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Bose-Einstein condensation in an external potential at zero temperature: General theory

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Bose-Einstein condensation is described in terms of the condensate wave function and the pair-excitation function, the latter being responsible for the existence of phonons. This minimal description in terms of these two functions is generalized to the case with an external potential. For a dilute gas with short-range pairwise repulsive interaction and at very 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. Experimentally, the external potential is used to trap the atoms, i.e., to keep them together. Since the trap is of macroscopic dimensions, the resulting external potential is often slowly varying. In these cases and when the condensate is in the lowest state, the partial differential equation for the condensate wave function and the integro-differential equation for the pair excitation are solved approximately for the case of a time-independent trap. [S1050-2947(98)04208-5]

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I. INTRODUCTION

Over a year ago, in a remarkable paper [1], Anderson, Ensher, Matthews, Wieman, and Cornell reported the first experimental observation of Bose-Einstein condensation in a weakly interacting system. The system used is a vapor of rubidium-87 atoms confined by a magnetic trap. Several similar experiments on various atomic vapors followed soon after [2].

From the theoretical point of view, the most important implication of the presence of the trap is that there is no translational invariance. Thirty-five years ago, Bose-Einstein condensation without translational invariance was treated for a low-density system of hard spheres at zero temperature [3]. It is the purpose of the present investigation to apply that approach to these recent cases of interest where a trap is present.

The key idea of the approach in Ref. [3] is the following. Let $\Phi(\mathbf{r},t)$ be the wave function for the Bose-Einstein condensate at time t, while $a_0^*(t)$ and $a_0(t)$ are the corresponding creation and annihilation operators for this $\Phi(\mathbf{r},t)$. Then the terms in the Hamiltonian due to boson-boson pair interaction are classified according to the number n of times that $a_0^*(t)$ and $a_0(t)$ appear, where this n can be 4, 3, 2, 1, or 0. To the first approximation, the equation of motion for $\Phi(\mathbf{r},t)$ is determined by the terms with $n=3$. In the usual case where the Bose-Einstein condensate is in the single-particle zero-momentum state, these $n=3$ terms are absent. See also Sec. II.

When the condensate is in the zero-momentum state, it is known that pair excitation plays an important role [4]. This is the process where two zero momentum bosons in the Bose-Einstein condensate scatter from each other to produce a pair of bosons of opposite momenta. In particular, from the atomic point of view, this is the process that is responsible for the existence of phonons and sound vibrations in a superfluid. When translational invariance does not hold, pair excitation remains equally important; however, since there is no pairing of equal but opposite momenta, this process is much more complicated [3]. The pair-excitation function, to be discussed in Sec. III, satisfies an integro-differential equation involving the external potential.

Experimentally, the external potential is used to keep a large number N of atoms together. It is therefore necessary to use this N for normalization. This is carried out in Sec. IV. Such external potentials are often time-independent and spatially slowly varying. When the condensate is in the lowest state, both the condensate wave function and the pair-excitation function can be found explicitly by solving approximately the nonlinear Schrödinger equation and the integro-differential equation of Secs. II and III. This is carried out in Sec. V.

This paper is devoted to the study of the simplest situation where the temperature is sufficiently low that the Bose-Einstein condensation is nearly 100%. The technique used here can be combined with the pioneering work of Lee and Yang [5] to treat the case where the Bose-Einstein condensation is less than 100%, i.e., the case where the superfluid and the normal fluid coexist. This is going to be presented in a later paper.

II. THE CONDENSATE

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

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

where

$$r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|, \tag{2.2}$$

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 $r_{ij}<a$. The external potential $V_e(\mathbf{r},t)$ may have explicit dependence on the time t.

In the late 1950s, Huang and Yang [6] initiated the application of the method of pseudopotentials to many-body problems. This method developed rapidly within a few years [7–9]. When this method is used, the Hamiltonian (2.1) is replaced approximately by

$$H' = T + V', \tag{2.3}$$

with

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

and

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

For the present purpose, it is sufficient to use

$$H = T + V, \tag{2.6}$$

where

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

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. [4] and [8].

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

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

and

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

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

Let $\Phi(\mathbf{r}, t)$ be the wave function at time t for the Bose-Einstein condensate, i.e., the wave function for the state that is macroscopically occupied. For the case under consideration, this macroscopic occupation is nearly 100%. In general, this wave function $\Phi(\mathbf{r}, t)$ depends on t and is complex. It is normalized by

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

for all t, where Ω is the volume of the box, and the creation and annihilation operators for this condensate state are

$$\begin{aligned} a_0^*(t) &= \Omega^{-1/2} \int d\mathbf{r} \; \Phi(\mathbf{r}, t) \psi^*(\mathbf{r}), \\ a_0(t) &= \Omega^{-1/2} \int d\mathbf{r} \; \Phi^*(\mathbf{r}, t) \psi(\mathbf{r}). \end{aligned} \tag{2.11}$$

Since $\Phi(\mathbf{r}, t)$ is in general time-dependent, so are $a_0^*(t)$ and $a_0(t)$. They, of course, satisfy the commutation rule

$$[a_0(t), a_0^*(t)] = 1 \tag{2.12}$$

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

$$\begin{aligned} \psi^*(\mathbf{r}) &= \Omega^{-1/2} \Phi^*(\mathbf{r}, t) a_0^*(t) + \psi_1^*(\mathbf{r}, t), \\ \psi(\mathbf{r}) &= \Omega^{-1/2} \Phi(\mathbf{r}, t) a_0(t) + \psi_1(\mathbf{r}, t). \end{aligned} \tag{2.13}$$

Since this state Φ is macroscopically occupied, for low densities these ψ_1^* and ψ_1 may be considered to be a small perturbation [3,4]. Moreover, at low temperatures very near zero, the relation

$$\begin{aligned} N &= \int d\mathbf{r} \; \psi^*(\mathbf{r}) \psi(\mathbf{r}) \\ &= a_0^*(t) a_0(t) + \int d\mathbf{r} \; \psi_1^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \end{aligned} \tag{2.14}$$

may be approximated by

$$N \sim a_0^*(t) a_0(t). \tag{2.15}$$

Clearly this approximation can be used only when the Bose-Einstein condensation is nearly complete.

