

Bose-Einstein Condensation in an External Potential I

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Abstract

The theory of Bose-Einstein condensation for a dilute gas with short-range pairwise repulsive interaction is developed when an external potential is present. At low temperatures when the Bose-Einstein condensation is nearly complete, a partial differential equation is obtained for the condensate wave function and an integro-differential equation for the pair excitation.

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I. INTRODUCTION

A most interesting development in physics last year was the first experimental observation of Bose-Einstein condensation [1,2] in dilute atomic gases [3–5]. From the point of view of statistical mechanics in general and Bose-Einstein condensation in particular, a novel feature of these experiments is the presence of a trap which supplies an external potential that keeps the atomic gas together. It is the purpose of this and the following papers to study Bose-Einstein condensation in the presence of such an external potential.

In the fifties and early sixties, there was a systematic effort to study theoretically the properties of a dilute Bose gas with short-range repulsion [6–15]. In most of these papers, periodic boundary conditions are assumed and play an important role. The case of the rigid wall where the wave function vanishes is briefly mentioned by Lee, Huang, and Yang [9] and studied further in Ref. [15]. Since such a rigid wall is described by an infinite potential, this case can be considered to be an example of an external potential. Accordingly, the method of Ref. [15] is to be generalized to treat the present case of the Bose-Einstein condensation in an external potential. This Paper I and the following Paper II are devoted to the study of the simplest situation where the Bose-Einstein condensation is nearly 100%.

II. THE CONDENSATE

When there is no external potential and the periodic boundary condition applies, the condensate is the zero-momentum state. In other words, the single-particle zero-momentum state has a macroscopic occupation number. Clearly, the first question to be answered is: In the presence of an external potential, what is the condensate wave function?

Consider a system of N pairwise interacting particles in an external potential V_e . The Hamiltonian is ($\hbar = 2m = 1$)

$$\sum_{i=1}^N p_i^2 + \sum_{i<j} V_0(r_{ij}) + \sum_{i=1}^N V_e(\mathbf{r}_i), \quad (2.1)$$

where

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|, \quad (2.2)$$

and V_0 is a short-range repulsive potential with scattering length $a > 0$. For example, V_0 may be the hard-sphere potential which is zero for $r_{ij} > a$ and infinite for $r_{ij} < a$. When the method of pseudopotential of Huang and Yang [6] is applied, the Hamiltonian (2.1) is replaced approximately by

$$H' = T + V', \quad (2.3)$$

with

$$T = \sum_i [p_i^2 + V_e(\mathbf{r}_i)] \quad (2.4)$$

and

$$V' = 4\pi a \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j) \frac{\partial}{\partial r_{ij}} r_{ij}. \quad (2.5)$$

For the present purpose, it is sufficient to use

$$H = T + V, \quad (2.6)$$

where

$$V = 4\pi a \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j). \quad (2.7)$$

The only difficulty involved in using H instead of H' is the appearance of a familiar type of divergence, which may be removed using the procedure of Refs. [9] and [11].

It is convenient to rewrite this H in the language of quantized fields:

$$T = \int d\mathbf{r} [|\nabla\psi(\mathbf{r})|^2 + V_e(\mathbf{r})|\psi(\mathbf{r})|^2] \quad (2.8)$$

and

$$V = 4\pi a \int d\mathbf{r} \psi^*(\mathbf{r})^2 \psi(\mathbf{r})^2, \quad (2.9)$$

where $\psi(\mathbf{r})$ satisfies the usual commutation rules for a boson field.

