Variational Approach to the Dynamics of Bose-Einstein Condensates. I

Variational Ansatz and Quantum Dynamics

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Abstract

Variational method is applied to describe Bose-Einstein condensates (BEC) interacting via a pseudo-potential, taking into account quantum fluctuations around the mean field by the Gaussian approximation. Contributions from the pair-wise scattering by the singular potential should be removed carefully to avoid double countings in the perturbation series in terms of original bare interaction. We show that this procedure removes all dangerous terms which contain divergences.

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§1. Introduction

Recent experimental breakthrough\(^1\) of manufacturing Bose-Einstein condensates (BEC) in magnetically trapped dilute gases of alkali-metal atoms has created new opportunities to test many-body theories in well-controlled experimental conditions. Although the phenomena can be considered as a spectacular realization of an old prediction of quantum statistical mechanics as applied to ideal Bose gases\(^2\), it is known that mutual interactions of particles still play important roles to determine characteristic properties of the systems.\(^3\), \(^4\)

In theoretical treatments the condensate is usually described by the dilute gas approximation in which the pair-wise short range interaction is fully accommodated by the use of the effective interaction, usually referred to as the pseudo-potential, defined by

\[ V_{\text{eff}}(\mathbf{r}) = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}) = g\delta(\mathbf{r}), \quad (1.1) \]

where \(a\) is the \(S\)-wave scattering length of the pair interaction and \(m\) is the mass of the particle, while the many-body collective dynamics of the condensate is described by the Gross-Pitaevskii equation\(^5\), also known as the non-linear Schrödinger equation, for a classical field \(\Phi(\mathbf{r}, t)\):

\[ i\hbar \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = \left[ -\frac{\hbar^2 \nabla^2}{2m} + g|\Phi(\mathbf{r}, t)|^2 \right] \Phi(\mathbf{r}, t). \quad (1.2) \]

This equation can be derived from the Heisenberg equation of motion of the quantum field \(\psi(\mathbf{r}, t)\)

\[ i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = [\psi(\mathbf{r}, t), \hat{H}] = -\frac{\hbar^2 \nabla^2 \psi(\mathbf{r}, t)}{2m} + g\psi(\mathbf{r}, t)\psi^2(\mathbf{r}, t) \quad (1.3) \]

by the replacement

\[ \psi(\mathbf{r}, t) \rightarrow \Phi(\mathbf{r}, t) = \langle \psi(\mathbf{r}, t) \rangle_{\text{coh}}. \]

where the expectation value is taken with a coherent state of the particle creation and annihilation operator of the lowest single particle state. This approximation is also known as the tree approximation in the language of the loop expansion\(^6\) and ignores quantum fluctuations around the mean field \(\Phi(\mathbf{r}, t)\). It is the purpose of the present work to investigate the effect of quantum corrections to the mean field by the variational method which we have developed for describing dynamics of quantum fields.\(^7\), \(^8\)

When the effective interaction of the form \((1.1)\) is used to calculate the effect of the quantum fluctuations, a special care is needed to avoid (ultraviolet) divergences which arises due to the singular nature of the potential which causes coupling of all momentum modes.\(^9\)-\(^11\) It has been shown by Lee, Huang and Yang\(^9\) that such divergences can be eliminated...
systematically by the proper use of the pseudo-potential defined by\textsuperscript{12)}

\[ V_{ps}(r) = g\delta(r)\frac{\partial}{\partial r}r = g\delta(r) + g\delta(r)r \frac{\partial}{\partial r}. \]  

(1.4)

The difference,

\[ \Delta V(r) = V_{ps}(r) - V_{eff}(r) = g\delta(r)r \frac{\partial}{\partial r}, \]  

(1.5)

which has only vanishing contribution in the first order, generates divergent terms in higher order and it is precisely these divergent terms which cancel the divergences which are contained in the higher order quantum corrections of \( V_{eff}(r) \).\textsuperscript{9)}

Physically this procedure is understood as the elimination of the double counting in the usual perturbation expansion in terms of the bare two particle interaction \( V_0(r) \): since the pair scattering (in vacuum) is already fully accounted for by the scattering length \( a \), one should not include, when performing many body calculation, contributions from repeated use of the effective interaction (1.1) in the two particle scattering channel.\textsuperscript{*}) For example, the contributions from the diagram in Fig. 1 (a) should not be included in the many body calculation, because it is a part of the diagrams Fig. 1 (b) which is already included in the lowest order diagrams Fig. 1 (c) in terms of \( V_{eff} \). The problem of ultraviolet divergence can of course be avoided if one starts from a bare two-body interaction of finite range; this approach would however involve much more elaborate calculations even for a static system.\textsuperscript{15)}

Elimination of the ultraviolet divergences due to the singular potential looks technically similar to the renormalization of the effective local couplings in quantum field theories to eliminate ultraviolet divergences.\textsuperscript{14)} This analogy was exploited further by Toyoda\textsuperscript{16)} and more recently by Braaten and Nieto.\textsuperscript{11)} However, here we choose to remove all divergences by simply avoiding double countings of pair scatterings, by inspection, based on the observation that the effective interaction (1.1) should be used only in the first Born “approximation” to describe two particle scattering.