To first order in $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$, the T and V of Eqs. (2.4) and (2.7) are approximated by

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

and

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

where

$$\begin{aligned} \overline{\zeta}(t) &= \Omega^{-1} \int d\mathbf{r} |\nabla \Phi(\mathbf{r}, t)|^2, \\ \zeta(t) &= \Omega^{-1} \int d\mathbf{r} |\Phi(\mathbf{r}, t)|^4, \\ \zeta_e(t) &= \Omega^{-1} \int d\mathbf{r} \; V_e(\mathbf{r}, t) |\Phi(\mathbf{r}, t)|^2. \end{aligned} \tag{2.18}$$

Note that Eq. (2.17) here is identical to Eq. (2.14) of Ref. [3], but T_1 is modified by the presence of the external potential $V_e(\mathbf{r},t)$.

Since the Hamiltonian T_1+V_1 is linear in $\psi_1^*(\mathbf{r},t)$ and $\psi_1(\mathbf{r},t)$, it is a simple matter to take a Schrödinger state vector of the form

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

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

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

The Schrödinger equation for Ψ,

$$(T_1+V_1)\Psi(t)=i(\partial/\partial t)\Psi(t), \tag{2.21}$$

then leads to a nonlinear Schrödinger equation for $\Phi(\mathbf{r},t)$:

$$i\left(\frac{\partial}{\partial t}\right)\Phi(\mathbf{r},t)=\left(-\nabla^2+V_e(\mathbf{r},t)+\frac{8\pi aN}{\Omega}|\Phi(\mathbf{r},t)|^2 -\frac{4\pi aN}{\Omega}\zeta(t)\right)\Phi(\mathbf{r},t). \tag{2.22}$$

This is essentially Eq. (2.21) of Ref. [3]. See also the papers of Pitaevskii [10] and Gross [11].

In the time-independent case, $\Phi(\mathbf{r},t)$ takes the form

$$\Phi(\mathbf{r},t)=\Phi(\mathbf{r})e^{-iEt}, \tag{2.23}$$

where E is the energy per particle for the condensate, and Eq. (2.22) reduces to

$$\left(-\nabla^2+V_e(\mathbf{r})+\frac{8\pi aN}{\Omega}|\Phi(\mathbf{r})|^2-\frac{4\pi aN}{\Omega}\zeta-E\right)\Phi(\mathbf{r})=0. \tag{2.24}$$

Note that $V_e(\mathbf{r},t)$ in Eq. (2.22) can have explicit time dependence, but not $V_e(\mathbf{r})$ in Eq. (2.24).

There are two basic lengths in Eq. (2.24): (i) the length over which $V_e(\mathbf{r})$ varies, and (ii) the length scale determined by $(4\pi aN/\Omega)|\Phi(\mathbf{r})|^2$. It is the interplay between these two lengths that is responsible for some of the interesting properties of this nonlinear Schrödinger equation. The simplest example of this interplay is the case of the rigid boundary [3,4].

III. PAIR PRODUCTION

Since the time-dependent formalism and the time-independent formalism are closely related, the choice is made to treat pair production in this section using the time-independent formalism. In the absence of the external potential, a possible approach is to use the Bogoliubov transformation [12]. An equivalent procedure as used in Ref. [4] involves diagonalizing a matrix. In the Appendix here, this procedure of Lee, Huang, and Yang [4], as discussed in their Appendix I, is recast in a form more suitable for generalization to the present case. See also Ref. [13].

In the time-independent formalism, the creation and annihilation operators for the condensate are

$$\begin{aligned} a_0^*&=\Omega^{-1/2}\int d\mathbf{r}\ \Phi(\mathbf{r})\psi^*(\mathbf{r}),\\ a_0&=\Omega^{-1/2}\int d\mathbf{r}\ \Phi^*(\mathbf{r})\psi(\mathbf{r}). \end{aligned} \tag{3.1}$$

By Eq. (2.23), these are related to $a_0^*(t)$ and $a_0(t)$ by

$$a_0^*(t)=e^{-iEt}a_0^*,\quad a_0(t)=e^{iEt}a_0. \tag{3.2}$$

Equations (2.16) and (2.17) give approximations to the T and V of Eqs. (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, Eq. (2.15) for N is no longer accurate enough, and Eq. (2.14) needs to be used. Thus,

$$\begin{aligned} T={}&N(\overline{\zeta}+\zeta_e)+\Omega^{-1/2}a_0\int d\mathbf{r}[-\nabla^2\Phi(\mathbf{r})+V_e(\mathbf{r})\Phi(\mathbf{r})]\psi_1^*(\mathbf{r})+\Omega^{-1/2}a_0^*\int d\mathbf{r}[-\nabla^2\Phi^*(\mathbf{r})+V_e(\mathbf{r})\Phi^*(\mathbf{r})]\psi_1(\mathbf{r})\\ &+\int d\mathbf{r}[|\nabla\psi_1(\mathbf{r})|^2+V_e(\mathbf{r})\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})-(\overline{\zeta}+\zeta_e)\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})] \end{aligned} \tag{3.3}$$

and

$$\begin{aligned} V_2={}&\frac{4\pi aN}{\Omega}\bigg[N\zeta+2\Omega^{-1/2}a_0\int d\mathbf{r}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r})\psi_1^*(\mathbf{r})+2\Omega^{-1/2}a_0^*\int d\mathbf{r}|\Phi(\mathbf{r})|^2\Phi^*(\mathbf{r})\psi_1(\mathbf{r})\\ &+\int d\mathbf{r}\{[-2\zeta+4|\Phi(\mathbf{r})|^2]\psi_1^*(\mathbf{r})\psi_1(\mathbf{r})+N^{-1}a_0^2\Phi(\mathbf{r})^2\psi_1^*(\mathbf{r})^2+N^{-1}a_0^{*\,2}\Phi^*(\mathbf{r})^2\psi_1(\mathbf{r})^2\}\bigg]. \end{aligned} \tag{3.4}$$

