m^\dagger \hat{a}_n^\dagger), \] (10)
where
\[ A_{mn} = (\mu_m - \mu_0) \delta_{mn} + d_{mn}, \] (11)
\[ B_{mn} = g N_0 \int d^3 \vec{r} \Phi_0(\vec{r}) \Phi_0^*(\vec{r}) \Phi_m^*(\vec{r}) \Phi_n^*(\vec{r}), \] (12)
\[ d_{mn} = g N_0 \int d^3 \vec{r} \Phi_m^*(\vec{r}) \Phi_0^*(\vec{r}) \Phi_0^*(\vec{r}) \Phi_n(\vec{r}). \] (13)
The scheme of diagonalizing the Hamiltonian as the form (10) has been extensively studied by Blaizot and Ripka. Here, their results will be briefly reviewed in the following for the use in our present discussion.
First, one write the Hamiltonian in a compact form
\[ \hat{H} \simeq -\frac{B_{00}}{2} N_0 + \frac{1}{2} \alpha^\dagger M \alpha - \frac{1}{2} \text{tr} A \] (14)
by introducing the vector operator
\[ \alpha^\dagger = \begin{pmatrix} \hat{a}_0^\dagger & \hat{a}_1^\dagger & \cdots & \hat{a}_{f-1}^\dagger \end{pmatrix}, \] (15)
the \(2f \times 2f\) coefficients matrix
\[ M = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}, A = A^\dagger, B = B^\dagger. \] (16)
In ref.[4], it is assumed that the matrix \(M\) is semi-definite positive. However, in our discussion, this condition on the matrix \(M\) is not necessary since it is only a condition for the stability of the mode of the ground state of BEC.
Second, a unitary canonical transformation is carried out to diagonalize the Hamiltonian,
\[ \beta = T \alpha \]  
where the operator vector
\[ \beta^\dagger = \left( \hat{b}_0^\dagger \hat{b}_1^\dagger \cdots \hat{b}_{f-1}^\dagger \hat{b}_0 \hat{b}_1 \cdots \hat{b}_{f-1} \right), \]  
the transformation matrix and its inverse matrix
\[ T = \begin{pmatrix} X^* & -Y^* \\ -Y & X \end{pmatrix}, \quad T^{-1} = \begin{pmatrix} \hat{X} & Y^\dagger \\ \hat{Y} & X^\dagger \end{pmatrix}, \]
the matrix satisfy the canonical condition
\[ T \eta T^\dagger \eta = 1, \]
and the matrix
\[ \eta = \begin{pmatrix} 1_f & 0 \\ 0 & -1_f \end{pmatrix}. \]

If the elements of the \( f \times f \) matrixes \( X \) and \( Y \) satisfy the following conditions\([4, 14]\)
\[ \eta M V^n = \varpi_n V^n, \]
where
\[ V^n = \begin{pmatrix} X^n \\ Y^n \end{pmatrix}, X^n_i = X_{ni}, Y^n_i = Y_{ni}, (i = 1, 2, \ldots, f) \]
especially, if the above equation have one special solution \( \{ \varpi = 0, V^0 = P \} \), i.e.
\[ \eta MP = 0 \]
the Hamiltonian can be written as
\[ \hat{H} \simeq -\frac{B_{00}}{2} N_0 + \sum_{n=1}^{f-1} \omega_n \hat{b}_n^\dagger \hat{b}_n + \frac{\varphi^2}{2 \mu} + \frac{1}{2} \sum_n \omega_n - \frac{1}{2} tr A \]  
where
\[ \varphi \equiv \alpha^\dagger \eta P, \]
and \( \mu \) is a positive constant, which can be determined by the following conditions
\[ \eta M Q^\dagger = -\frac{i P}{\mu}, \]
\[ Q^\dagger \eta P = i, \]
where the vector $Q$ is orthogonal to all the eigenvectors of the matrix $\eta M$.

In Hamiltonian (24), the second term is the Hamiltonian of a system of independent oscillators, which represent elementary excitations of the system; However, the third term has the form of a free kinetic energy, which is connected with a collective motion in Fock space arising from a broken $U(1)$ symmetry in the procedure of the mean field approximation [1]. Usually, the third term is termed with *spurious state* [4] or zero mode [3] for the corresponding eigenvalue and the norm of the vector $P$ both are zero. The physical meaning of this term will be discussed in details in Sec. 3.

In fact, we can determine the vector $P$ through observation. Notice that in principle, we can solve the the eigenvalues $\{\omega_n\}$ and the corresponding eigenvectors defined by $\{X_m^n, Y_m^n\}$ of eqs. (22), which consist of $2 \times f \times f$ homogeneous linear equations. Obviously, the eigenvalue $\omega_0 = 0$ and the corresponding vector $P$ denoted by $\{X_0^m = \delta_{m0}, Y_0^m = -\delta_{m0}\}$ is a specific solution of the above equations. Hence

$$\varphi = \hat{a}_0 + \hat{a}_0^\dagger, \quad (28)$$

which is in agreement with that in ref. [3].

