Bose-Einstein Condensation in an External Potential at Finite Temperatures

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Abstract

At finite but sufficiently low temperatures where there is macroscopic occupation of a single-particle quantum state, Bose-Einstein condensation in the presence of an external potential is described in terms of (i) $\Phi(\mathbf{r},t)$, the wave function of the macroscopically occupied state, referred to as the condensate; (ii) $\phi_i(\mathbf{r},t)$, $i = 1, 2, \ldots$, the single-particle wave functions that pertain to excitations from this condensate; and (iii) $K_0(\mathbf{r},\mathbf{r}';t)$, the pair-excitation function which is responsible for the existence of phonons and sound vibrations. For a dilute atomic gas with short-range pairwise repulsive interactions, partial differential equations are given for the condensate and single-particle excitation wave functions, and an integro-differential equation for the pair-excitation function.

I. INTRODUCTION

The first experimental observations of Bose-Einstein condensation in dilute atomic gases were reported in 1995 [1]. Many similar experiments followed soon after.

From the theoretical point of view, the two most important features of these experiments are the following: (i) The presence of the trap. The trap is necessary in order to keep the atoms together. Because of its presence, there is no translational invariance of the boson system. (ii) Finite temperature. Although the actual temperatures are very low, in the range of nanodegrees Kelvin, the Bose-Einstein condensation is not complete. An alternative way of stating this fact in the language of superfluid helium is that the superfluid and the normal fluid coexist.

In connection with the first feature, a quantum-mechanical treatment of Bose-Einstein condensation for systems without translational symmetry was given forty years ago [2], with focus on the condensate wave function $\Phi(\mathbf{r}, t)$ and the pair-excitation function $K_0(\mathbf{r}, \mathbf{r}'; t)$. The former is the wave function of the macroscopically occupied quantum state, henceforth referred to as the condensate, while the latter describes the scattering of two atoms from the condensate into other states at positions $\mathbf{r}$ and $\mathbf{r}'$. The method introduced in Ref. [2] was recently applied to Bose-Einstein condensation in an external potential [3]. Both papers deal with the case of extremely low temperatures, where the presence of the normal fluid can be ignored.

For systems with translational invariance and periodic boundary conditions, much of the present knowledge and insight in Bose-Einstein condensation is due to the work of Lee, Huang and Yang in the 1950s [4–8]. In such cases, the condensate wave function is that of the zero-momentum state. This is true at all temperatures below the Bose-Einstein phase transition. Using the method of pseudopotentials developed in Ref. [4], Lee, Huang and Yang in Ref. [6] approximate the many-body Hamiltonian in the momentum representation for zero temperature and then diagonalize it; the ensuing many-body wave function describes the excitation of pairs of atoms from the condensate into states of opposite nonzero momenta. By considering pair excitations, Lee and Yang [7, 8] soon after extended the approach to finite temperatures below the transition point in order to study some equilibrium [7] and nonequilibrium properties such as first and second sound [8]. Approximating the Hamiltonian is much more involved in this case of finite temperatures, and is achieved in Ref. [7] through the introduction of the fraction of particles in the condensate, ξ, which is treated as a fixed parameter in the approximation scheme. This ξ is subsequently determined as a function of temperature [7].

In the absence of translational invariance at extremely low temperatures, a minimal description of the boson system should employ the condensate wave function $\Phi(\mathbf{r}, t)$ and the pair-excitation function $K_0(\mathbf{r}, \mathbf{r}'; t)$ [2, 3, 9]; both of these functions are not known a priori and need to be determined by solving a partial differential equation and an integro-differential equation. At finite temperatures below the transition point, one needs to determine, in addition to these two quantities, the single-particle excitation wave functions $\phi_i(\mathbf{r}, t)$ $(i = 1, 2, \ldots)$ that correspond to the various nonzero-momentum eigenstates of the case with translational symmetry and periodic boundary conditions.

It is the purpose of the present paper to generalize the treatment of Ref. [3] to finite temperatures below the Bose-Einstein phase transition in the presence of an external potential. The proposed approach is a combination of Ref. [3] with the work of Lee and Yang [7] to treat the case where the superfluid and the normal fluid are simultaneously present, by taking into account the pair excitation.

The existing bibliography attests to the variety of methods employed in the past for certain aspects of this problem. Besides the work of Lee, Huang and Yang [4–8], noteworthy is Popov's diagrammatic approach [10] for translationally invariant, weakly interacting Bose-Einstein systems at finite temperatures. His approach is an extension of a previous technique by Beliaev [11] for the case of zero temperature. In the early 1980s, theoretical analyses of systems lacking translational symmetry were motivated by experiments involving spin-polarized atomic hydrogen in traps at low temperatures. By minimizing a free-energy functional that originated from the self-consistent Hartree-Fock and Bogoliubov theory, as described for example in Ref. [12], Goldman, Silvera, and Leggett [13] obtained approximate equations for the time-independent condensate and single-particle excitation wave functions. In their equations, terms that preserve orthogonality between the condensate and other states are neglected. Of the same nature is the method elaborated by Huse and Siggia [14], where additional terms are retained to ensure orthogonality. Their equation of motion for the condensate wave function contains the chemical potential as a parameter. In both of these papers [13, 14] the pair excitation is neglected. Similar calculations by Bagnato, Pritchard, and Kleppner [15] concentrate on the critical temperature, condensate fraction, and heat capacity of atomic gases confined by power-law external potentials. A different method by Oliva [16] makes use of the "local-density approximation," where the dependence of the required functionals on the local density is assumed to be that in a translationally invariant system of weakly interacting atoms.