The first terms in Eqs. (3.3) and (3.4) are constants, while the sum of those terms involving a factor of $\Omega^{-1/2}$ also leads to a constant by virtue of the nonlinear Schrödinger equation (2.24) for $\Phi(\mathbf{r})$. We therefore concentrate on the terms that are quadratic in $\psi_1^*(\mathbf{r})$ and $\psi_1(\mathbf{r})$:

$$H_2 = \int d\mathbf{r} \left\{ |\nabla \psi_1(\mathbf{r})|^2 + \left[-\overline{\zeta} - \zeta_e - \frac{8\pi a N}{\Omega} \zeta + V_e(\mathbf{r}) \right] \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + \frac{4\pi a N}{\Omega} [4|\Phi(\mathbf{r})|^2 \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + N^{-1} a_0^2 \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 + N^{-1} a_0^{*\,2} \Phi^*(\mathbf{r})^2 \psi_1(\mathbf{r})^2] \right\}. \tag{3.5}$$

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

Following the procedure in the Appendix, define

$$H_2' = e^{-P} H_2 e^{P}, \tag{3.6}$$

where [3]

$$P = (2N)^{-1} \int d\mathbf{r}\, d\mathbf{r}'\, \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') K_0(\mathbf{r},\mathbf{r}') a_0^2. \tag{3.7}$$

Without loss of generality, choose K_0 to satisfy

$$K_0(\mathbf{r},\mathbf{r}') = K_0(\mathbf{r}',\mathbf{r}) \tag{3.8}$$

and

$$\int d\mathbf{r}\, \Phi^*(\mathbf{r}) K_0(\mathbf{r},\mathbf{r}') = 0. \tag{3.9}$$

Since it follows from Eq. (2.13) that

$$[\psi_1(\mathbf{r}), \psi_1^*(\mathbf{r}')] = \delta^3(\mathbf{r}-\mathbf{r}') - \Omega^{-1} \Phi(\mathbf{r}) \Phi^*(\mathbf{r}'), \tag{3.10}$$

it is straightforward to verify that

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

$$[\psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}), e^P] = N^{-1} \int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') e^P a_0^2, \tag{3.12}$$

$$[|\nabla \psi_1(\mathbf{r})|^2, e^P] = N^{-1} \int d\mathbf{r}'\, \nabla_r K_0(\mathbf{r},\mathbf{r}') \times \nabla_r \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') e^P a_0^2, \tag{3.13}$$

and

$$[\psi_1(\mathbf{r})^2, e^P] = N^{-1} e^P \left[K_0(\mathbf{r},\mathbf{r}) + 2 \int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}') + N^{-1} \int d\mathbf{r}'\, d\mathbf{r}''\, K_0(\mathbf{r},\mathbf{r}') K_0(\mathbf{r},\mathbf{r}'') \times \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}'') a_0^2 \right] a_0^2. \tag{3.14}$$

Using these commutation relations, the H_2' of Eq. (3.6) is given by

$$H_2' = H_2 + e^{-P} [H_2, e^P] = H_2'' + H_{2c}', \tag{3.15}$$

where

$$H_2'' = \int d\mathbf{r} \left\{ |\nabla \psi_1(\mathbf{r})|^2 + \left[-\overline{\zeta} - \frac{8\pi a N}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) \right] \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + \frac{4\pi a N}{\Omega} [4|\Phi(\mathbf{r})|^2 \psi_1^*(\mathbf{r}) \psi_1(\mathbf{r}) + N^{-1} \Phi^*(\mathbf{r})^2 a_0^{*\,2} \psi_1(\mathbf{r})^2] + \Phi^*(\mathbf{r})^2 \frac{4\pi a N}{\Omega} \left[K_0(\mathbf{r},\mathbf{r}) + 2 \int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \right] \right\}, \tag{3.16}$$

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

$$H_{2c}' = N^{-1} \int d\mathbf{r} \left\{ \frac{4\pi a N}{\Omega} \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 - \int d\mathbf{r}' [\nabla_r^2 K_0(\mathbf{r},\mathbf{r}')] \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') + \left[-\overline{\zeta} - \frac{8\pi a N}{\Omega} \zeta - \zeta_e + V_e(\mathbf{r}) \right] \int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') + \frac{4\pi a N}{\Omega} \left[4|\Phi(\mathbf{r})|^2 \int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') + \Phi^*(\mathbf{r})^2 \int d\mathbf{r}'\, d\mathbf{r}''\, K_0(\mathbf{r},\mathbf{r}') K_0(\mathbf{r},\mathbf{r}'') \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}'') \right] \right\} a_0^2. \tag{3.17}$$

Similar to Eqs. (3.7)–(3.9), define $L(\mathbf{r},\mathbf{r}')$ by

$$H_{2c}' = (2N)^{-1} \int d\mathbf{r}\, d\mathbf{r}'\, L(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') a_0^2, \tag{3.18}$$

$$L(\mathbf{r},\mathbf{r}')=L(\mathbf{r}',\mathbf{r}), \tag{3.19}$$

and

$$\int d\mathbf{r}\ \Phi^*(\mathbf{r}')L(\mathbf{r},\mathbf{r}')=0. \tag{3.20}$$

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

$$L(\mathbf{r},\mathbf{r}')=0. \tag{3.21}$$

It only remains to rewrite Eq. (3.21) in the form of an integro-differential equation for $K_0(\mathbf{r},\mathbf{r}')$:

$$\begin{aligned}L(\mathbf{r},\mathbf{r}')=&-\nabla^2K_0(\mathbf{r},\mathbf{r}')-\nabla'^{\,2}\ K_0(\mathbf{r},\mathbf{r}')+\frac{8\pi aN}{\Omega}\Phi(\mathbf{r})^2\delta(\mathbf{r}-\mathbf{r}')\\&+\left\{-2\bar{\zeta}-\frac{16\pi aN}{\Omega}\zeta-2\zeta_e+V_e(\mathbf{r})+V_e(\mathbf{r}')+\frac{16\pi aN}{\Omega}[|\Phi(\mathbf{r})|^2+|\Phi(\mathbf{r}')|^2]\right\}K_0(\mathbf{r},\mathbf{r}')\\&+\frac{8\pi aN}{\Omega}\int d\mathbf{r}''\Phi^*(\mathbf{r}'')^2K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}',\mathbf{r}'')-\lambda(\mathbf{r})\Phi(\mathbf{r}')-\lambda(\mathbf{r}')\Phi(\mathbf{r})\\=&\,0,\end{aligned} \tag{3.22}$$

where $\lambda(\mathbf{r})$ is to be determined by Eq. (3.20).