This does not mean, however, that we should discard the quantum fluctuations entirely: the many-body interaction such as Fig. 2 should be still retained in the calculation. For example, the well-known Bogoliubov theory\textsuperscript{17)} contains the effect of quantum fluctuations as zero-point oscillations of quasi-particle modes; the contribution to the energy density of this fluctuation would diverge if one uses the potential of the form (1.1). This divergence can be eliminated by the above procedure leaving behind non-analytic \( a^{5/2} \) correction which originates from the sum of genuine many-body interaction contributions.\textsuperscript{9)}

\textsuperscript{*}) Although the procedure to eliminate the ultraviolet divergence found in the literature\textsuperscript{13), 14)} is very suggestive, this interpretation of the subtraction of the double counting terms was never explicitly mentioned elsewhere to the best of our knowledge.
Fig. 1. The one-loop diagram depicted in (a) should not be included in the calculation since it is a part of (b) which is already included in the first order (tree) diagram (c).

Fig. 2. Some diagrams which cannot be reduced to the pair interaction like Fig. 1 (b) and therefore should be included in the calculation.

In this paper we present the basic formulation of the variational method and derive the equations of motion which generalizes the Gross-Pitaevskii mean field equation (1.2) to include the effect of quantum fluctuations in terms of the reduced density matrix. The resultant equations are similar to those known as the Hartree-Fock-Bogoliubov equations for fermions in nuclear many-body theory\textsuperscript{21} and are identical, although slightly disguised, to the ones obtained for interacting bose-systems by Blaizot and Ripka\textsuperscript{22}, and more recently by Griffin\textsuperscript{23}. The general static solutions of these equations are given in terms of the mode functions. We then perform an explicit calculation for a uniform condensate and show how the divergent terms appear by the use of the effective potential (1.1). By the inspection of the origin of these divergences in perturbation series we will demonstrate that all these divergences can be eliminated by the systematic removal of the terms which correspond to the double counting of pair scattering. By this method we obtain a gap equation free of divergence, (6.20), a new result obtained in this paper: To the best of our knowledge, this equation has never been written explicitly in the literature. In the forthcoming paper, we shall apply the present method to compute the density response function of the system.

The rest of the paper is organized as follows. In the next section, we construct the Gaussian variational wave functional for condensates in a general trapping external potential. In section 3, we derive the equations of motion which consist of a generalized Gross-Pitaevskii equation for the condensate and the Liouville equation for the reduced density matrix. Our
generalized Gross-Pitaevskii equations consist of two coupled non-linear equations: one is the equation of motion for $\Phi(x, t)$ similar to the Gross-Pitaevskii equation (1.2), but it also contains the mean field terms associated with the fluctuations, and the other is the equation of motion for the fluctuations, written in the form of the Liouville equation for the reduced density matrix consisting of fluctuations, these equations are often called the time-dependent Hartree-Bogoliubov equation. In section 4, we show that these equations can be easily extended to finite temperatures using the Gaussian density matrix which is determined self-consistently. In section 5, we express the static solutions of these equations in terms of the mode functions. In section 6 we examine the static solution in uniform system in detail and compare the results to the well-known Bogoliubov's mean field theory. We illustrate how the divergence can be eliminated by the removal of the double counting terms in the diagrams of perturbative series. A brief summary is given in section 7.

§2. Gaussian wave functional

In this and following sections we shall apply the variational method developed earlier in the functional Schrödinger picture to derive an extended form of the Gross-Pitaevskii equation which contain the effect of quantum fluctuations in a minimal fashion.

We consider a non-relativistic gas of bose particles of mass $m$ interacting via contact interaction in the form of (1.1). The dynamics of system is described by the following second quantized Hamiltonian:

$$
\hat{H} = \int d^3x \left\{ -\frac{1}{2m} \psi^\dagger(x) \nabla^2 \psi(x) + \psi^\dagger(x)V_{\text{ext}}(x)\psi(x) + \frac{g}{2} \psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x) \right\}.
$$

Here, $V_{\text{ext}}$ represents an external confining potential provided by the magnetic trap and the mutual interaction of particle is given by the effective interaction of the form (1.1). The fields $\psi(x)$ are quantized by the commutation relation : $[\psi(x), \psi^\dagger(y)] = \delta^3(x - y)$ and the other combinations are equal to 0. Hereafter, we take $\hbar = 1$.

In order to apply the Gaussian wave functional method, which has been developed in our previous work, we need to rewrite the Hamiltonian in terms of canonical coordinates and their associate momenta. There is some earlier attempt to define such coordinates, but we choose here the representation which diagonalize the bilinear
part of the Hamiltonian.

\[
\hat{H}_0 \equiv \int d^3x \left\{ -\frac{\hbar^2}{2m} \psi^\dagger(x) \nabla^2 \psi(x) + \psi^\dagger(x) V_{\text{ext}}(x) \psi(x) \right\} = \sum_{\alpha} \omega_\alpha a^\dagger_\alpha a_\alpha \tag{2.2}
\]

The field operator is decomposed as

\[
\psi(x) = \sum_\alpha \varphi_\alpha(x) a_\alpha \tag{2.3}
\]

where \( \varphi_\alpha(x) \) is the normalized eigen wave function of free bosons in external potential. We then introduce the following Hermitian operators:

\[
Q_\alpha \equiv \frac{1}{\sqrt{2\omega_\alpha}} (a_\alpha + a^\dagger_\alpha),
\]

\[
P_\alpha \equiv -i\sqrt{\frac{\omega_\alpha}{2}} (a_\alpha - a^\dagger_\alpha). \tag{2.4}
\]