Let $\Phi(\mathbf{r})$ be the wave function of the condensate, normalized by

$$\Omega^{-1} \int d\mathbf{r} |\Phi(\mathbf{r})|^2 = 1, \quad (2.10)$$

where Ω is the volume of the box. The creation and annihilation operators for this condensate are

$$a_0^* = \Omega^{-1/2} \int d\mathbf{r} \Phi(\mathbf{r}) \psi^*(\mathbf{r}), \quad a_0 = \Omega^{-1/2} \int d\mathbf{r} \Phi^*(\mathbf{r}) \psi(\mathbf{r}). \quad (2.11)$$

They, of course, satisfy

$$[a_0, a_0^*] = 1. \quad (2.12)$$

With the parts of $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$ corresponding to this Φ singled out, define $\psi_1^*(\mathbf{r})$ and $\psi_1(\mathbf{r})$ by

$$\psi^*(\mathbf{r}) = \Omega^{-1/2} \Phi^*(\mathbf{r}) a_0^* + \psi_1^*(\mathbf{r}), \quad \psi(\mathbf{r}) = \Omega^{-1/2} \Phi(\mathbf{r}) a_0 + \psi_1(\mathbf{r}). \quad (2.13)$$

Since this state Φ is macroscopically occupied, for low densities these ψ_1^* and ψ_1 may be considered to be a small perturbation [9,15]. Moreover, at low temperatures very near zero, the relation

$$N = \int d\mathbf{r} \psi^*(\mathbf{r}) \psi(\mathbf{r}) = a_0^* a_0 + \int d\mathbf{r} \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \quad (2.14)$$

may be approximated by

$$N \sim a_0^* a_0. \quad (2.15)$$

This means that the Bose-Einstein condensation is nearly 100%.

To first order in $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$, the T and V are approximated by

$$\begin{aligned} T_1 &= N(\bar{\zeta} + \zeta_e) + \Omega^{-1/2} a_0 \int d\mathbf{r} [-\nabla^2 \Phi(\mathbf{r}) + V_e(\mathbf{r}) \Phi(\mathbf{r})] \psi_1^*(\mathbf{r}) \\ &\quad + \Omega^{-1/2} a_0^* \int d\mathbf{r} [-\nabla^2 \Phi^*(\mathbf{r}) + V_e(\mathbf{r}) \Phi^*(\mathbf{r})] \psi_1(\mathbf{r}) \end{aligned} \quad (2.16)$$

and

$$\begin{aligned} V_1 &= \frac{4\pi a N}{\Omega} \left\{ N\zeta + 2\Omega^{-1/2} a_0 \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \Phi(\mathbf{r}) \psi_1^*(\mathbf{r}) \right. \\ &\quad \left. + 2\Omega^{-1/2} a_0^* \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \Phi^*(\mathbf{r}) \psi_1(\mathbf{r}) \right\}, \end{aligned} \quad (2.17)$$

where

$$\bar{\zeta} = \Omega^{-1} \int d\mathbf{r} |\nabla \Phi(\mathbf{r})|^2, \quad \zeta = \Omega^{-1} \int d\mathbf{r} |\Phi(\mathbf{r})|^4, \quad \zeta_e = \Omega^{-1} \int d\mathbf{r} V_e(\mathbf{r}) |\Phi(\mathbf{r})|^2. \quad (2.18)$$

Note that eq. (2.17) here is identical to eq. (2.14) of Ref. [15], but T_1 is modified by the presence of the external potential $V_e(\mathbf{r})$.

Since the Hamiltonian $T_1 + V_1$ is linear in $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$, it is a simple matter to take a Schrödinger state vector of the form

$$\Psi = (N!)^{-1/2} a_0^{*N} |\text{vac}\rangle, \quad (2.19)$$

where $|\text{vac}\rangle$ is defined by

$$\psi(\mathbf{r}) |\text{vac}\rangle = 0. \quad (2.20)$$

The Schrödinger equation for Ψ ,

$$(T_1 + V_1)\Psi = NE\Psi, \quad (2.21)$$

then leads to a non-linear Schrödinger equation for $\Phi(\mathbf{r})$:

$$\left[-\nabla^2 + V_e(\mathbf{r}) + \frac{8\pi a N}{\Omega} |\Phi(\mathbf{r})|^2 - \frac{4\pi a N}{\Omega} \zeta - E \right] \Phi(\mathbf{r}) = 0. \quad (2.22)$$

This is the desired equation for the condensate wave function in the presence of the external potential $V_e(\mathbf{r})$.