In many recent researches [17] that are stimulated by the experiments [1], the formal self-consistent Hartree-Fock theory [12] is essentially simplified under the Popov approximation at finite temperatures [10]. A perturbation theory intended to go beyond the Popov approximation is given in Ref. [18]. A comprehensive critical analysis of such schemes in the light of the Hohenberg-Martin [19] classification of approximations, namely, their distinction into "conserving" and "gapless" ones, is provided by Griffin [20]. Other works include a variational approach [21] as well as adaptations [22, 23] of Oliva's local-density approximation [16]. In Ref. [24], an attempt is made for inclusion in the equations of motion of terms beyond the Popov approximation, but the required expectation values of operator products are essentially left undetermined. Again, there in no systematic treatment of pair excitation in these works.

From the point of view of quantum field theory, Bose-Einstein condensation provides an explicit example of non-perturbative effects [2, 3]. This means that the treatment of some operators as small compared to others leads to results that go beyond the ordinary perturbation expansion in a small physical parameter, here the s-wave scattering length. A feature that renders the present analysis distinctly different from other studies for finite temperatures is the systematic consideration of pair excitation in an external potential by methods of quantum field theory. The pair-excitation function describes pairs correlated due to interactions and is essential in treating physical effects such as phonon excitations and sound vibrations [2, 7, 8]. Note that the standard Hartree-Fock analysis does not include pair excitation, as is also pointed out in Ref. [25]. In order to determine all the required quantities to the lowest order, a first, natural step is to work out a suitable approximation to the many-body Hamiltonian; so far as the authors are aware, the proposed scheme is new. This task can be outlined roughly as follows.

By generalizing Ref. [2] for zero temperature, the various terms in the Hamiltonian are classified according to the number of times ψ_1^* and ψ_1 appear, where $\psi_1(\mathbf{r}, t)$ is the boson field operator in the Schrödinger picture corresponding to the space orthogonal to the condensate wave function. A complication in the case of finite temperatures arises from the use of the fraction of particles in the condensate, ξ, which is a fixed parameter with $0 < \xi \leq 1$ [7]. As discussed by Lee and Yang [7], the occupation numbers of the states other than the condensate do not fluctuate excessively, and these numbers are taken to be of the order of 1 while their sum is of course $N(1-\xi)$. The density of the thermal component, $A(\mathbf{r}, t)$, defined by Eq. (2.36) below, is then introduced explicitly as a time-dependent quantity. Products of two or more operators ψ_1 or ψ_1^* are subsequently simplified by treating $\psi_1^*(\mathbf{r}, t)\psi_1(\mathbf{r}, t) - A(\mathbf{r}, t)$ as small. In the first-order theory, it is necessary to retain terms that include up to two of the operators ψ_1^* or ψ_1, since atoms are distributed both over the condensate and the states pertaining to the single-particle wave functions ϕ_i, while pair creation from the condensate is neglected at this stage. In the next step, this process is taken into account by introducing the pair-excitation function $K_0(\mathbf{r}, \mathbf{r}'; t)$, in much the same way as the corresponding function at zero temperature [3]. An outline of the paper is provided below.

Section 2 deals with the step-by-step approximation to the many-body Hamiltonian. In Sec. 3, a part of the approximate Hamiltonian is used in combination with the many-body Schrödinger equation in order to obtain a system of lowest-order, time-dependent coupled partial differential equations for the condensate wave function $\Phi(\mathbf{r}, t)$ and the single-particle excitation wave functions $\phi_i(\mathbf{r}, t)$. By following the derivation in Ref. [3] for zero temperature, an integro-differential equation is determined in Sec. 4 for the time-independent pair-excitation function $K_0(\mathbf{r}, \mathbf{r}')$, with an effective potential to account for the presence of the thermal cloud. In Sec. 5, the equations of motion for the time-independent $\Phi(\mathbf{r})$ and $\phi_i(\mathbf{r})$ are discussed; the atoms are taken to obey the Bose-Einstein distribution law over the states i. The approximations in Sec. 2 for the more demanding case with an external potential run parallel to those presented in Appendix A where translational symmetry and periodic boundary conditions apply. The approximate Hamiltonian given in Appendix A correctly yields the energy spectrum of Lee and Yang [7]. Finally, Appendix B provides a detailed derivation of the equation for the pair-excitation function in Sec. 4 along the lines of Ref. [3]. Throughout the analysis, the external potential is taken to be sufficiently smooth and increasing rapidly at large distances. The interactions among the bosons are pairwise, repulsive, and of short range.