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

$$\int d\mathbf{r}'K_0(\mathbf{r},\mathbf{r}')\left[-\nabla'^{\,2}+V_e(\mathbf{r}')+\frac{16\pi aN}{\Omega}|\Phi(\mathbf{r}')|^2\right]\Phi^*(\mathbf{r}')+\frac{8\pi aN}{\Omega}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r})=\lambda(\mathbf{r})\Omega+\Phi(\mathbf{r})\int d\mathbf{r}'\Phi^*(\mathbf{r}')\lambda(\mathbf{r}'). \tag{3.23}$$

Equation (2.24) may be used to give

$$\lambda(\mathbf{r})=\frac{8\pi aN}{\Omega^2}\left[|\Phi(\mathbf{r})|^2\Phi(\mathbf{r})+\int d\mathbf{r}'K_0(\mathbf{r},\mathbf{r}')|\Phi(\mathbf{r}')|^2\Phi^*(\mathbf{r}')-\tfrac{1}{2}\zeta\Phi(\mathbf{r})\right]. \tag{3.24}$$

The integro-differential equation for $K_0(\mathbf{r},\mathbf{r}')$ is explicitly

$$\begin{aligned}&-\nabla^2K_0(\mathbf{r},\mathbf{r}')-\nabla'^{\,2}\ K_0(\mathbf{r},\mathbf{r}')+\frac{8\pi aN}{\Omega}\Phi(\mathbf{r})^2\delta(\mathbf{r}-\mathbf{r}')+\left\{-2\bar{\zeta}-\frac{16\pi aN}{\Omega}\zeta-2\zeta_e+V_e(\mathbf{r})+V_e(\mathbf{r}')\right.\\&\quad\left.+\frac{16\pi aN}{\Omega}[|\Phi(\mathbf{r})|^2+|\Phi(\mathbf{r}')|^2]\right\}K_0(\mathbf{r},\mathbf{r}')+\frac{8\pi aN}{\Omega}\int d\mathbf{r}''\Phi^*(\mathbf{r}'')^2K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}',\mathbf{r}'')\\&=\frac{8\pi aN}{\Omega^2}\left\{\Phi(\mathbf{r})\Phi(\mathbf{r}')[|\Phi(\mathbf{r})|^2+|\Phi(\mathbf{r}')|^2-\zeta]+\Phi(\mathbf{r})\int d\mathbf{r}''K_0(\mathbf{r}',\mathbf{r}'')|\Phi(\mathbf{r}'')|^2\Phi^*(\mathbf{r}'')\right.\\&\quad\left.+\Phi(\mathbf{r}')\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'')|\Phi(\mathbf{r}'')|^2\Phi^*(\mathbf{r}'')\right\}.\end{aligned} \tag{3.25}$$

For completeness, we write down the corresponding equation for the time-dependent case. In this case, the V is approximated by

$$\begin{aligned}V_2=\frac{4\pi aN}{\Omega}\Bigg[&N\zeta(t)+2\Omega^{-1/2}a_0(t)\int d\mathbf{r}|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t)\psi_1^*(\mathbf{r},t)+2\Omega^{-1/2}a_0^*(t)\int d\mathbf{r}|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\\&+\int d\mathbf{r}\{[-2\zeta(t)+4|\Phi(\mathbf{r},t)|^2]\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)+N^{-1}a_0(t)^2\Phi(\mathbf{r},t)^2\psi_1^*(\mathbf{r},t)^2+N^{-1}a_0^*(t)^2\Phi^*(\mathbf{r},t)^2\psi_1(\mathbf{r},t)^2\}\Bigg],\end{aligned} \tag{3.26}$$

and the N-body wave function takes the form

$$\mathbf{\Psi}(t)=\mathcal{N}(t)e^{\mathcal{P}(t)}(N!)^{-1/2}a_0^*(t)^N|\mathrm{vac}\rangle, \tag{3.27}$$

where $\mathcal{P}(t)$ describes the creation of pairs from the condensate

$$\mathcal{P}(t)=(2N)^{-1}\int d\mathbf{r}\,d\mathbf{r}'\,\psi_1^*(\mathbf{r},t)\psi_1^*(\mathbf{r}',t)K_0(\mathbf{r},\mathbf{r}';t)a_0(t)^2, \tag{3.28}$$

and $\mathcal{N}(t)$ is the normalization constant. It should be noted that the reduction to the time-independent case involves the phase factor

$$K_0(\mathbf{r},\mathbf{r}';t)=e^{-2iEt}K_0(\mathbf{r},\mathbf{r}'). \tag{3.29}$$

The time-dependent version of Eq. (3.25) is

$$\begin{aligned}\left[i\frac{\partial}{\partial t}-2E(t)\right]K_0(\mathbf{r},\mathbf{r}';t)={}&-\nabla^2K_0(\mathbf{r},\mathbf{r}';t)-\nabla'^2K_0(\mathbf{r},\mathbf{r}';t)+\frac{8\pi aN}{\Omega}\Phi(\mathbf{r},t)^2\delta(\mathbf{r}-\mathbf{r}')+\left\{-2\overline{\zeta}(t)-\frac{16\pi aN}{\Omega}\zeta(t)-2\zeta_e(t)\right.\\&\left.+V_e(\mathbf{r},t)+V_e(\mathbf{r}',t)+\frac{16\pi aN}{\Omega}[|\Phi(\mathbf{r},t)|^2+|\Phi(\mathbf{r}',t)|^2]\right\}K_0(\mathbf{r},\mathbf{r}';t)\\&+\frac{8\pi aN}{\Omega}\int d\mathbf{r}''\Phi^*(\mathbf{r}'',t)^2K_0(\mathbf{r},\mathbf{r}'';t)K_0(\mathbf{r}',\mathbf{r}'';t)-\frac{8\pi aN}{\Omega^2}\left\{\Phi(\mathbf{r},t)\Phi(\mathbf{r}',t)\right.\\&\times[|\Phi(\mathbf{r},t)|^2+|\Phi(\mathbf{r}',t)|^2-\zeta(t)]+\Phi(\mathbf{r},t)\int d\mathbf{r}''K_0(\mathbf{r}',\mathbf{r}'';t)|\Phi(\mathbf{r}'',t)|^2\Phi^*(\mathbf{r}'',t)\\&\left.+\Phi(\mathbf{r}',t)\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'';t)|\Phi(\mathbf{r}'',t)|^2\Phi^*(\mathbf{r}'',t)\right\},\end{aligned} \tag{3.30}$$

where $E(t)$ on the left-hand side is defined by

$$E(t)=i\Omega^{-1}\int d\mathbf{r}\frac{\partial\Phi(\mathbf{r},t)}{\partial t}\Phi^*(\mathbf{r},t). \tag{3.31}$$

Compare with Sec. 7 of Ref. [3].