With \( \int dx \varphi^\ast_\alpha(x) \varphi_\beta(x) = \delta_{\alpha,\beta} \) these operators satisfy the canonical commutation relations:

\[
[Q_\alpha, P_\beta] = i\delta_{\alpha,\beta},
\]

an analogue to that of the position and momentum operator in quantum mechanics, and convert the free Hamiltonian into a sum of uncoupled harmonic oscillators:

\[
\hat{H}_0 = \sum_\alpha \frac{1}{2} \left( P^2_\alpha + \omega^2_\alpha Q^2_\alpha \right). \tag{2.5}
\]

In the \( Q \)-representation, corresponding to the coordinate representation in quantum mechanics, the field momentum operator is expressed by the functional differential:

\[
P_\alpha = -i \frac{\delta}{\delta Q_\alpha}.
\]

The vacuum state of the Hamiltonian \( \hat{H}_0 \) is expressed as a product of Gaussian:

\[
\Psi_0[\phi] = \langle \phi | 0 \rangle = \mathcal{N}_0 \exp \left[ -\frac{1}{2} \sum_\alpha \omega_\alpha Q^2_\alpha \right] = \mathcal{N}_0 \exp \left[ -\frac{1}{2} \int d^3x d^3y \phi^\dagger(x) W_0(x, y) \phi(y) \right] \tag{2.6}
\]

where in the last line we have used the complex \( \phi \)-field defined by\(^*)

\[
\phi(x) = \sum_\alpha \varphi_\alpha(x) Q_\alpha
\]

and the kernel of the integral is defined by

\[
W_0(x, y) = \sum_\alpha \varphi_\alpha(x) \omega_\alpha \varphi^\ast_\alpha(y). \tag{2.7}
\]

\(^*)\) Do not confuse \( \phi(x) \) with the original bose field \( \psi(x) \): it obeys the commutation relation, \([\phi(x), \pi^\dagger(y)] = i\delta(x - y)\) where the \( \pi \)-field is defined by \( \pi(x) = \sum_\alpha \varphi_\alpha(x) P_\alpha \).
Indeed, this state will be annihilated when we operate the particle annihilation operator \( a_\alpha \) from the left for any \( \alpha \). In the uniform system \( (V_{\text{ext.}} = V_0) : \varphi_\alpha(x) \to \frac{1}{\sqrt{\lambda}} e^{ikx} \), \( \omega_\alpha \to k^2/2m + V_0 \), and \( W_0(x, y) \to \delta(x - y)(-\nabla_x^2/2m + V_0) \).

Our time-dependent variational wave functional in the functional Schrödinger picture is written as a straightforward generalization of the time-dependent Gaussian wave function in quantum mechanics: \(^7\)

\[
\Psi[\phi] = \mathcal{N} \exp \left[ i \langle \pi | \phi - \bar{\phi} \rangle - \langle \phi - \bar{\phi} | \frac{1}{4G} + i \Sigma | \phi - \bar{\phi} \rangle \right] \tag{2.8}
\]

where we have used abbreviate notations for integrals such as

\[
\langle \pi | \phi - \bar{\phi} \rangle = \sum_\alpha P_\alpha(t) \left( Q_\alpha - Q_\alpha(t) \right) = \int d^3x \pi^*(x,t) \left( \phi(x) - \bar{\phi}(x,t) \right),
\]

\[
\langle \phi | K | \phi \rangle = \sum_{\alpha,\beta} Q_\alpha K_{\alpha,\beta}(t) Q_\beta = \int d^3x d^3y \phi^*(x) K(x,y;t) \phi(y)
\]

for \( K = G^{-1}, \Sigma \). Here two (complex) functions,

\[
\bar{\phi}(x,t) = \sum_\alpha \varphi_\alpha(x) \bar{Q}_\alpha(t), \quad \pi(x,t) = \sum_\alpha \varphi_\alpha(x) \bar{P}_\alpha(t),
\]

and two kernels,

\[
G^{-1}(x,y;t) = \sum_\alpha \varphi_\alpha(x) G^{-1}_{\alpha,\beta}(t) \varphi^*_\beta(y)
\]

\[
\Sigma(x,y;t) = \sum_\alpha \varphi_\alpha(x) \Sigma_{\alpha,\beta}(t) \varphi^*_\beta(y)
\]

are to be considered as time-dependent variational parameters of the wave functional.

The expectation value of a composite operator \( \mathcal{O}(\phi, \pi) \) is given by the functional integral

\[
\langle \mathcal{O} \rangle = \int [d\phi] [\pi^*][\phi] \mathcal{O} \left( \phi, -i \frac{\delta}{\delta \bar{\phi}} \right) \Psi[\phi]
\]

which becomes a functional of the variational parameters \( \bar{\phi}(x,t) \), \( \pi(x,t) \), \( G(x,y,t) \) and \( \Sigma(x,y,t) \). For example, the expectation values of the field \( \phi(x) \) and its canonical momentum \( \pi(x) \) are given by

\[
\langle \phi(x) \rangle = \bar{\phi}(x,t) \tag{2.9}
\]

\[
\langle \pi(x) \rangle = \pi(x,t) \tag{2.10}
\]

respectively, and

\[
\langle \phi(x) \rangle = \sum_\alpha \sqrt{\frac{\omega_\alpha}{2}} \varphi_\alpha(x) \left( Q_\alpha(t) + \frac{i}{\omega_\alpha} P_\alpha(t) \right) \equiv \Phi(x,t) \tag{2.11}
\]

\[
\langle \psi(x) \rangle = \sum_\alpha \sqrt{\frac{\omega_\alpha}{2}} \varphi_\alpha(x) \left( \bar{Q}_\alpha(t) - \frac{i}{\omega_\alpha} \bar{P}_\alpha(t) \right) \equiv \Phi^*(x,t) \tag{2.12}
\]
The nonvanishing expectation value of the particle creation and annihilation operators implies that our wave functional is not an eigen state of the particle number. Our Gaussian state corresponds to a squeezed state, or a generalized coherent state, in quantum optics.