II. APPROXIMATE HAMILTONIAN

Consider a system of N pairwise interacting bosons at positions $\mathbf{r}_j$ $(j = 1, 2, \ldots, N)$ in an external potential V_e. In units where $\hbar = 2m = 1$, the Hamiltonian of the system is

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

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 $(a > 0)$. Similar to Ref. [3], the external potential $V_e(\mathbf{r}, t)$ may have explicit dependence on the time t.

In the late 1950s, Huang, Yang, and Luttinger [4] initiated the application of the method of pseudopotentials to many-body problems. 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 purposes as well as those of Refs. [2, 3], it is sufficient to employ

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

where the operator $(\partial/\partial r_{ij}) r_{ij}$ is omitted, viz.,

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

The only difficulty arising from the use of H in place of H' is the appearance of a familiar type of divergence, which may be removed using the procedures of Refs. [6] and [26].

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

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

and

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

where the field operator $\psi(\mathbf{r})$ satisfies the usual commutation relations for a boson field, i.e., $[\psi(\mathbf{r}), \psi^*(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$.

Let $\Phi(\mathbf{r}, t)$ be the wave function of the condensate, which is macroscopically but incompletely occupied. This wave function satisfies the normalization condition

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

The creation and annihilation operators for this condensate are

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

Of course, $[a_0(t), a_0^*(t)] = 1$. With the parts of $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$ corresponding to $\Phi(\mathbf{r}, t)$ singled out, the field operators $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$ are defined by the equations

$$\begin{aligned} \psi^*(\mathbf{r}) &= \Omega^{-1/2} \Phi^*(\mathbf{r}, t) a_0^*(t) + \psi_1^*(\mathbf{r}, t), \\ \psi(\mathbf{r}) &= \Omega^{-1/2} \Phi(\mathbf{r}, t) a_0(t) + \psi_1(\mathbf{r}, t). \end{aligned} \tag{2.12}$$

Clearly, $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$ correspond to the space orthogonal to the condensate wave function Φ. In terms of $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$, the total number N of particles is given by

$$N = a_0^*(t) a_0(t) + \int d\mathbf{r}\, \psi_1^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t). \tag{2.13}$$

It is the purpose of this section to find an approximation to H that is quadratic in $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$. Since the T of Eq. (2.8) is already in this form, it suffices to concentrate on the V of Eq. (2.9). By use of Eqs. (2.12), V is decomposed as

$$V = V_0 + V_1 + V_2 + V_3 + V_4, \tag{2.14}$$

where each subscript indicates the total number of times $\psi_1^*(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$ appear. Explicitly the terms V_i ($i = 0,\ 1,\ 2,\ 3,\ 4$) are given by

$$V_0 = 4\pi a \Omega^{-1} \zeta(t) a_0^*(t)^2 a_0(t)^2, \tag{2.15}$$

$$V_1 = 8\pi a \Omega^{-3/2} a_0^*(t) \int d\mathbf{r}\, |\Phi(\mathbf{r},t)|^2 [\Phi^*(\mathbf{r},t) a_0^*(t) \psi_1(\mathbf{r},t) + \Phi(\mathbf{r},t) \psi_1^*(\mathbf{r},t) a_0(t)] a_0(t), \tag{2.16}$$

$$V_2 = 4\pi a \Omega^{-1} \int d\mathbf{r}\, [\Phi^*(\mathbf{r},t)^2 a_0^*(t)^2 \psi_1(\mathbf{r},t)^2 + \Phi(\mathbf{r},t)^2 \psi_1^*(\mathbf{r},t)^2 a_0(t)^2 + 4|\Phi(\mathbf{r},t)|^2 a_0^*(t) \psi_1^*(\mathbf{r},t) \psi_1(\mathbf{r},t) a_0(t)], \tag{2.17}$$

$$V_3 = 8\pi a \Omega^{-1/2} \int d\mathbf{r}\, [\Phi^*(\mathbf{r},t) a_0^*(t) \psi_1^*(\mathbf{r},t) \psi_1(\mathbf{r},t)^2 + \Phi(\mathbf{r},t) \psi_1^*(\mathbf{r},t)^2 \psi_1(\mathbf{r},t) a_0(t)], \tag{2.18}$$

and

$$V_4 = 4\pi a \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)^2 \psi_1(\mathbf{r},t)^2. \tag{2.19}$$

In the above,

$$\zeta(t) = \Omega^{-1} \int d\mathbf{r}\, |\Phi(\mathbf{r},t)|^4. \tag{2.20}$$

Following the idea of Lee and Yang [7] for zero external potential and periodic boundary conditions, let $a_0^*(t)a_0(t)$ be approximated by $N\xi$ with $0 < \xi \le 1$. In this case, all five terms of Eqs. (2.15)–(2.19) contribute, contrary to the situation described in Ref. [3]. In this section, all five contributions are considered separately. In Appendix A, they are written down when translational invariance obtains; their sum is of course the one given in Ref. [7].