Note that eq. (2.22) differs from the non-linear Schrödinger equation (2.21) of Ref. [15] only in the addition of the term $V_e(\mathbf{r})$ due to the external potential. This $V_e(\mathbf{r})$ does not lead to any complication in the derivation of (2.22); for a more detailed discussion, see Appendix A of Ref. [15].

There are two basic lengths in eq. (2.22): (i) the length over which $V_e(\mathbf{r})$ varies; and (ii) the length scale determined by $(4\pi a N/\Omega) |\Phi(\mathbf{r})|^2$. It is the interplay between these two lengths that is responsible for some of the interesting properties of this non-linear Schrödinger equation. The simplest example of this interplay is the case of the rigid boundary [9,15]. Some further cases are studied in Sec. III.

III. PAIR PRODUCTION

In the absence of an external potential, pair production of particles with opposite momenta plays an important role [9,10,15]. In Appendix A here, the procedure of dealing with pair production as discussed by Lee, Huang, and Yang in Appendix I of Ref. [9] is recast in a form more suitable for generalization to the present case.

Equations (2.16) and (2.17) give approximations to the T and V of (2.8) and (2.9) to the first order in $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$. In order to study pair production, what is needed is the second-order approximation to T and V . Here (2.15) for N is no longer accurate enough, and (2.14) needs to be used. Thus,

$$\begin{aligned}
T &= N(\bar{\zeta} + \zeta_e) + \Omega^{-1/2} a_0 \int d\mathbf{r} [-\nabla^2 \Phi(\mathbf{r}) + V_e(\mathbf{r})\Phi(\mathbf{r})] \psi_1^*(\mathbf{r}) \\
&\quad + \Omega^{-1/2} a_0^* \int d\mathbf{r} [-\nabla^2 \Phi^*(\mathbf{r}) + V_e(\mathbf{r})\Phi^*(\mathbf{r})] \psi_1(\mathbf{r}) \\
&\quad + \int d\mathbf{r} [|\nabla \psi_1(\mathbf{r})|^2 + V_e(\mathbf{r})\psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) - (\bar{\zeta} + \zeta_e)\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})]
\end{aligned} \tag{3.1}$$

and

$$\begin{aligned}
V_2 &= \frac{4\pi a N}{\Omega} \left[N\bar{\zeta} + 2\Omega^{-1/2} a_0 \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \Phi(\mathbf{r})\psi_1^*(\mathbf{r}) \right. \\
&\quad + 2\Omega^{-1/2} a_0^* \int d\mathbf{r} |\Phi(\mathbf{r})|^2 \Phi^*(\mathbf{r})\psi_1(\mathbf{r}) \\
&\quad + \int d\mathbf{r} \{ [-2\bar{\zeta} + 4|\Phi(\mathbf{r})|^2] \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) \\
&\quad \left. + N^{-1} a_0^2 \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 + N^{-1} a_0^{*2} \Phi^*(\mathbf{r})^2 \psi_1(\mathbf{r})^2 \} \right].
\end{aligned} \tag{3.2}$$

The first terms in (3.1) and (3.2) are constants, while the sum of those terms involving a factor of $\Omega^{-1/2}$ also leads to a constant by virtue of the non-linear Schrödinger equation (2.22) for $\Phi(\mathbf{r})$. We therefore concentrate on the terms that are quadratic in $\psi_1^*(\mathbf{r})$ and $\psi_1(\mathbf{r})$:

$$\begin{aligned}
H_2 &= \int d\mathbf{r} \left\{ |\nabla \psi_1(\mathbf{r})|^2 + \left[-\bar{\zeta} - \zeta_e - \frac{8\pi a N}{\Omega} \bar{\zeta} + V_e(\mathbf{r}) \right] \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) \right. \\
&\quad \left. + \frac{4\pi a N}{\Omega} [4|\Phi(\mathbf{r})|^2 \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) + N^{-1} a_0^2 \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 + N^{-1} a_0^{*2} \Phi^*(\mathbf{r})^2 \psi_1(\mathbf{r})^2] \right\}.
\end{aligned} \tag{3.3}$$