In order to describe field fluctuations it is convenient to introduce

\[ \hat{\psi}(x, t) \equiv \psi(x) - \Phi(x, t) \quad (2.13) \]

For example, we obtain

\[ \langle \psi^\dagger(x) \psi(y) \rangle = \Phi^\ast(x, t) \Phi(y, t) + \langle \hat{\psi}^\dagger(x, t) \hat{\psi}(y, t) \rangle \quad (2.14) \]

and so on, where \( \langle \hat{\psi}^\dagger(x, t) \hat{\psi}(y, t) \rangle \) is the two-point correlation function at time \( t \) and represents the quantum fluctuation. The fluctuation is determined by the width parameter of the Gaussian wave functional. The explicit forms may be obtained from the following relations:

\begin{align*}
\langle \hat{Q}_\alpha \hat{Q}_\beta \rangle &= G_{\alpha,\beta}(t) \\
\langle \hat{P}_\alpha \hat{P}_\beta \rangle &= \frac{1}{4} G^{-1}_{\alpha,\beta}(t) + 4 (\Sigma \Sigma)_{\alpha,\beta}(t) \\
\langle \hat{Q}_\alpha \hat{P}_\beta \rangle &= -2 (G \Sigma)_{\alpha,\beta}(t) + \frac{1}{2} i \delta_{\alpha,\beta} \\
\langle \hat{P}_\alpha \hat{Q}_\beta \rangle &= -2 (\Sigma G)_{\alpha,\beta}(t) - \frac{1}{2} i \delta_{\alpha,\beta}
\end{align*}

where \( \hat{Q}_\alpha = Q_\alpha - \bar{Q}_\alpha \) and \( \hat{P}_\alpha = P_\alpha - \bar{P}_\alpha \). For example,

\[ \langle \hat{\phi}(x) \hat{\phi}^\dagger(y) \rangle = \sum_{\alpha,\beta} \varphi_\alpha(x) \langle \hat{Q}_\alpha \hat{Q}_\beta \rangle \varphi^\ast_\beta(y) = \sum_{\alpha,\beta} \varphi_\alpha(x) G_{\alpha,\beta}(t) \varphi^\ast_\beta(y) = G(x, y; t) \]

and similar relations can be obtained for \( \langle \hat{\phi}^\dagger(x) \hat{\pi}(y) \rangle \) etc. However, we do not need such explicit forms in the following discussion.

With the Gaussian form of the variational wave functional, expectation value of all higher products of the field operators are expressed in terms of the center (the mean field) and the width (the two-point correlation function) of the Gaussian. This feature, characteristic of the Gaussian Ansatz of the fluctuations, enables one to truncate otherwise infinite set of coupled equations of the motion for the expectation values of the products of the quantum fields into a set of coupled equations of motion for the mean field \( \Phi(x, t) \) and the two-point functions of fluctuations \( G(x, y; t) \).
§3. Equations of motion

The equations of motion can be derived from the time-dependent variational principle as applied to the action:

\[ S = \int dt \langle \hat{\Psi} | i \frac{\partial}{\partial t} - \hat{H} + \mu \hat{N} | \hat{\Psi} \rangle, \tag{3.1} \]

where \( \mu \) is the chemical potential of the bosons introduced to enforce that the total number of the bosons \( N = \langle \hat{\Psi} | \hat{N} | \hat{\Psi} \rangle \), defined with \( \hat{N} = \int dx \hat{\psi}^\dagger(x) \hat{\psi}(x) \), is conserved. Minimization of (3.1) with respect to the variational parameters leads to the equations of motion of \( \bar{\phi}(x, t) \) and \( \pi(x, t) \), \( G^{-1}(x, y; t) \) and \( \Sigma(x, y; t) \) which can be rewritten for the mean field and the fluctuations.

Alternatively, one can derive the equations of motion written in terms of the mean field and fluctuation directly from: \( i \dot{\Phi} = \delta \langle \hat{H}' \rangle / \delta (\Phi^*) \) and \( i \Phi^* = -\delta \langle \hat{H}' \rangle / \delta \Phi \). Here, \( \langle \hat{H}' \rangle \) is the expectation value of the effective Hamiltonian \( \hat{H}' = \hat{H} - \mu \hat{N} \). Then one finds:

\[ i \dot{\Phi}(x, t) = -\frac{1}{2m} \nabla^2 \Phi(x, t) + (V_{\text{ext}}(x) - \mu) \Phi(x, t) + g |\Phi(x, t)|^2 \Phi(x, t) \]
\[ + 2g \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle \Phi(x, t) + g \langle \dot{\psi}(x) \hat{\psi}(x) \rangle \Phi^*(x, t), \tag{3.2} \]

which is a generalized form of the Gross-Pitaevskii equation (1.2) including the effect of fluctuations.