Among these five terms, V_1 is the simplest to deal with since its approximation simply involves replacement of the $a_0^*(t)a_0(t)$ in Eq. (2.16) by $N\xi$. Thus,

$$V_1 \sim \frac{8\pi a N\xi}{\Omega} \int d\mathbf{r}\, |\Phi(\mathbf{r},t)|^2 [\Phi^*(\mathbf{r},t) a_0^*(t) \Omega^{-1/2} \psi_1(\mathbf{r},t) + \Phi(\mathbf{r},t) \Omega^{-1/2} \psi_1^*(\mathbf{r},t) a_0(t)]. \tag{2.21}$$

For V_0, the procedure of approximation is that of formula (A13) of Appendix A by use of Eq. (2.13):

$$\begin{aligned} V_0 &= 4\pi a \zeta(t) \Omega^{-1} \{[a_0^*(t)a_0(t)]^2 - a_0^*(t)a_0(t)\} \\ &\sim 4\pi a \zeta(t) \Omega^{-1} [a_0^*(t)a_0(t)]^2 \\ &\sim 4\pi a \zeta(t) \Omega^{-1} \left\{ N\xi + \left[N(1-\xi) - \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \right] \right\}^2 \\ &\sim 4\pi a \zeta(t) \Omega^{-1} \left\{ N^2\xi^2 + 2N\xi \left[N(1-\xi) - \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \right] \right\} \\ &= 4\pi a \zeta(t) \Omega^{-1} \left[N^2\xi(2-\xi) - 2N\xi \int d\mathbf{r}\, \psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \right]. \end{aligned} \tag{2.22}$$

Note that the term $a_0^*(t)a_0(t)$ inside the braces in the first line of this equation contributes $O(N\xi)$ to the constant and $O(1)$ to the c-number multiplying $\psi_1^*\psi_1$, and is therefore neglected.

In analogy with Eqs. (A10)–(A12) of Appendix A, the V_2 of Eq. (2.17) is recast in the form

$$V_2 = V_{21} + V_{22}, \tag{2.23}$$

where

$$\begin{aligned} V_{21} &= 4\pi a\Omega^{-1} \int d\mathbf{r}\, [\Phi^*(\mathbf{r},t)^2 a_0^*(t)^2 \psi_1(\mathbf{r},t)^2 \\ &\quad + \Phi(\mathbf{r},t)^2 \psi_1^*(\mathbf{r},t)^2 a_0(t)^2] \end{aligned} \tag{2.24}$$

and

$$V_{22} = 16\pi a\Omega^{-1} \int d\mathbf{r}\, |\Phi(\mathbf{r},t)|^2 a_0^*(t)\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)a_0(t). \tag{2.25}$$

While nothing further needs to be done for V_{21}, it is necessary to find approximations to V_{22}, V_3, and V_4.

At this point, two difficulties are encountered:

(i) Because $|\Phi(\mathbf{r},t)|^2$ is in general not a constant, the integral on the right-hand side of Eq. (2.25) is not proportional to that on the right-hand side of Eq. (2.13). Therefore, the straightforward procedure followed in order to obtain the approximation (A14) does not work for the V_{22} of Eq. (2.25).

(ii) In the case with translational invariance, the steps that lead to the approximation (A6) from Eq. (A5) and to the approximation (A16) from Eq. (A9) invoke the momentum representation. Such approximations depend on the choice of the representation. While the use of the momentum representation is quite natural for that case, it is necessary to ascertain, in the presence of an external potential, what single-particle states should be employed to replace the eigenstates of the momentum.

These two difficulties are related. Instead of attempting to address these issues directly at this stage of the calculations, let $\phi_i(\mathbf{r},t)$, $i = 1, 2, 3, \ldots$, denote the single-particle wave functions that play the role of $e^{i\mathbf{k}\cdot\mathbf{r}}$, $\mathbf{k} \neq 0$, when translational invariance holds. These functions satisfy the orthonormality conditions

$$\int d\mathbf{r}\, \Phi^*(\mathbf{r},t)\phi_i(\mathbf{r},t) \;=\; 0$$

and

$$\Omega^{-1}\int d\mathbf{r}\,\phi_i^*(\mathbf{r},t)\phi_j(\mathbf{r},t) \;=\; \delta_{ij}. \tag{2.26}$$

For the time being, the question is deferred as to what these $\phi_i(\mathbf{r},t)$ are. In terms of the $\phi_i(\mathbf{r},t)$, the field operators $\psi_1^*(\mathbf{r},t)$ and $\psi_i(\mathbf{r},t)$ of Eqs. (2.12) are expanded as

$$\begin{aligned}\psi_1^*(\mathbf{r},t) \;&=\; \Omega^{-1/2}\sum_{i=1}^{\infty}\phi_i^*(\mathbf{r},t)a_i^*(t),\\ \psi_1(\mathbf{r},t) \;&=\; \Omega^{-1/2}\sum_{i=1}^{\infty}\phi_i(\mathbf{r},t)a_i(t),\end{aligned} \tag{2.27}$$

where $a_i^*(t)$ and $a_i(t)$ satisfy the usual commutation relations for bosons, i.e., $[a_i(t), a_j^*(t)] = \delta_{ij}$. Then, in accord with the steps involved in going from Eq. (A9) to the approximation (A16), the V_4 of Eq. (2.19) rewritten as