IV. ATOMIC TRAP

One immediate consequence of the trapping potential is that the volume Ω no longer has a well-defined meaning. It is indeed possible to assign a somewhat arbitrary value to Ω, and the final results will be independent of this arbitrarily assigned value. A better procedure is to use N, the total number of particles, as the normalization instead of Ω. In terms of the condensate wave function of Eq. (2.10), define

$$\tilde{\Phi}(\mathbf{r},t)=(N/\Omega)^{1/2}\Phi(\mathbf{r},t), \tag{4.1}$$

so that Eq. (2.10) becomes

$$N^{-1}\int d\mathbf{r}|\tilde{\Phi}(\mathbf{r},t)|^2=1. \tag{4.2}$$

Note that, while $\Phi(\mathbf{r},t)$ is dimensionless, the $\tilde{\Phi}(\mathbf{r},t)$ here has the dimension of $(\text{length})^{-3/2}$. Similar to the $\zeta(t)$ of Eq. (2.18), define

$$\tilde{\zeta}(t)=N^{-1}\int d\mathbf{r}|\tilde{\Phi}(\mathbf{r},t)|^4, \tag{4.3}$$

which is equal to $N\zeta(t)/\Omega$.

In terms of this $\tilde{\Phi}(\mathbf{r},t)$, the basic equations of motion (2.22) and (3.30) for $\tilde{\Phi}$ and K_0 are, respectively,

$$\begin{aligned}i\left(\frac{\partial}{\partial t}\right)\tilde{\Phi}(\mathbf{r},t)={}&[-\nabla^2+V_e(\mathbf{r},t)+8\pi a|\tilde{\Phi}(\mathbf{r},t)|^2\\&-4\pi a\tilde{\zeta}(t)]\tilde{\Phi}(\mathbf{r},t),\end{aligned} \tag{4.4}$$

and

$$\begin{aligned}\left[i\frac{\partial}{\partial t}-2E(t)\right]K_0(\mathbf{r},\mathbf{r}';t)={}&-\nabla^2K_0(\mathbf{r},\mathbf{r}';t)-\nabla'^2K_0(\mathbf{r},\mathbf{r}';t)+8\pi a\tilde{\Phi}(\mathbf{r},t)^2\delta(\mathbf{r}-\mathbf{r}')+\{-2\overline{\zeta}(t)-16\pi a\tilde{\zeta}(t)-2\zeta_e(t)\\&+V_e(\mathbf{r},t)+V_e(\mathbf{r}',t)+16\pi a[|\tilde{\Phi}(\mathbf{r},t)|^2+|\tilde{\Phi}(\mathbf{r}',t)|^2]\}K_0(\mathbf{r},\mathbf{r}';t)\\&+8\pi a\int d\mathbf{r}''\tilde{\Phi}^*(\mathbf{r}'',t)^2K_0(\mathbf{r},\mathbf{r}'';t)K_0(\mathbf{r}',\mathbf{r}'';t)-\frac{8\pi a}{N}\left\{\tilde{\Phi}(\mathbf{r},t)\tilde{\Phi}(\mathbf{r}',t)\right.\\&\times[|\tilde{\Phi}(\mathbf{r},t)|^2+|\tilde{\Phi}(\mathbf{r}',t)|^2-\tilde{\zeta}(t)]+\tilde{\Phi}(\mathbf{r},t)\int d\mathbf{r}''K_0(\mathbf{r}',\mathbf{r}'';t)|\tilde{\Phi}(\mathbf{r}'',t)|^2\tilde{\Phi}^*(\mathbf{r}'',t)\\&\left.+\tilde{\Phi}(\mathbf{r}',t)\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'';t)|\tilde{\Phi}(\mathbf{r}'',t)|^2\tilde{\Phi}^*(\mathbf{r}'',t)\right\},\end{aligned} \tag{4.5}$$

where $\overline{\zeta(t)}$ and $\zeta_e(t)$ are defined in Eq. (2.18), and

$$E(t)=iN^{-1}\int d\mathbf{r}\frac{\partial\tilde{\Phi}(\mathbf{r},t)}{\partial t}\tilde{\Phi}^*(\mathbf{r},t). \tag{4.6}$$

In the time-independent case given by Eq. (3.29) and

$$\tilde{\Phi}(\mathbf{r},t)=\tilde{\Phi}(\mathbf{r})e^{-iEt}, \tag{4.7}$$

the above equations of motion reduce to

$$[-\nabla^2+V_e(\mathbf{r})+8\pi a|\tilde{\Phi}(\mathbf{r})|^2-4\pi a\tilde{\zeta}-E]\tilde{\Phi}(\mathbf{r})=0, \tag{4.8}$$

and

$$\begin{aligned}&-\nabla^2K_0(\mathbf{r},\mathbf{r}')-\nabla'^2K_0(\mathbf{r},\mathbf{r}')+8\pi a\tilde{\Phi}(\mathbf{r})^2\delta(\mathbf{r}-\mathbf{r}')+\{-2\overline{\zeta}-16\pi a\tilde{\zeta}-2\zeta_e+V_e(\mathbf{r})+V_e(\mathbf{r}')\\&\quad+16\pi a[|\tilde{\Phi}(\mathbf{r})|^2+|\tilde{\Phi}(\mathbf{r}')|^2]\}K_0(\mathbf{r},\mathbf{r}')+8\pi a\int d\mathbf{r}''\tilde{\Phi}^*(\mathbf{r}'')^2K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}',\mathbf{r}'')\\&=8\pi aN^{-1}\Big\{\tilde{\Phi}(\mathbf{r})\tilde{\Phi}(\mathbf{r}')[|\tilde{\Phi}(\mathbf{r})|^2+|\tilde{\Phi}(\mathbf{r}')|^2-\tilde{\zeta}]+\tilde{\Phi}(\mathbf{r})\int d\mathbf{r}''K_0(\mathbf{r}',\mathbf{r}'')|\tilde{\Phi}(\mathbf{r}'')|^2\tilde{\Phi}^*(\mathbf{r}'')\\&\quad+\tilde{\Phi}(\mathbf{r}')\int d\mathbf{r}''K_0(\mathbf{r},\mathbf{r}'')|\tilde{\Phi}(\mathbf{r}'')|^2\tilde{\Phi}^*(\mathbf{r}'')\Big\}.\end{aligned} \tag{4.9}$$

In Eqs. (4.2)–(4.9), the volume Ω does not appear anywhere.