This is a quadratic form in $\psi_1^*(\mathbf{r})$ and $\psi_1(\mathbf{r})$.

Following the procedure in Appendix A, define

$$H'_2 = e^{-P} H_2 e^P, \tag{3.4}$$

where [15]

$$P = (2N)^{-1} \int d\mathbf{r} d\mathbf{r}' \psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') a_0^2. \tag{3.5}$$

Without loss of generality, choose K_0 to satisfy

$$K_0(\mathbf{r}, \mathbf{r}') = K_0(\mathbf{r}', \mathbf{r}) \quad (3.6)$$

and

$$\int d\mathbf{r} \Phi^*(\mathbf{r}) K_0(\mathbf{r}, \mathbf{r}') = 0. \quad (3.7)$$

Since it follows from (2.13) that

$$[\psi_1(\mathbf{r}), \psi_1^*(\mathbf{r}')] = \delta^3(\mathbf{r} - \mathbf{r}') - \Omega^{-1} \Phi(\mathbf{r}) \Phi^*(\mathbf{r}'), \quad (3.8)$$

it is straightforward to verify that

$$[\psi_1(\mathbf{r}), e^P] = N^{-1} \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}') e^P a_0^2, \quad (3.9)$$

$$[\psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}), e^P] = N^{-1} \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') e^P a_0^2, \quad (3.10)$$

$$[|\nabla \psi_1(\mathbf{r})|^2, e^P] = N^{-1} \int d\mathbf{r}' \nabla_r K_0(\mathbf{r}, \mathbf{r}') \cdot \nabla_r \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}') e^P a_0^2, \quad (3.11)$$

and

$$\begin{aligned} [\psi_1(\mathbf{r})^2, e^P] = & N^{-1} e^P \left[K_0(\mathbf{r}, \mathbf{r}) + 2 \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \right. \\ & \left. + N^{-1} \int d\mathbf{r}' d\mathbf{r}'' K_0(\mathbf{r}, \mathbf{r}') K_0(\mathbf{r}, \mathbf{r}'') \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}'') a_0^2 \right] a_0^2. \end{aligned} \quad (3.12)$$

Using these commutation relations, the H'_2 of (3.4) is given by

$$H'_2 = H_2 + e^{-P} [H, e^P] = H''_2 + H'_{2c}, \quad (3.13)$$

where

$$\begin{aligned} H''_2 = & \int d\mathbf{r} \left\{ |\nabla \psi_1(\mathbf{r})|^2 + \left[-\bar{\zeta} - \frac{8\pi a N}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) \right] \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \right. \\ & + \frac{4\pi a N}{\Omega} [4|\Phi(\mathbf{r})|^2 \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + N^{-1} \Phi^*(\mathbf{r})^2 a_0^2 \psi_1(\mathbf{r})^2] \\ & \left. + \Phi^*(\mathbf{r})^2 \frac{4\pi a N}{\Omega} \left[K_0(\mathbf{r}, \mathbf{r}) + 2 \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}') \right] \right\}, \end{aligned} \quad (3.14)$$

and H'_{2c} contains all the terms that are quadratic in $\psi_1^*(\mathbf{r})$ and hence no $\psi_1(\mathbf{r})$:

$$\begin{aligned} H'_{2c} = & N^{-1} \int d\mathbf{r} \left\{ \frac{4\pi a N}{\Omega} \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 - \int d\mathbf{r}' [\nabla_r^2 K_0(\mathbf{r}, \mathbf{r}')] \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') \right. \\ & + \left[-\bar{\zeta} - \frac{8\pi a N}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) \right] \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') \\ & + \frac{4\pi a N}{\Omega} \left[4|\Phi(\mathbf{r})|^2 \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') \right. \\ & \left. \left. + \Phi^*(\mathbf{r})^2 \int d\mathbf{r}' d\mathbf{r}'' K_0(\mathbf{r}, \mathbf{r}') K_0(\mathbf{r}, \mathbf{r}'') \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}'') \right] \right\} a_0^2. \end{aligned} \quad (3.15)$$

Similar to (3.5)–(3.7), define $L(\mathbf{r}, \mathbf{r}')$ by

$$H'_{2c} = (2N)^{-1} \int d\mathbf{r} d\mathbf{r}' L(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') a_0^2, \quad (3.16)$$

$$L(\mathbf{r}, \mathbf{r}') = L(\mathbf{r}', \mathbf{r}), \quad (3.17)$$

and

$$\int d\mathbf{r} \Phi^*(\mathbf{r}') L(\mathbf{r}, \mathbf{r}') = 0. \quad (3.18)$$

As a generalization of (A4) in Appendix A, the pair-production distribution $K_0(\mathbf{r}, \mathbf{r}')$ is determined by the condition

$$L(\mathbf{r}, \mathbf{r}') = 0. \quad (3.19)$$

It only remains to rewrite (3.19) in the form of an integro-differential equation for $K_0(\mathbf{r}, \mathbf{r}')$:

$$\begin{aligned} L(\mathbf{r}, \mathbf{r}') &= -\nabla^2 K_0(\mathbf{r}, \mathbf{r}') - \nabla'^2 K_0(\mathbf{r}, \mathbf{r}') + \frac{8\pi a N}{\Omega} \Phi(\mathbf{r})^2 \delta(\mathbf{r} - \mathbf{r}') \\ &+ \left\{ -2\bar{\zeta} - \frac{16\pi a N}{\Omega} \zeta - 2\zeta_e + V_e(\mathbf{r}) + V_e(\mathbf{r}') + \frac{16\pi a N}{\Omega} [|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2] \right\} K_0(\mathbf{r}, \mathbf{r}') \\ &+ \frac{8\pi a N}{\Omega} \int d\mathbf{r}'' \Phi^*(\mathbf{r}'')^2 K_0(\mathbf{r}, \mathbf{r}'') K_0(\mathbf{r}', \mathbf{r}'') - \lambda(\mathbf{r}) \Phi(\mathbf{r}') - \lambda(\mathbf{r}') \Phi(\mathbf{r}) \\ &= 0, \end{aligned} \quad (3.20)$$

where $\lambda(\mathbf{r})$ is to be determined by (3.18).

This determination is carried out by multiplying by $\Phi^*(\mathbf{r}')$ and then integrating over \mathbf{r}' . An integration by parts gives

$$\begin{aligned} &\int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \left[-\nabla'^2 + V_e(\mathbf{r}') + \frac{16\pi a N}{\Omega} |\Phi(\mathbf{r}')|^2 \right] \Phi^*(\mathbf{r}') + \frac{8\pi a N}{\Omega} |\Phi(\mathbf{r})|^2 \Phi(\mathbf{r}) \\ &= \lambda(\mathbf{r}) \Omega + \Phi(\mathbf{r}) \int d\mathbf{r}' \Phi^*(\mathbf{r}') \lambda(\mathbf{r}'). \end{aligned} \quad (3.21)$$

Equation (2.22) may be used to give

$$\lambda(\mathbf{r}) = \frac{8\pi a N}{\Omega^2} \left[|\Phi(\mathbf{r})|^2 \Phi(\mathbf{r}) + \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') |\Phi(\mathbf{r}')|^2 \Phi^*(\mathbf{r}') - \frac{1}{2} \zeta \Phi(\mathbf{r}) \right]. \quad (3.22)$$