$$\begin{aligned}V_4 \;&=\; 4\pi a\Omega^{-2}\sum_{i,j,k,l}a_i^*(t)a_j^*(t)a_k(t)a_l(t)\\ &\quad\times\int d\mathbf{r}\,\phi_i^*(\mathbf{r},t)\phi_j^*(\mathbf{r},t)\phi_k(\mathbf{r},t)\phi_l(\mathbf{r},t)\end{aligned} \tag{2.28}$$

is approximated by

$$\begin{aligned}V_4 \;&\sim\; 8\pi a\Omega^{-2}\sum_{i,j=1}^{\infty}a_i^*(t)a_j^*(t)a_i(t)a_j(t)\\ &\quad\times\int d\mathbf{r}\,|\phi_i(\mathbf{r},t)\phi_j(\mathbf{r},t)|^2\\ &\sim\; 8\pi a\int d\mathbf{r}\left[\Omega^{-1}\sum_{i=1}^{\infty}a_i^*(t)a_i(t)|\phi_i(\mathbf{r},t)|^2\right]^2.\end{aligned} \tag{2.29}$$

Note the factor of 2 between the $4\pi a$ in Eq. (2.28) and the $8\pi a$ in the approximation (2.29).

Attention is now turned to difficulty (i). In the present notation, the fact that $|\phi_i(\mathbf{r},t)|^2$ is in general not independent of $\mathbf{r}$ means that the sum on the right-hand side of the approximation (2.29) cannot be simply approximated by $N(1-\xi)$. This difficulty can be circumvented in view of the following considerations. First, in the same way that (2.29) is obtained from Eq. (2.28), the expression

$$\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) = \Omega^{-1}\sum_{i,j=1}^{\infty}\phi_i^*(\mathbf{r},t)\phi_j(\mathbf{r},t)a_i^*(t)a_j(t) \tag{2.30}$$

may be approximated to the lowest order in the particle density by

$$\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \;\sim\; \Omega^{-1}\sum_{i=1}^{\infty}|\phi_i(\mathbf{r},t)|^2 n_i(t), \qquad n_i(t) = a_i^*(t)a_i(t). \tag{2.31}$$

Second, as discussed by Lee and Yang in Sec. 3 of Ref. [7], it is desirable to start with an N-body state with the occupation numbers

$$n_0 = N\xi \quad \text{and} \quad n_i = n_i^0 = O(1), \tag{2.32}$$

for $i \geq 1$, where

$$\sum_{i=1}^{\infty} n_i^0 = N(1-\xi). \tag{2.33}$$

For low densities, the occupation numbers $n_i(t)$ do not fluctuate excessively, and hence to zeroth order in the particle density,

$$\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i(t) \sim \Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0. \tag{2.34}$$

Finally, the approximations (2.31) and (2.34) are used to simplify the right-hand side of formula (2.29) for V_4. This is somewhat tricky; for example, it is clearly not allowed to use formula (2.31) in the right-hand side of formula (2.29) directly. Instead, the proposed sequence of steps is

$$\begin{aligned}
V_4 \sim\ & 8\pi a \int d\mathbf{r} \left\{ \Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 \right. \\
& \left. + \left[\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i(t) - \Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 \right] \right\}^2 \\
\sim\ & 8\pi a \int d\mathbf{r} \left\{ \left[\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 \right]^2 \right. \\
& \left. + 2 \left[\Omega^{-1} \sum_{j=1}^{\infty} |\phi_j(\mathbf{r},t)|^2 n_j^0 \right] \left[\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i(t) - \Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 \right] \right\} \\
=\ & 8\pi a \int d\mathbf{r} \left[\Omega^{-1} \sum_{j=1}^{\infty} |\phi_j(\mathbf{r},t)|^2 n_j^0 \right] \left[-\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 + 2\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i(t) \right] \\
\sim\ & 8\pi a \int d\mathbf{r} \left[\Omega^{-1} \sum_{j=1}^{\infty} |\phi_j(\mathbf{r},t)|^2 n_j^0 \right] \left[-\Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0 + 2\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \right].
\end{aligned} \tag{2.35}$$

This is the desired result for V_4. Use of expression (2.31) in the last step of approximation (2.35) is due to the multiplication of $\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)$ by c-numbers only.

At this point, it is convenient to define

$$A(\mathbf{r},t) = \Omega^{-1} \sum_{i=1}^{\infty} |\phi_i(\mathbf{r},t)|^2 n_i^0. \tag{2.36}$$

In terms of $A(\mathbf{r},t)$, the V_4 of (2.35) is recast in the form

$$V_4 \sim 8\pi a \int d\mathbf{r}\, A(\mathbf{r},t)[-A(\mathbf{r},t) + 2\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)]. \tag{2.37}$$