From eqs. (24,28), a direct conclusion is that the approximate vacuum state $|\text{Vac}\rangle = \prod_i \otimes |\text{Vac}\rangle_i$ of BEC satisfies the following conditions

$$\hat{b}_i |\text{Vac}\rangle_i = 0, \quad (29)$$

$$\varphi |\text{Vac}\rangle_0 = 0. \quad (30)$$

To sum up, in this section, we give a new formalism for elementary excitations in trapped BEC, which is equivalent to the standard linearized GP equation. This equivalence can be easily verified when the complex wave functions $\left(\begin{array}{c} u(\vec{r}) \\ v(\vec{r}) \end{array}\right)$ in traditional method are expanded with the specific complete wave functions defined by eqs.(6). In this sense, our formalism is a specific representation of the traditional method.

### 3 Homogeneous case $V_{tr}(\vec{r}) = 0$

In this section, the general formalism obtained in the above section will be demonstrated in the homogeneous case.

In this case, the ground wave function satisfy

$$\left(-\frac{\hbar^2 \nabla^2}{2M} + gN_0 \Phi_0^*(\vec{r})\Phi_0(\vec{r})\right)\Phi_0(\vec{r}) = \mu_0 \Phi_0(\vec{r}). \quad (31)$$
Therefore, the ground wave function and the chemical potential are given by

$$\Phi_0(\vec{r}) = \frac{1}{\sqrt{V}}, \mu_0 = g \frac{N_0}{V}. \quad (32)$$

Eq. (3) which give the complete wave functions now becomes

$$(-\frac{\hbar^2 \nabla^2}{2M} + \mu_0)\Phi_k(\vec{r}) = \mu_k \Phi_k(\vec{r}) \quad (33)$$

By solving the above equations, the eigen wave functions and the corresponding eigen values are given by

$$\Phi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}},$$

$$\mu_k = \mu_0 + \frac{\hbar^2 k^2}{2M}. \quad (34)$$

Formulas (12,13) become

$$B_{\vec{k} \vec{k}'} = gN_0 \int d^3 \vec{r} \Phi_0(\vec{r}) \Phi_0(\vec{r}) \Phi_k^*(\vec{r}) \Phi_k'(\vec{r}) = g \frac{N_0}{V} \delta_{\vec{k},-\vec{k}'},$$

$$d_{\vec{k} \vec{k}'} = gN_0 \int d^3 \vec{r} \Phi_k^*(\vec{r}) \Phi_0(\vec{r}) \Phi_k(\vec{r}) \Phi_k'(\vec{r}) = g \frac{N_0}{V} \delta_{\vec{k},\vec{k}'} \quad (35)$$

Due to the fact the mode denoted by $\vec{k}$ is only coupled to the mode denoted by $-\vec{k}$ implied by the above equation, eqs. (22) can be simplified as

$$\left(\frac{\hbar^2 k'^2}{2M} + g \frac{N_0}{V} - \omega_{\vec{k}'}\right)X_{\vec{k}}^{\vec{k}'} + g \frac{N_0}{V} Y_{\vec{k}} = 0$$

$$\left(\frac{\hbar^2 k'^2}{2M} + g \frac{N_0}{V} + \omega_{\vec{k}'}\right)Y_{\vec{k}}^{\vec{k}'} + g \frac{N_0}{V} X_{\vec{k}'} = 0 \quad (36)$$

When $\vec{k}' \neq 0$, the eigenvalue can be calculated by requiring that the above equations have nontrivial solution,

$$\omega_{\vec{k}'} = \omega_{-\vec{k}'} = \sqrt{\left(\frac{\hbar^2 k'^2}{2M} + g \frac{N_0}{V}\right)^2 - (g \frac{N_0}{V})^2} \quad (37)$$

The corresponding annihilation operators of the elementary excitation are

$$\hat{b}_{\vec{k}'} = \sqrt{\frac{1}{2} \left(\frac{\hbar^2 k'^2}{2M} + g \frac{N_0}{V} + 1\right)} \hat{a}_{\vec{k}'} - \sqrt{\frac{1}{2} \left(\frac{\hbar^2 k'^2}{2M} + g \frac{N_0}{V} - 1\right)} \hat{a}^\dagger_{-\vec{k}'}.$$
or
\[
\hat{b}_{-\vec{k}'} = \sqrt{\frac{1}{2} \left( \frac{\hbar^2 k'^2}{2M} + \frac{g N_0}{V} \right) + 1} \hat{a}_{-\vec{k}'} - \sqrt{\frac{1}{2} \left( \frac{\hbar^2 k'^2}{2M} + \frac{g N_0}{V} \right) - 1} \hat{a}_{-\vec{k}'}^\dagger
\]

Clearly, it comes back to the familiar form \[2\], which supports that our formalism is equivalent to the traditional one.