In the next section, Eqs. (4.8) and (4.9) will be studied under the assumption that the external potential $V_e(\mathbf{r})$ is sufficiently slowly varying. This case is of interest because in the experiments [1,2] the magnetic traps are necessarily of macroscopic dimensions. Note that in the following section, only the simpler time-independent cases are treated.

V. CONDENSATE IN A TRAP

When the condensate is in the lowest state, its wave function $\tilde{\Phi}(\mathbf{r})$ can be chosen to be non-negative. Thus, Eq. (4.8) is

$$[-\nabla^2+V_e(\mathbf{r})+8\pi a\tilde{\Phi}(\mathbf{r})^2-4\pi a\tilde{\zeta}-E]\tilde{\Phi}(\mathbf{r})=0. \tag{5.1}$$

When $V_e(\mathbf{r})$ is slowly varying, a first approximation to Eq. (5.1) is obtained by neglecting the first term $-\nabla^2\tilde{\Phi}(\mathbf{r})$ [14], i.e.,

$$[V_e(\mathbf{r})+8\pi a\tilde{\Phi}(\mathbf{r})^2-4\pi a\tilde{\zeta}-E]\tilde{\Phi}(\mathbf{r})=0. \tag{5.2}$$

This means that

$$\tilde{\Phi}(\mathbf{r})=\{[4\pi a\tilde{\zeta}+E-V_e(\mathbf{r})]/(8\pi a)\}^{1/2} \tag{5.3a}$$

in some region, say R_0, and

$$\tilde{\Phi}(\mathbf{r})=0 \tag{5.3b}$$

outside of R_0. It follows from Eq. (5.3a) that

$$V_e(\mathbf{r})\leqslant 4\pi a\tilde{\zeta}+E \tag{5.4}$$

in R_0. Furthermore, since $\tilde{\Phi}(\mathbf{r})$ is necessarily continuous,

$$V_e(\mathbf{r})=4\pi a\tilde{\zeta}+E \tag{5.5}$$

on the boundary of R_0.

Multiplying Eq. (5.2) by $\tilde{\Phi}(\mathbf{r})$ and integrating over $\mathbf{r}$ give

$$E=\zeta_e+4\pi a\tilde{\zeta}. \tag{5.6}$$

Given N, the value of $\tilde{\zeta}$ is determined by Eqs. (4.2) and (4.3). With Eq. (5.6), the approximate solution (5.3) is

$$\tilde{\Phi}(\mathbf{r})=\begin{cases}\{\tilde{\zeta}+(8\pi a)^{-1}[\zeta_e-V_e(\mathbf{r})]\}^{1/2} & \text{inside } R_0\\ 0 & \text{outside } R_0.\end{cases} \tag{5.7}$$

As mentioned above, in writing down Eq. (5.2), the term $-\nabla^2\tilde{\Phi}(\mathbf{r})$ has been neglected. However, if the approximate solution (5.3), or equivalently Eq. (5.7), is used, this neglected term $-\nabla^2\tilde{\Phi}(\mathbf{r})$ is in general not even bounded on

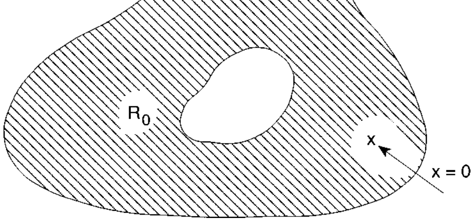

FIG. 1. Geometry for the condensate wave function.

the boundary of R_0. An improved solution is thus needed near this boundary. Let x be the rectangular coordinate normal to the boundary, chosen such that the positive x axis points toward the interior of R_0. The geometry is shown schematically in Fig. 1. Instead of neglecting $-\nabla^2\tilde{\Phi}(\mathbf{r})$, replace it by the corresponding second derivative with respect to x. Expand the potential $V_e(\mathbf{r})$ near $x=0$ on the boundary of R_0 to get

$$V_e(x,y,z)=V_e(0,y,z)-\kappa(y,z)x+o(x), \tag{5.8}$$

where $\kappa(y,z)$ is assumed to be positive. By Eq. (5.5) and suppressing the variables y and z, Eq. (5.8) is

$$V_e(x)\sim 4\pi a\tilde{\zeta}+E-\kappa x. \tag{5.9}$$

The substitution of Eq. (5.9) into Eq. (5.1) gives the ordinary differential equation

$$\left[-\frac{d^2}{dx^2}+8\pi a\tilde{\Phi}(x)^2-\kappa x\right]\tilde{\Phi}(x)=0. \tag{5.10}$$

This differential equation can be put in a canonical form by the scaling

$$x=\kappa^{-1/3}\eta$$

and

$$\tilde{\Phi}(x)=(4\pi a)^{-1/2}\kappa^{1/3}\tau(\eta). \tag{5.11}$$

The equation for τ is then

$$\tau''(\eta)-2\tau(\eta)^3+\eta\tau(\eta)=0, \tag{5.12}$$

with the boundary conditions

$$\lim_{\eta\to-\infty}\tau(\eta)=0 \tag{5.13}$$

and

$$\lim_{\tau\to\infty}\eta^{-1/2}\tau(\eta)=2^{-1/2}. \tag{5.14}$$

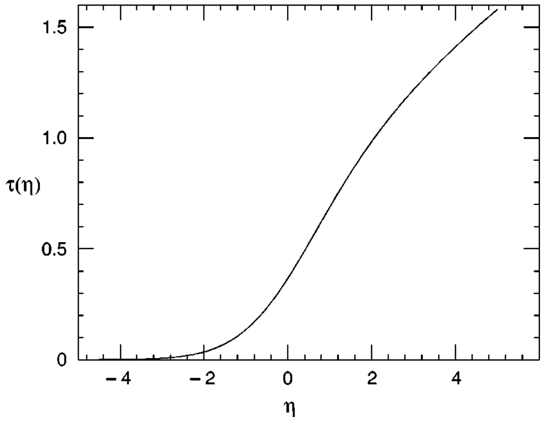

FIG. 2. The universal function $\tau(\eta)$ that describes the behavior of the condensate wave function near the boundary of the region R_0.