Similar procedures can be applied to the V_3 and V_{22} of Eqs. (2.18) and (2.25). Taking again into account the factor of 2, the approximations for V_3 read

$$\begin{aligned}
V_3 \;&=\; 8\pi a\Omega^{-1/2} \int d\mathbf{r} \left[\Phi^*(\mathbf{r},t)a_0^*(t)\Omega^{-3/2}\sum_{i,j,k}\phi_i^*(\mathbf{r},t)\phi_j(\mathbf{r},t)\phi_k(\mathbf{r},t)a_i^*(t)a_j(t)a_k(t)\right.\\
&\quad \left. +\, \Phi(\mathbf{r},t)\Omega^{-3/2}\sum_{i,j,k}\phi_i^*(\mathbf{r},t)\phi_j^*(\mathbf{r},t)\phi_k(\mathbf{r},t)a_i^*(t)a_j^*(t)a_k(t)a_0(t)\right]\\
&\sim\; 8\pi a\Omega^{-1/2} \int d\mathbf{r} \left[2\Phi^*(\mathbf{r},t)a_0^*(t)\Omega^{-3/2}\sum_{i,j}\phi_i^*(\mathbf{r},t)\phi_i(\mathbf{r},t)\phi_j(\mathbf{r},t)a_i^*(t)a_i(t)a_j(t)\right.\\
&\quad \left. +\, 2\Phi(\mathbf{r},t)\Omega^{-3/2}\sum_{i,j}\phi_i^*(\mathbf{r},t)\phi_j^*(\mathbf{r},t)\phi_j(\mathbf{r},t)a_i^*(t)a_j^*(t)a_j(t)a_0(t)\right]\\
&=\; 16\pi a\Omega^{-1/2} \int d\mathbf{r} \left[\Phi^*(\mathbf{r},t)a_0^*(t)\Omega^{-1}\sum_{i=1}^{\infty}|\phi_i(\mathbf{r},t)|^2 n_i(t)\psi_1(\mathbf{r},t)\right.\\
&\quad \left. +\, \Phi(\mathbf{r},t)\psi_1^*(\mathbf{r},t)a_0(t)\Omega^{-1}\sum_{j=1}^{\infty}|\phi_j(\mathbf{r},t)|^2 n_j(t)\right]\\
&\sim\; 16\pi a\Omega^{-1/2} \int d\mathbf{r}\, A(\mathbf{r},t)[\Phi^*(\mathbf{r},t)a_0^*(t)\psi_1(\mathbf{r},t) + \Phi(\mathbf{r},t)\psi_1^*(\mathbf{r},t)a_0(t)].
\end{aligned} \tag{2.38}$$

The corresponding calculation for V_{22} is

$$\begin{aligned}
V_{22} \;&=\; 16\pi a\Omega^{-1}a_0^*(t)a_0(t)\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\\
&=\; 16\pi a\Omega^{-1}\left\{N\xi + \left[N(1-\xi) - \int d\mathbf{r}\,\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\right]\right\}\\
&\quad \times \int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2\{A(\mathbf{r},t) + [\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) - A(\mathbf{r},t)]\}\\
&\sim\; 16\pi a\Omega^{-1}\int d\mathbf{r}\,\left\{N\xi|\Phi(\mathbf{r},t)|^2A(\mathbf{r},t) + N\xi|\Phi(\mathbf{r},t)|^2[\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) - A(\mathbf{r},t)]\right.\\
&\quad \left. +\, |\Phi(\mathbf{r},t)|^2A(\mathbf{r},t)\left[N(1-\xi) - \int d\mathbf{r}'\,\psi_1^*(\mathbf{r}',t)\psi_1(\mathbf{r}',t)\right]\right\}\\
&=\; 16\pi a\Omega^{-1}\left\{N(1-\xi)\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2A(\mathbf{r},t) + N\xi\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\right.\\
&\quad \left. -\left[\int d\mathbf{r}'\,|\Phi(\mathbf{r}',t)|^2A(\mathbf{r}',t)\right]\int d\mathbf{r}\,\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\right\}.
\end{aligned} \tag{2.39}$$

The desired approximation to the V of Eq. (2.9) is therefore given by Eqs. (2.14) and

(2.23) together with expressions (2.22), (2.21), (2.24), (2.39), (2.38), and (2.37). Explicitly,

$$
\begin{aligned}
V \;\sim\; & 4\pi a\left\{\zeta(t)N^2\Omega^{-1}[1-(1-\xi)^2] + 4N\Omega^{-1}(1-\xi)\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2 A(\mathbf{r},t)\right.\\
& \left. -\,2\int d\mathbf{r}\,[A(\mathbf{r},t)]^2\right\} + \Omega^{-1/2}a_0(t)\int d\mathbf{r}\,[8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t)\\
& +\,16\pi a A(\mathbf{r},t)\Phi(\mathbf{r},t)]\psi_1^*(\mathbf{r},t) + \Omega^{-1/2}a_0^*(t)\int d\mathbf{r}\,[8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t)\\
& +\,16\pi a A(\mathbf{r},t)\Phi^*(\mathbf{r},t)]\psi_1(\mathbf{r},t) + \int d\mathbf{r}\,\left[-8\pi a\zeta(t)N\xi\Omega^{-1} + 16\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\right.\\
& \left. +\,16\pi a A(\mathbf{r},t) - 16\pi a\Omega^{-1}\int d\mathbf{r}'\,|\Phi(\mathbf{r}',t)|^2 A(\mathbf{r}',t)\right]\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\\
& +\,4\pi a\Omega^{-1}a_0(t)^2\int d\mathbf{r}\,\Phi(\mathbf{r},t)^2\psi_1^*(\mathbf{r},t)^2 + 4\pi a\Omega^{-1}a_0^*(t)^2\int d\mathbf{r}\,\Phi^*(\mathbf{r},t)^2\psi_1(\mathbf{r},t)^2. \quad (2.40)
\end{aligned}
$$