Since the operators \( \hat{a}_0 \) and \( \hat{a}_0^\dagger \) are only coupled each other, we can limit ourself in the subspace of the wave vector \( \vec{k}' = 0 \). The matrix \( \eta M \) in this subspace is

\[
\eta M = \begin{pmatrix}
g \frac{N_0}{V} & g \frac{N_0}{V} \\
-\frac{g N_0}{2V} & -\frac{g N_0}{2V}
\end{pmatrix}
\]

Obviously, the eigen vector \( P \) of the zero mode and the corresponding momentum operator \( \varphi \) are obtained as

\[
P = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \varphi = \hat{a}_0 + \hat{a}_0^\dagger = (\hat{A}_0 + \hat{A}^\dagger_0) - 2\sqrt{N_0}.
\]

According to eqs. \[28,27\], the other independent vector \( Q \) and the constant \( \mu \) are obtained as

\[
Q = -\frac{i}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \mu = \frac{N_0}{V}.
\]

In sum, the Hamiltonian can be written as

\[
\hat{H} \simeq -\frac{g N_0^2}{2V} + \sum_{\vec{k} \neq 0} \omega_{\vec{k}} \hat{b}_{\vec{k}}^\dagger \hat{b}_{\vec{k}} + \frac{\varphi^2}{2 \mu} + \frac{1}{2} \sum_{\vec{k} \neq 0} \omega_{\vec{k}} - \frac{1}{2} \sum_{\vec{k}} \left( \frac{\hbar^2 k^2}{2M} + g \frac{N_0}{V} \right).
\] (38)

Now, the approximate vacuum state \( |\text{Vac}\rangle = \prod_{\vec{k}} |\text{Vac}\rangle_{\vec{k}} \) of BEC can be obtained analytically by solving eqs.\([28,24]\). When the wave vector \( \vec{k} \neq 0 \), the vacuum state \( |\text{Vac}\rangle_{\vec{k}} \) is given by solving the equations \( \hat{b}_{\vec{k}}^\dagger |\text{Vac}\rangle_{\vec{k}} = \hat{b}_{-\vec{k}}^\dagger |\text{Vac}\rangle_{-\vec{k}} = 0 \),

\[
|\text{Vac}\rangle_{\vec{k}} = \sum_n A_{\vec{k}} \left( \frac{k^2}{2M} + \frac{g N_0}{V} - \omega_{\vec{k}} \right)^\frac{n}{2} |n\rangle_{\vec{k}} \otimes |n\rangle_{-\vec{k}},
\]

where \( A_{\vec{k}} \) is the constant of normalization, the vector \( |n\rangle_{\vec{k}} \) (\(|n\rangle_{-\vec{k}}\)) is the eigenstate of the number operator \( \hat{a}_{\vec{k}}^\dagger \hat{a}_{\vec{k}} \) (\( \hat{a}_{-\vec{k}}^\dagger \hat{a}_{-\vec{k}} \)). When the wave vector \( \vec{k} = 0 \), \( \varphi |\text{Vac}\rangle_0 = 0 \). Therefore,
\[ |Vac\rangle_0 = \frac{1}{\sqrt{2\pi}} \sum_n |n\rangle_0 \int dx e^{i\sqrt{2N_0 x}} \langle x|n|^{*}, \]

where the state vector \( |n\rangle_0 \) is the eigen state of the number operator \( \hat{A}_0 \hat{A}_0^{\dagger} \),

\[ \langle x|n \rangle = \left[ \frac{1}{\sqrt{\pi 2^n n!}} \right]^{\frac{1}{2}} e^{-\frac{1}{2}x^2} H_n(x), \]

and \( H_n(x) \) is Hermit polynomial.

In this section, we explicitly solve the elementary excitations of BEC in the homogeneous case. In this case, it is easy to see that the term of the zero mode in Hamiltonian (38) originate from the quantum fluctuation of the mode denoted by macroscopic wave function \( \Phi_0(\vec{r}) \). In fact, if we adopt the usual Bogoliubov approximation, i.e. \( \hat{A}_0 \sim \hat{A}_0^{\dagger} \sim \sqrt{N_0} \), thus the momentum operator \( \Phi_0 \equiv 0 \). However, we have no specific reasons to ignore this quantum fluctuation while maintaining those of the other modes. In our treatment, the conservation of the particle number is destroyed, which is easily seen from the approximate vacuum state \( |Vac\rangle \). The kinetic term appearing in the Hamiltonian is originated from this symmetry breaking, which represents a collective motion, not an intrinsic elementary excitation of the system[4].

\section{Conclusion}

In this paper, based on a natural choice of the complete wave functions, we expand the atomic field operator and obtain a new formalism for the excitations of trapped BEC system near zero temperature. We argue that our formalism is equivalent to the standard linearized GP equation. In terms of this formalism, we illustrate the relation between the zero mode and the other excited modes. Essentially, the zero mode originates from the quantum fluctuations of the mode denoted by the condensate wave function. When applying the formalism to the homogeneous case, the formalism comes back to the usual Bogoliubov excitation spectrum, which identifies our theory.. Especially, in this case, the physical meaning of zero mode become obvious and the ground state of BEC can be calculate explicitly up to second order of the quantum fluctuations.

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