Equation (5.12) with the boundary conditions (5.13) and (5.14) defines a unique universal function $\tau(\eta)$. It is plotted in Fig. 2 and describes through Eq. (5.11) the behavior of the condensate wave function near the boundary of R_0. This result is similar to the findings of Dalfovo, Pitaevskii, and Stringari [15] using the chemical potential as a parameter.

Note the important point that Eq. (5.12) is a special case of the Painlevé equation of the second type [16].

The next step is to study the integro-differential equation (4.9) when the external potential $V_e(\mathbf{r})$ is slowly varying. In this case, it is convenient to use the ''center-of-mass'' coordinate by defining

$$P(\mathbf{R},\mathbf{r})=K_0(\mathbf{r}_1,\mathbf{r}_2), \tag{5.15}$$

where

$$\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2),\quad \mathbf{r}=\mathbf{r}_1-\mathbf{r}_2.$$

In terms of these coordinates, Eq. (4.9) is

$$\begin{aligned}
&-\tfrac{1}{2}\nabla_R^2P(\mathbf{R},\mathbf{r})-2\nabla^2P(\mathbf{R},\mathbf{r})+8\pi a\tilde{\Phi}(\mathbf{R})^2\delta(\mathbf{r})+\{-2\overline{\zeta}-16\pi a\tilde{\zeta}-2\zeta_e+V_e(\mathbf{R}+\tfrac{1}{2}\mathbf{r})+V_e(\mathbf{R}-\tfrac{1}{2}\mathbf{r})+16\pi a[|\tilde{\Phi}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})|^2\\
&\quad+|\tilde{\Phi}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})|^2]\}P(\mathbf{R},\mathbf{r})+8\pi a\int d\mathbf{r}'\,\tilde{\Phi}^*(\mathbf{R}+\mathbf{r}')^2P(\mathbf{R}+\tfrac{1}{4}\mathbf{r}+\tfrac{1}{2}\mathbf{r}',\tfrac{1}{2}\mathbf{r}-\mathbf{r}')P(\mathbf{R}-\tfrac{1}{4}\mathbf{r}+\tfrac{1}{2}\mathbf{r}',-\tfrac{1}{2}\mathbf{r}-\mathbf{r}')\\
&=8\pi aN^{-1}\Big\{\tilde{\Phi}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})\tilde{\Phi}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})[|\tilde{\Phi}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})|^2+|\tilde{\Phi}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})|^2-\tilde{\zeta}]+\tilde{\Phi}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})\int d\mathbf{r}'\,P(\mathbf{R}-\tfrac{1}{4}\mathbf{r}+\tfrac{1}{2}\mathbf{r}',-\tfrac{1}{2}\mathbf{r}-\mathbf{r}')\\
&\quad\times|\tilde{\Phi}(\mathbf{R}+\mathbf{r}')|^2\tilde{\Phi}^*(\mathbf{R}+\mathbf{r}')+\tilde{\Phi}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})\int d\mathbf{r}'\,P(\mathbf{R}+\tfrac{1}{4}\mathbf{r}+\tfrac{1}{2}\mathbf{r}',\tfrac{1}{2}\mathbf{r}-\mathbf{r}')|\tilde{\Phi}(\mathbf{R}+\mathbf{r}')|^2\tilde{\Phi}^*(\mathbf{R}+\mathbf{r}')\Big\},
\end{aligned} \tag{5.16}$$

where ∇^2 means ∇_r^2.

Motivated by Eq. (5.2), simplify Eq. (5.16) by the following approximations: (i) neglect the first term $-\tfrac{1}{2}\nabla_R^2P(\mathbf{R},\mathbf{r})$; (ii) replace $V_e(\mathbf{R}+\tfrac{1}{2}\mathbf{r})+V_e(\mathbf{R}-\tfrac{1}{2}\mathbf{r})$ by $2V_e(\mathbf{R})$, and similarly replace $|\tilde{\Phi}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})|^2+|\tilde{\Phi}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})|^2$ by $2|\tilde{\Phi}(\mathbf{R})|^2$; (iii) in the same spirit, simplify the last term on the left-hand side to

$$8\pi a\int d\mathbf{r}'\,\tilde{\Phi}^*(\mathbf{R})^2P(\mathbf{R},\tfrac{1}{2}\mathbf{r}-\mathbf{r}')P(\mathbf{R},-\tfrac{1}{2}\mathbf{r}-\mathbf{r}');$$

and, finally, (iv) neglect the entire right-hand side because of the factor N^{-1}.

With (i)–(iv), Eq. (5.16) becomes

$$-\nabla^2 P(\mathbf{R},\mathbf{r})+4\pi a\tilde{\Phi}(\mathbf{R})^2\delta(\mathbf{r})+[-\bar{\zeta}-8\pi a\tilde{\zeta}-\zeta_e+V_e(\mathbf{R})+16\pi a|\tilde{\Phi}(\mathbf{R})|^2]P(\mathbf{R},\mathbf{r})+4\pi a\tilde{\Phi}^*(\mathbf{R})^2\times\int d\mathbf{r}'\,P(\mathbf{R},\mathbf{r}-\mathbf{r}')P(\mathbf{R},\mathbf{r}')=0. \tag{5.17}$$

In this approximation, **R** can be considered to be a parameter and the ideas of Lee, Huang, and Yang [4] can be applied.