For completeness, we write down explicitly the integro-differential equation for $K_0(\mathbf{r}, \mathbf{r}')$:

$$\begin{aligned} &-\nabla^2 K_0(\mathbf{r}, \mathbf{r}') - \nabla'^2 K_0(\mathbf{r}, \mathbf{r}') + \frac{8\pi a N}{\Omega} \Phi(\mathbf{r})^2 \delta(\mathbf{r} - \mathbf{r}') \\ &+ \left\{ -2\bar{\zeta} - \frac{16\pi a N}{\Omega} \zeta - 2\zeta_e + V_e(\mathbf{r}) + V_e(\mathbf{r}') + \frac{16\pi a N}{\Omega} [|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2] \right\} K_0(\mathbf{r}, \mathbf{r}') \\ &+ \frac{8\pi a N}{\Omega} \int d\mathbf{r}'' \Phi^*(\mathbf{r}'')^2 K_0(\mathbf{r}, \mathbf{r}'') K_0(\mathbf{r}', \mathbf{r}'') \\ &= \frac{8\pi a N}{\Omega^2} \left\{ \Phi(\mathbf{r}) \Phi(\mathbf{r}') [|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2 - \zeta] \right. \\ &\quad \left. + \Phi(\mathbf{r}) \int d\mathbf{r}'' K_0(\mathbf{r}', \mathbf{r}'') |\Phi(\mathbf{r}'')|^2 \Phi^*(\mathbf{r}'') + \Phi(\mathbf{r}') \int d\mathbf{r}'' K_0(\mathbf{r}, \mathbf{r}'') |\Phi(\mathbf{r}'')|^2 \Phi^*(\mathbf{r}'') \right\}. \end{aligned} \quad (3.23)$$

IV. LOW-LYING EXCITATIONS

When (3.23) is satisfied, $H'_{2c} = 0$ and hence

$$H'_2 = H''_2. \quad (4.1)$$

From (3.14), H''_2 contains three types of terms:

i) a constant

$$\frac{4\pi aN}{\Omega} \int d\mathbf{r} \Phi^*(\mathbf{r})^2 K_0(\mathbf{r}, \mathbf{r});$$

ii) a pair interaction that creates two condensate particles

$$\frac{4\pi a}{\Omega} a_0^{*2} \int d\mathbf{r} \Phi^*(\mathbf{r})^2 \psi_1(\mathbf{r})^2; \quad \text{and}$$

iii) the rest of the terms.

Terms of the types i) and ii) have no effect on the energies of the low-lying excitations. It is therefore useful to consider terms of type iii) first:

$$\begin{aligned} H_2''' = \int d\mathbf{r} \left\{ |\nabla \psi_1(\mathbf{r})|^2 + \left[-\bar{\zeta} - \frac{8\pi aN}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) + \frac{16\pi aN}{\Omega} |\Phi(\mathbf{r})|^2 \right] \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) \right. \\ \left. + \frac{8\pi aN}{\Omega} \Phi^*(\mathbf{r})^2 \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \right\}. \end{aligned} \quad (4.2)$$

Since this H_2''' is linear in $\psi_1^*(\mathbf{r})$ and also linear in $\psi_1(\mathbf{r})$, the excitations can be described by a creation operator of the form

$$a^* = \int d\mathbf{r} \varphi(\mathbf{r}) \psi_1^*(\mathbf{r}), \quad (4.3)$$

where $\varphi(\mathbf{r})$ is a c -number wave function for the excitation. Similar to (3.7) and (3.18), it is convenient to choose $\varphi(\mathbf{r})$ so that