Our next task is to derive equations of motion for the two-point functions: \( \langle \hat{\psi}^\dagger(x) \hat{\psi}(y) \rangle \) and \( \langle \dot{\psi}(x) \hat{\psi}(y) \rangle \). This can be done from the equations of motion of the kernel functions \( G(x, y, t) \) and \( \Sigma(x, y, t) \). For this purpose we introduce the 2 \( \times \) 2 reduced density matrix defined as

\[ \mathcal{M}(x, y, t) + \frac{1}{2} \delta^3(x - y) = \left( \begin{array}{cc} \langle \hat{\psi}(x) \hat{\psi}^\dagger(y) \rangle & -\langle \dot{\psi}(x) \hat{\psi}(y) \rangle \\ \langle \hat{\psi}^\dagger(x) \hat{\psi}(y) \rangle & -\langle \dot{\psi}^\dagger(x) \hat{\psi}(y) \rangle \end{array} \right). \tag{3.3} \]

Then one can show that the equation of motion for the reduced density matrix \( \mathcal{M} \) is expressed in the form of the Liouville equation:

\[ i \dot{\mathcal{M}} = [ \mathcal{H}, \mathcal{M} ], \tag{3.4} \]

where the Hamiltonian density \( \mathcal{H} \) is defined by

\[ \mathcal{H}(x, y, t) \equiv \delta^3(x - y) \left( \begin{array}{cc} W(x) & \Delta(x) \\ -\Delta^*(x) & -W^*(x) \end{array} \right) \tag{3.5} \]

with

\[ W(x) \equiv -\frac{1}{2m} \nabla^2 x + V_{\text{ext}}(x) - \mu + 2g |\Phi(x, t)|^2 + 2g \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle \]
\[ = W^*(x) \tag{3.6} \]
\[ \Delta(x) \equiv g \langle \dot{\Phi}(x, t)^2 + \langle \dot{\psi}(x) \hat{\psi}(x) \rangle \rangle. \tag{3.7} \]
As we shall show, this equation reproduces the quasiparticle excitations in the Bogoliubov theory when the term induced by the fluctuations are discarded.

Equations (3.2) and (3.4) with (2.11), (3.3), (3.5), (3.6), and (3.7), form a closed set of equations which describe non-linear time evolution of the Bose-Einstein condensate and its fluctuations described by the Gaussian state. They are an extension of the Gross-Pitaevskii equation to include quantum fluctuations.

§4. Inclusion of thermal fluctuations

Foregoing derivation based on the pure state (2.8) can be extended to include thermal fluctuations by introducing statistical average with a Gaussian density matrix for mixed states.\(^{20}\) If the system is near equilibrium, it is equivalent to introduce the density operator in the form:

\[
D(t) = \frac{1}{Z} e^{-\beta \overline{H}(t)} , \quad \text{with} \quad Z = \text{Tr} e^{-\beta \overline{H}(t)} , \tag{4.1}
\]

where \(\beta = 1/k_B T\) is the inverse temperature and \(\overline{H}(t)\) is the (time-dependent) mean field Hamiltonian given by

\[
\overline{H}(t) = \int d^3x \left\{-\frac{1}{2m} \psi^\dagger(x) \nabla^2 \psi(x) + (V_{\text{ext}}(x) - \mu) \psi^\dagger(x) \psi(x) \right. + \frac{g}{2} \left[ \langle \psi^\dagger(x) \psi^\dagger(x) \rangle \psi(x) \psi(x) + \langle \psi(x) \psi(x) \rangle \psi^\dagger(x) \psi^\dagger(x) \right. \\
+ 4 \langle \psi^\dagger(x) \psi(x) \rangle \psi^\dagger(x) \psi(x) \right\}. \tag{4.2}
\]

Here, \(\langle \psi^\dagger(x) \psi(x) \rangle = \Phi^*(x,t) \Phi(x,t) + \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle\), \(\langle \psi^\dagger(x) \psi^\dagger(x) \rangle = \Phi^*(x,t) \Phi^*(x,t) + \langle \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \rangle\) and \(\langle \psi(x) \psi(x) \rangle = \Phi(x,t) \Phi(x,t) + \langle \hat{\psi}(x) \hat{\psi}(x) \rangle\). The mean field and the fluctuations are now defined by

\[
\Phi(x,t) = \langle \psi(x) \rangle = \text{Tr} (D(t) \psi(x)) \tag{4.3}
\]
\[
\langle \hat{\phi}(x) \hat{\phi}(y) \rangle = \text{Tr} \left( D(t) \hat{\phi}(x) \hat{\phi}(y) \right) \quad \text{etc.} \tag{4.4}
\]

One can derive the equation of motion from the Liouville equation of the non-equilibrium density matrix \(D\),

\[
i \frac{\partial D}{\partial t} = [\overline{H}, D] . \tag{4.5}
\]

For example, the equation of motion of the mean field can be obtained from

\[
\frac{\partial \Phi}{\partial t} = i \text{Tr} \left( D(t) \psi(x) \right) = \text{Tr} \left( [\overline{H}, D] \psi(x) \right) = \text{Tr} \left( D \left[ \psi(x), \overline{H} \right] \right) . \tag{4.6}
\]
Upon insertion of the (4.2) to compute the commutator \([\mathcal{H}, \psi(x)]\) we reproduce the generalized Gross-Pitaevskii equation in the form as (3.2) which we have obtained for the pure state evolution. Similarly, by replacing \(\psi(x)\) by \(\hat{\psi}(x)\hat{\psi}(y)\), etc. one can derive the equation of motion for the reduced density matrix \(\mathcal{M}\) defined by (3.3) with (4.4) which becomes precisely the same as the equation (3.4).