For completeness, the T of Eq. (2.8) is given by

$$
\begin{aligned}
T \;=\; & N[\bar{\zeta}(t)+\zeta_e(t)] + \Omega^{-1/2}a_0(t)\int d\mathbf{r}\,[-\nabla^2\Phi(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi(\mathbf{r},t)]\psi_1^*(\mathbf{r},t)\\
& +\,\Omega^{-1/2}a_0^*(t)\int d\mathbf{r}\,[-\nabla^2\Phi^*(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi^*(\mathbf{r},t)]\psi_1(\mathbf{r},t)\\
& +\int d\mathbf{r}\,\{|\nabla\psi_1(\mathbf{r},t)|^2 + V_e(\mathbf{r},t)\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) - [\bar{\zeta}(t)+\zeta_e(t)]\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)\}, \quad (2.41)
\end{aligned}
$$

where

$$
\bar{\zeta}(t) \;=\; \Omega^{-1}\int d\mathbf{r}\,|\nabla\Phi(\mathbf{r},t)|^2, \qquad \zeta_e(t) = \Omega^{-1}\int d\mathbf{r}\,V_e(\mathbf{r},t)|\Phi(\mathbf{r},t)|^2. \quad (2.42)
$$

Attention is herein restricted to boundary conditions for which integration by parts does not produce any surface terms.

Accordingly, the approximate Hamiltonian, called H_2, is given by

$$
H_2 = H^{(0)} + H^{(1)} + H^{(2)}, \quad (2.43)
$$

where

$$
\begin{aligned}
H^{(0)} \;=\; & N[\bar{\zeta}(t)+\zeta_e(t)] + 4\pi a\left\{\zeta(t)N^2\Omega^{-1}[1-(1-\xi)^2]\right.\\
& \left. +\,4N\Omega^{-1}(1-\xi)\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2 A(\mathbf{r},t) - 2\int d\mathbf{r}\,[A(\mathbf{r},t)]^2\right\}, \quad (2.44)
\end{aligned}
$$

$$
\begin{aligned}
H^{(1)} \;=\; & \Omega^{-1/2}a_0(t)\int d\mathbf{r}\,[-\nabla^2\Phi(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi(\mathbf{r},t)\\
& +\,8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t) + 16\pi a A(\mathbf{r},t)\Phi(\mathbf{r},t)]\psi_1^*(\mathbf{r},t)\\
& +\,\Omega^{-1/2}a_0^*(t)\int d\mathbf{r}\,[-\nabla^2\Phi^*(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi^*(\mathbf{r},t)\\
& +\,8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t) + 16\pi a A(\mathbf{r},t)\Phi^*(\mathbf{r},t)]\psi_1(\mathbf{r},t), \quad (2.45)
\end{aligned}
$$

and

$$
\begin{aligned}
H^{(2)} \;=\; & \int d\mathbf{r}\, \Bigg\{ |\nabla\psi_1(\mathbf{r},t)|^2 + \bigg[V_e(\mathbf{r},t) - \bar{\zeta}(t) - \zeta_e(t) - 8\pi a \zeta(t) N\xi\Omega^{-1} \\
& + 16\pi a N\xi\Omega^{-1} |\Phi(\mathbf{r},t)|^2 + 16\pi a A(\mathbf{r},t) \\
& -\; 16\pi a\Omega^{-1} \int d\mathbf{r}'\, |\Phi(\mathbf{r}',t)|^2 A(\mathbf{r}',t) \bigg] \psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \Bigg\} \\
& + 4\pi a\Omega^{-1} a_0(t)^2 \int d\mathbf{r}\, \Phi(\mathbf{r},t)^2 \psi_1^*(\mathbf{r},t)^2 \\
& + 4\pi a\Omega^{-1} a_0^*(t)^2 \int d\mathbf{r}\, \Phi^*(\mathbf{r},t)^2 \psi_1(\mathbf{r},t)^2 .
\end{aligned} \tag{2.46}
$$

III. FIRST-ORDER THEORY

In this first-order theory, the last two terms of Eq. (2.46) involving $a_0(t)^2$ and $a_0^*(t)^2$ are neglected. These terms describe pair creation and annihilation to be addressed in Sec. 4. The resulting Hamiltonian, called H_1, is

$$H_1 = H^{(0)} + H^{(1)} + \bar{H}^{(2)}, \tag{3.1}$$

where

$$
\begin{aligned}
\bar{H}^{(2)} \;=\; & \int d\mathbf{r}\, \Bigg\{ |\nabla\psi_1(\mathbf{r},t)|^2 + \bigg[V_e(\mathbf{r},t) - \bar{\zeta}(t) - \zeta_e(t) \\
& - 8\pi a \zeta(t) N\xi\Omega^{-1} + 16\pi a N\xi\Omega^{-1} |\Phi(\mathbf{r},t)|^2 + 16\pi a A(\mathbf{r},t) \\
& -\; 16\pi a\Omega^{-1} \int d\mathbf{r}'\, |\Phi(\mathbf{r}',t)|^2 A(\mathbf{r}',t) \bigg] \psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t) \Bigg\} .
\end{aligned} \tag{3.2}
$$

Note that H_1 is linear in $a_0^*(t)\psi_1(\mathbf{r},t)$, $\psi_1^*(\mathbf{r},t)a_0(t)$, and $\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)$, a fact which makes it possible to obtain the equations of motion for $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$.