$$\int d\mathbf{r} \Phi^*(\mathbf{r}) \varphi(\mathbf{r}) = 0. \quad (4.4)$$

This wave function $\varphi(\mathbf{r})$ is determined by

$$[H_3''', a^*] = \lambda a^*, \quad (4.5)$$

where λ is the energy of the excitation. This is the generalization of the phonon spectrum. It follows from (4.5) that $\varphi(\mathbf{r})$ satisfies the linear integro-differential equation

$$\begin{aligned} \left[-\nabla^2 - \bar{\zeta} - \frac{8\pi aN}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) + \frac{16\pi aN}{\Omega} |\Phi(\mathbf{r})|^2 \right] \varphi(\mathbf{r}) \\ + \frac{8\pi aN}{\Omega} \int d\mathbf{r}' K_0(\mathbf{r}, \mathbf{r}') \Phi^*(\mathbf{r}')^2 \varphi(\mathbf{r}') \\ = \lambda \varphi(\mathbf{r}) + \mu \Phi(\mathbf{r}), \end{aligned} \quad (4.6)$$

where μ is to be determined so that (4.4) is satisfied

$$\mu = \Omega^{-1} \int d\mathbf{r} \Phi^*(\mathbf{r}) \left[-\nabla^2 + V_e(\mathbf{r}) + \frac{16\pi aN}{\Omega} |\Phi(\mathbf{r})|^2 \right] \varphi(\mathbf{r}). \quad (4.7)$$

Note that (4.6) describes a low-lying excitation due to the addition of a boson to the system.

V. CONCLUSION

Using the method of the pseudo-potential as applied to many-body problems [6,7], the effects of an external potential have been incorporated in the theory of Bose-Einstein condensation for a dilute gas with short-range pairwise repulsive interaction. The condensate wave function $\Phi(\mathbf{r})$ is found first by solving the non-linear Schrödinger equation (2.22); the pair production as described by $K_0(\mathbf{r}, \mathbf{r}')$ of (3.5) is then determined by the non-linear integro-differential equation (3.23); and finally, the wave function $\varphi(\mathbf{r})$ for low-lying excitations is governed by (4.7) here.

As is often the case for a dilute boson gas, the expansion parameter is typically $(Na^3/\Omega)^{1/2}$. In terms of this expansion parameter, (2.22) and (3.5) give essentially the leading order and the next-to-leading order description of the system. Extension to higher orders, where the logarithm of this expansion parameter will appear, has not been accomplished.

This present work has been motivated by the beautiful experiments on Bose-Einstein condensation in dilute atomic gases [3–5]. In the following paper, the results obtained here will be applied to the case where the external potential is a trap to keep the atoms together.

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APPENDIX A

Consider the Hamiltonian

$$H = \frac{1}{2} (a^* a + b^* b) + y(a^* b^* + ab), \quad (\text{A1})$$

where (a^*, a) and (b^*, b) are a pair of independent creation and annihilation boson operators. Let us calculate

$$H' = e^{\alpha a^* b^*} H e^{-\alpha a^* b^*}, \quad (\text{A2})$$

where the constant α remains to be chosen. This H' is of course not hermitian. The result is

$$H' = \left(\frac{1}{2} - \alpha y\right)(a^* a + b^* b) + yab - \alpha y + (y - \alpha + \alpha^2 y)a^* b^*. \quad (\text{A3})$$

Let α be chosen such that the coefficient of $a^* b^*$ vanishes:

$$y - \alpha + \alpha^2 y = 0. \quad (\text{A4})$$

This gives

$$\alpha = \frac{1}{2y} [1 - (1 - 4y^2)^{1/2}], \quad (\text{A5})$$

which is (A12) of Lee, Huang, and Yang [9]. With this α , H' is

$$H' = -\frac{1}{2} + \frac{1}{2} (1 - 4y^2)^{1/2} (a^* a + b^* b + 1) + yab. \quad (\text{A6})$$

Since the last term yab has no effect on the energy spectrum, H' leads immediately to the ground-state energy per particle and the phonons.

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