We can therefore reinterpret that the equations, (3.2) and (3.4), also describe the non-equilibrium time evolution of the perturbation introduced in the system which has been in equilibrium at temperature \(T\) and the chemical potential \(\mu\).

§5. Static solutions

We first consider the case in which the mean field \(\Phi\) and the fluctuation \(\mathcal{M}\) do not depend on time, that is, the system is in the thermal equilibrium. In this case, the equation of motion for \(\mathcal{M}\) becomes

\[
[\mathcal{H}, \mathcal{M}] = 0 .
\]  

(5.1)

This implies that the Hamiltonian density \(\mathcal{H}\) and the reduced density matrix \(\mathcal{M}\) can be simultaneously diagonalized. This is achieved explicitly by introducing the mode functions.

The mode functions, \(u(x, t)\) and \(v(x, t)\), for the Hamiltonian matrix \(\mathcal{H}\) are defined by:

\[
\begin{pmatrix}
  W(x) & \Delta(x) \\
  -\Delta^*(x) & -W^*(x)
\end{pmatrix}
\begin{pmatrix}
  u(x, t) \\
  v(x, t)
\end{pmatrix} = \begin{pmatrix}
  E_\alpha(u_\alpha(x)) \\
  v_\alpha(x)
\end{pmatrix},
\]  

(5.2)

For the stationary state, we write

\[
\begin{align*}
u(x, t) &= e^{-iEt}u(x), \\
v(x, t) &= e^{-iEt}v(x).
\end{align*}
\]  

(5.3)

The eigenvalue equation is then obtained as

\[
\begin{pmatrix}
  W(x) & \Delta(x) \\
  -\Delta^*(x) & -W^*(x)
\end{pmatrix}
\begin{pmatrix}
  u_\alpha(x) \\
  v_\alpha(x)
\end{pmatrix} = E_\alpha
\begin{pmatrix}
  u_\alpha(x) \\
  v_\alpha(x)
\end{pmatrix},
\]  

(5.4)

where \(\alpha\) represents quantum numbers. By taking a complex conjugate of the above eigenvalue equation, it can be shown that the following equation is also satisfied :

\[
\begin{pmatrix}
  W(x) & \Delta(x) \\
  -\Delta^*(x) & -W^*(x)
\end{pmatrix}
\begin{pmatrix}
  v_\alpha^*(x) \\
  u_\alpha^*(x)
\end{pmatrix} = -E_\alpha
\begin{pmatrix}
  v_\alpha^*(x) \\
  u_\alpha^*(x)
\end{pmatrix}.
\]  

(5.5)

Namely, there exist negative energy solutions. The eigenvector \((u, v)\) is also the eigenvector for the reduced density matrix \(\mathcal{M}\) because \(\mathcal{H}\) and \(\mathcal{M}\) commute :

\[
\int d^3y \left( \mathcal{M}(x, y) + \frac{1}{2}\delta^3(x - y) \right)
\begin{pmatrix}
  u_\alpha(y) \\
  v_\alpha(y)
\end{pmatrix} = (f_\alpha(x) + 1/2)
\begin{pmatrix}
  u_\alpha(x) \\
  v_\alpha(x)
\end{pmatrix}.
\]  

(5.6)

\(^*) These equations describe the coherent, adiabatic evolution of the system, while kinetic aspects (e.g. the growth of the condensate\(^{24-26}\)) are beyond the scope of the present method.
where, by construction (3.3), the eigenvalues of $\mathcal{M}$ are related to the quasi-particle distribution $n_\alpha$ by $^7, ^8$)

$$f_\alpha = n_\alpha + \frac{1}{2}, \quad n_\alpha = \frac{1}{e^{\beta E_\alpha} - 1}.$$  \hspace{1cm} (5.7)

Taking the complex conjugate of the eigenvalue equation for $\mathcal{M} + 1/2$, we also obtain

$$\int d^3 y \left( \mathcal{M}(x, y) + \frac{1}{2} \delta^3(x - y) \right) \left( \begin{array}{c} v_\alpha^*(y) \\ u_\alpha^*(y) \end{array} \right) = -\left( f_\alpha(x) - 1/2 \right) \left( \begin{array}{c} v_\alpha^*(x) \\ u_\alpha^*(x) \end{array} \right).$$  \hspace{1cm} (5.8)

Here the ortho-normalization relation is given by

$$\int d^3 x \left( u_\alpha^*(x) u_\beta(x) - v_\alpha^*(x) v_\beta(x) \right) = \pm \delta_{\alpha \beta}, $$  \hspace{1cm} (5.9)

where $\alpha > 0 (< 0)$ and $\beta > 0 (< 0)$ corresponds to $+$ ($-$) on the right-hand side and it is implied that $\alpha > 0 (< 0)$ represents the positive (negative) energy solution. The reduced density matrix $\mathcal{M}$ can be expressed in terms of the mode functions $u$ and $v$ as

$$\mathcal{M}(x, y) + \frac{1}{2} \delta^3(x - y) = \sum_{\alpha > 0} \left\{ \begin{array}{c} u_\alpha(x) \\ v_\alpha(x) \end{array} \right\} \left( f_\alpha(x) + 1/2 \right) \left( \begin{array}{c} u_\alpha^*(y), & -v_\alpha^*(y) \\ v_\alpha^*(y), & u_\alpha(y) \end{array} \right)$$  \hspace{1cm} (5.10)