Since there is translational invariance in the variable **r**, define the Fourier transform

$$\bar{P}(\mathbf{R},\mathbf{k})=\int d\mathbf{r}\; e^{i\mathbf{k}\cdot\mathbf{r}}P(\mathbf{R},\mathbf{r}). \tag{5.18}$$

In terms of this $\bar{P}$, Eq. (5.17) is a quadratic equation

$$4\pi a\tilde{\Phi}^*(\mathbf{R})^2\bar{P}(\mathbf{R},\mathbf{k})^2+[k^2+k_0(\mathbf{R})^2]\bar{P}(\mathbf{R},\mathbf{k})+4\pi a\tilde{\Phi}(\mathbf{R})^2=0, \tag{5.19}$$

where

$$k_0(\mathbf{R})^2=-\bar{\zeta}-8\pi a\tilde{\zeta}-\zeta_e+V_e(\mathbf{R})+16\pi a|\tilde{\Phi}(\mathbf{R})|^2. \tag{5.20}$$

Therefore

$$\bar{P}(\mathbf{R},\mathbf{k})=[8\pi a\tilde{\Phi}^*(\mathbf{R})^2]^{-1}(-k^2-k_0(\mathbf{R})^2+\{[k^2+k_0(\mathbf{R})^2]^2-(8\pi a)^2|\tilde{\Phi}(\mathbf{R})|^4\}^{1/2}). \tag{5.21}$$

So far, no property of $\tilde{\Phi}$ has been used except that it is slowly varying. Let us now use the approximate solution (5.7). With this approximation, it follows from Eq. (5.19) that

$$K_0(\mathbf{r},\mathbf{r}')=0 \tag{5.22}$$

if $\frac{1}{2}(\mathbf{r}+\mathbf{r}')$ is outside of the region R_0. If it is inside, then, with $\bar{\zeta}$ negligible because $\tilde{\Phi}$ is slowly varying, Eq. (5.20) reduces simply to

$$k_0(\mathbf{R})^2=8\pi a\tilde{\Phi}(\mathbf{R})^2, \tag{5.23}$$

and the substitution into Eq. (5.21) gives

$$\bar{P}(\mathbf{R},\mathbf{k})=-k_0(\mathbf{R})^{-2}\{k^2+k_0(\mathbf{R})^2-k[k^2+2k_0(\mathbf{R})^2]^{1/2}\}, \tag{5.24}$$

very similar to the result of Lee, Huang, and Yang [4].

It is of some interest to carry out the inverse Fourier transform to get $P(\mathbf{R},\mathbf{r})$ explicitly. The result is

$$P(\mathbf{R},\mathbf{r})=\pi^{-2}(4\pi a)^{3/2}\tilde{\Phi}(\mathbf{R})^3\chi^{-1}\mathrm{Im}[S_{04}(i\chi)-S_{00}(i\chi)], \tag{5.25}$$

where

$$\chi=(16\pi a)^{1/2}\tilde{\Phi}(\mathbf{R})|\mathbf{r}|, \tag{5.26}$$

and S_{04} and S_{00} are Lommel's functions [17].

VI. DISCUSSION AND CONCLUSION

In the case of the system of hard-sphere bosons with periodic boundary conditions and without any external potential, the Bose-Einstein condensate is in the single-particle zero-momentum state and the many-body ground state is characterized by the pair-excitation function [4–9,12]. This pair excitation is essential for the existence of phonons and sound vibrations. Therefore, the minimal description of Bose-Einstein condensation of a dilute system in an external potential consists of the condensate wave function and the pair-excitation function. The former is a function of one spatial variable, while the latter is that of two spatial variables. In this paper, the equations satisfied by these two fundamental functions are given in the lowest-order approximation by Eqs. (2.22) and (3.30), respectively. More precisely, Eq. (2.22) is the nonlinear Schrödinger equation for the condensate wave function, while (3.30) is the integro-differential equation for the pair-excitation function.

It should perhaps be emphasized that, since Bose-Einstein condensation is a quantum phenomenon, the present treatment is also entirely quantum in nature, without the introduction of any classical concepts.

These lowest-order equations acquire corrections in higher orders, the leading corrections being of order $[\rho(\mathbf{r},t)a^3]^{1/2}$, where ρ is the local particle density, which is assumed to be small. As the simplest example, the pair excitation necessarily acts back on the wave function for the Bose-Einstein condensate, and therefore modifies the equation of motion for this condensate. While the first correction to Eq. (2.22) is manageable, higher corrections are likely to involve the logarithms of the expansion parameter [8,18,19] and therefore pose a challenge to our physical insight.

A word of caution should be added about the equations for the condensate wave function and the pair-excitation function. The approximate Hamiltonian used in this paper does not contain, for example, the decay of a phonon into two phonons. Therefore, in the present treatment, as well as those of Lee, Huang, and Yang [4] and Lee and Yang [5], the phonons are stable. This implies, as previously discussed in Sec. 6C of Ref. [3], that Eqs. (2.22) and (3.30) are valid only on a moderate time scale. There are many open questions both for shorter time scales and for longer time scales.

When the external potential is time-independent and slowly varying, as is often the case because of the macroscopic nature of the trap, both the nonlinear Schrödinger equation and the integro-differential equation are solved approximately in terms of known functions. Since the bosons are kept inside the trap, strictly speaking thermodynamics does not apply. However, since the number of atoms in the condensate ranges from the thousands to the millions [1,2], it is not unreasonable to use approximations based on N being large. On the other hand, for future technological applications, it is likely that the case of a moderate value of N will be most important. One example of such applications is perhaps to quantum computing [20].

Since the present treatment is limited to zero temperature, the most important next step is to remove this limitation so that the properties of Bose-Einstein condensation at nonzero temperatures can also be studied in the presence of an external potential. An equivalent way of stating this generalization is to deal with a mixture of superfluids and normal fluids.

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APPENDIX

Consider the Hamiltonian

$$H=\tfrac{1}{2}(a^*a+b^*b)+y(a^*b^*+ab), \tag{A1}$$

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

$$H'=e^{\alpha a^*b^*}He^{-\alpha a^*b^*}, \tag{A2}$$

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

$$\begin{aligned} H'=&(\tfrac{1}{2}-\alpha y)(a^*a+b^*b)+yab\\ &-\alpha y+(y-\alpha+\alpha^2 y)a^*b^*. \end{aligned} \tag{A3}$$

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

$$y-\alpha+\alpha^2 y=0. \tag{A4}$$

This gives

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

which is Eq. (A12) of Lee, Huang, and Yang [4]. With this α, H' is

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

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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