Here, summation is taken only over the positive energy eigenstates. This result implies, from the definition (3.3), the matrix elements of the reduced density matrix are expressed in terms of the mode functions and the Bose distribution function $n_\alpha$:

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}(y) \rangle = \sum_{\alpha > 0} \left[ (n_\alpha(x) + 1) v_\alpha(x) v_\alpha^*(y) + n_\alpha(x) u_\alpha^*(x) u_\alpha(y) \right]$$

$$\langle \hat{\psi}(x) \hat{\psi}(y) \rangle = \sum_{\alpha > 0} \left[ (n_\alpha(x) + 1) u_\alpha(x) v_\alpha^*(y) + n_\alpha(x) v_\alpha^*(x) u_\alpha(y) \right]$$

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \rangle = \sum_{\alpha > 0} \left[ (n_\alpha(x) + 1) u_\alpha(x) u_\alpha^*(y) + n_\alpha(x) v_\alpha^*(x) v_\alpha(y) \right]$$

$$\langle \hat{\psi}(x) \hat{\psi}^\dagger(y) \rangle = \sum_{\alpha > 0} \left[ (n_\alpha(x) + 1) u_\alpha(x) u_\alpha^*(y) + n_\alpha(x) v_\alpha^*(x) v_\alpha(y) \right].$$  \hspace{1cm} (5.11)

The equations (3.2), (5.4) and (5.11) with (5.7) form a basic set of equations for the static Bose-Einstein condensates which need to be solved self-consistently.

§6. Uniform condensate

In this section, we consider a simple uniform system, neglecting external confining potential, $V_{\text{ext}} = 0$, in order to illustrate how our method works. In this case, the condensate
is spatially uniform: $\Phi(x) = \Phi_0$ and all mode functions are reduced to simple plane waves. The indices $\alpha$ are regarded as momenta $k$ and the mode functions $u$ and $v$ may be written as

$$u_\alpha \rightarrow u_k(x) = \frac{1}{\sqrt{V}} e^{i k \cdot x} u_k, \quad v_\alpha \rightarrow v_k(x) = \frac{1}{\sqrt{V}} e^{i k \cdot x} v_k,$$

(6.1)

where $V$ is the volume of the system. Further, we take the continuum limit ($V \rightarrow \infty$) with the prescription $\sum_k \rightarrow V/(2\pi)^3 \cdot \int d^3k$ and $\delta_{\alpha\beta} \rightarrow \delta(k-k')$.

The generalized Gross-Pitaevskii equation now takes the form,

$$(-\mu + g|\Phi_0|^2 + 2g\langle \hat{\psi}^\dagger \hat{\psi} \rangle)\Phi_0 + g\langle \hat{\psi}^\dagger \hat{\psi} \rangle \Phi_0^* = 0,$$

(6.2)

where

$$\langle \hat{\psi}^\dagger \hat{\psi} \rangle = \int \frac{d^3k}{(2\pi)^3} [(n_k + 1)|v_k|^2 + n_k|u_k|^2],$$

(6.3)

$$\langle \hat{\psi} \hat{\psi} \rangle = \int \frac{d^3k}{(2\pi)^3} (2n_k + 1) u_kv_k^*,$$

(6.4)

and the mode functions and their eigenvalues are easily obtained from (5.4) as

$$u_k = \frac{\sqrt{W_k + E_k}}{2E_k}, \quad v_k = -\frac{\sqrt{W_k - E_k} \Delta^*}{2E_k |\Delta|},$$

(6.5)

with

$$E_k = \sqrt{W_k^2 - |\Delta|^2},$$

(6.6)

where

$$W_k = \frac{k^2}{2m} - \mu + 2g(|\Phi_0|^2 + \langle \hat{\psi}^\dagger \hat{\psi} \rangle),$$

(6.7)

$$\Delta = g(\Phi_0^2 + \langle \hat{\psi} \hat{\psi} \rangle).$$

(6.8)

Inserting (6.4) into (6.8) and then using (6.5), we obtain the “gap equation” for the anomalous density:

$$\frac{\Delta}{g} = \langle \psi \psi \rangle = \Phi_0^2 + \langle \hat{\psi} \hat{\psi} \rangle,$$

$$= \Phi_0^2 - \Delta \int \frac{d^3k}{(2\pi)^3} n_k + 1/2 \frac{W_k}{E_k}. $$

(6.9)

On the other hand, the particle number density is given by

$$n = \langle \psi^\dagger \psi \rangle = |\Phi_0|^2 + \langle \hat{\psi}^\dagger \hat{\psi} \rangle,$$

$$= |\Phi_0|^2 + \int \frac{d^3k}{(2\pi)^3} (n_k \frac{W_k}{E_k} + \frac{W_k - E_k}{2E_k}),$$

(6.10)
where we have used (6.5) again. Equations, (6.2) and (6.9), together with the constraint (6.10) and with the quasi-particle distribution function (5.7), determine $\Delta$, $\Phi_0$ and $\mu$, self-consistently for a given value of particle density $n$ and temperature $T$.

We can show that the well-known Bogoliubov spectrum of the quasi-particle can be reproduced from (6.6) by removing all fluctuations. For simplicity, we consider the ground state, $n_k = 0$ for all $k \neq 0$ and assume that $\Phi_0$ is real. Then, by setting $\langle \hat{\psi}^\dagger \hat{\psi} \rangle = \langle \hat{\psi} \hat{\psi} \rangle = \langle \hat{\psi}^\dagger \hat{\psi}^\dagger \rangle = 0$, we find

$$\mu = |\Delta| = g|\Phi_0|^2,$$  

(6.11)

and

$$E_k = \sqrt{W_k^2 - |\Delta|^2} = \sqrt{\frac{k^2}{2m} \left( \frac{k^2}{2m} + 2g|\Phi_0|^2 \right)},$$  

(6.12)

where we have used

$$W_k = \frac{k^2}{2m} - \mu + 2g|\Phi_0|^2 = \frac{k^2}{2m} + g|\Phi_0|^2,$$  

(6.13)

which precisely coincides with the Bogoliubov dispersion relation for quasi-particle excitations. For small $|k|$, with $g > 0$, the phonon dispersion relation $\omega = ck$ is obtained, where the sound velocity $c$ is

$$c = \sqrt{\frac{g|\Phi_0|^2}{m}}.$$  

(6.14)

This is the well-known result of the Bogoliubov theory.

The appearance of the phonon dispersion relation is a consequence of spontaneous breakdown of the continuous $U(1)$ symmetry of the Hamiltonian associated with the phase change of the boson field: $\psi(x) \rightarrow e^{i\delta} \psi(x)$. The phonon can be regarded as a Nambu-Goldstone mode of the broken $U(1)$ (or $O(2)$) symmetry.

Our formula (6.6) for the spectrum of the mode functions with the Gaussian fluctuation, however, does not reproduce phonon spectrum, but instead exhibits a gap at $k \rightarrow 0$, violating Goldstone’s theorem. This shortcoming is rather inherent in the Gaussian wave functional approach, *) but this defect can be remedied by computing the excitation spectrum. 8)

We now turn our discussion on the removal of divergences. The expression (6.4) for the fluctuations in the reduced density matrix actually contain a divergent integral, and so does the gap equation (6.9). To see this explicitly, we observe that at large $|k|$, 

$$E_k \simeq W_k - \frac{|\Delta|^2}{2W_k},$$  

(6.15)

*) According to the classification of Hohenberg and Martin27), our approximation corresponds to the conserving (or $\Phi$-derivable28) approximation, as opposed to the gapless approximation 29). The origin of the violation of the Goldstone theorem is traced back to the "Fock" term which may be suppressed by keeping the leading term in the $1/N$ expansion 30) for a system with $O(N)$ symmetry. 31)
so that

\[ u_k \simeq 1 + \frac{|\Delta|^2}{4W_k^2}, \quad v_k \simeq -\frac{\Delta^*}{2W_k}. \quad (6.16) \]

Inserting this expression in (6.4), we find that the off-diagonal component of the density matrix becomes

\[ \langle \hat{\psi} \hat{\psi} \rangle = \int \frac{d^3k}{(2\pi)^3} (2n_k + 1) u_k v_k^* \simeq -\int \frac{d^3k}{(2\pi)^3} (2n_k + 1) \frac{\Delta}{2W_k}, \quad (6.17) \]

which indeed contains a linearly divergent integral,

\[ \langle \hat{\psi} \hat{\psi} \rangle_{\text{div.}} = -\Delta \int \frac{d^3k}{(2\pi)^3} \frac{m}{k^2}. \quad (6.18) \]

This divergent integral is associated with the diagram shown in Fig. 3. It originates from a repeated use of the effective potential as we have mentioned in the introduction. This divergence should be removed in order to avoid the double counting of the perturbation series in terms of the bare potential. Therefore we define the renormalized density matrix by subtracting the divergent term:

\[ \langle \hat{\psi} \hat{\psi} \rangle_{\text{ren.}} = \langle \hat{\psi} \hat{\psi} \rangle - \langle \hat{\psi} \hat{\psi} \rangle_{\text{div.}}. \quad (6.19) \]

This procedure is equivalent to replace the gap equation by:

\[ \frac{\Delta}{g} = \phi_0^2 - \Delta \int \frac{d^3k}{(2\pi)^3} \left( \frac{n_k + 1/2}{E_k} - \frac{m}{k^2} \right). \quad (6.20) \]

With this replacement and all other relations untouched, all divergences associated with double counting of the pair scatterings are removed from the previous equations. The “renormalized gap equation” (6.20) is one of our new findings in this paper.

\[ \S 7. \quad \text{Summary} \]

In this paper we have formulated the variational method to describe the dynamics of the Bose-Einstein condensate interacting via short-range effective interaction. With the Gaussian variational wave functional we have derived the equations of motion which consist
of a generalized Gross-Pitaevskii equation for the condensate and a Liouville-von Neumann equation for the density matrix of the quantum and thermal fluctuations. The static solutions of these equations are examined in terms of the mode functions for the fluctuations. In the case of uniform condensate, these mode functions are reduced to simple plane waves, and we are able to perform the calculation explicitly. We have shown that the spectrum of the mode functions reduces to the Bogoliubov phonon spectrum when we neglect the effect of quantum fluctuations; it does not contain however phonon mode in the presence of quantum fluctuation. In these calculations we have shown that the divergent integrals which arise due to the use of singular effective interaction can be eliminated systematically by removing the repeated pair scattering terms to avoid the double counting of the diagrams in terms of the bare interaction. In the forthcoming paper, we will show how to apply the present method to compute the linear response of the system to external perturbation and to extract the phonon dispersion relation of the collective excitations in the system.

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