In the first-order theory for zero temperature, the N-body Schrödinger state vector is [2, 3]

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

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

$$\psi(\mathbf{r})|\text{vac}\rangle = 0. \tag{3.3}$$

For the present case, the N-body Schrödinger state vector is chosen to be

$$\Psi(t) = e^{-i\theta(t)}\, \frac{a_0^*(t)^{N\xi}}{[(N\xi)!]^{1/2}} \prod_{i=1}^{\infty} \frac{a_i^*(t)^{n_i^0}}{(n_i^0!)^{1/2}}\, |\text{vac}\rangle, \tag{3.4}$$

where $\theta(t)$ is a c-number function of time.

Several comments on this expression are in order:

(i) The n_i^0 are non-negative integers that satisfy Eq. (2.33). Therefore, only a finite number of these n_i^0 can be nonzero, and hence the product over i in Eq. (3.4) is actually a finite product.

(ii) Since the n_i^0 are integers, dn_i^0/dt can only be delta functions. However, in the present approximation, no such delta functions are present in the Hamiltonian. Hence, all n_i^0 are independent of the time t.

(iii) This time independence of n_i^0 gives an explicit illustration of an important point already discussed in Refs. [2] and [3], namely, that the present approach is valid only on a moderate time scale. This is true for both zero and nonzero temperatures, and there are many open questions for both shorter time scales and longer time scales.

(iv) Finally, the factor $e^{-i\theta(t)}$ is introduced for the following reason. Since the right-hand side of Eq. (3.4) is a product of the distinct creation operators $a_0^*(t)$ and $a_i^*(t)$, there is no restriction that can prevent the shifting of exponential factors from one creation operator to another. This is to be contrasted with the case at zero temperature, where only $a_0^*(t)^N$ appears in the first-order Schrödinger state vector. It is therefore convenient to include the factor $e^{-i\theta(t)}$ in order to obtain relatively simple equations of motion for $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$.

The N-particle Schrödinger equation in the first order is

$$i(\partial/\partial t)\Psi(t) = H_1\Psi(t). \tag{3.5}$$

In order to calculate the right-hand side, define

$$\Psi_0(t) = e^{-i\theta(t)} N\xi \, \frac{a_0^*(t)^{N\xi-1}}{[(N\xi)!]^{1/2}} \prod_{i=1}^{\infty} \frac{a_i^*(t)^{n_i^0}}{(n_i^0!)^{1/2}} \, |\mathrm{vac}\rangle \tag{3.6}$$

and, for $i = 1, 2, 3, \ldots,$

$$\Psi_i(t) = e^{-i\theta(t)} \, \frac{a_0^*(t)^{N\xi}}{[(N\xi)!]^{1/2}} \, n_i^0 \, \frac{a_i^*(t)^{n_i^0-1}}{(n_i^0!)^{1/2}} \prod_{j\neq i} \frac{a_j^*(t)^{n_j^0}}{(n_j^0!)^{1/2}} \, |\mathrm{vac}\rangle. \tag{3.7}$$

Note that $\Psi_i(t) = 0$ if $n_i^0 = 0$. Thus, there is only a finite number of nonzero $\Psi_i(t)$. With these definitions, the left-hand side of Eq. (3.5) becomes

$$i(\partial/\partial t)\Psi(t) \;=\; \theta'(t)\Psi(t) + i\,\frac{\partial a_0^*(t)}{\partial t}\,\Psi_0(t) + \sum_{j=1}^{\infty} i\,\frac{\partial a_j^*(t)}{\partial t}\,\Psi_j(t). \tag{3.8}$$

The combination of Eqs. (2.45), (3.2), (3.5), and (3.8) suggests that it is useful to define the creation operators

$$\begin{aligned} b_0^*(t) &= i(\partial/\partial t)a_0^*(t) - \Omega^{-1/2}\int d\mathbf{r}\,[-\nabla^2\Phi(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi(\mathbf{r},t) \\ &\quad + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t) + 16\pi a A(\mathbf{r},t)\Phi(\mathbf{r},t)]\psi_1^*(\mathbf{r},t) \end{aligned} \tag{3.9}$$

and, for $i = 1, 2, 3, \ldots,$

$$\begin{aligned} b_i^*(t) &= i(\partial/\partial t)a_i^*(t) - \Omega^{-1}a_0^*(t)\int d\mathbf{r}\,[-\nabla^2\Phi^*(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi^*(\mathbf{r},t) \\ &\quad + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi^*(\mathbf{r},t) + 16\pi a A(\mathbf{r},t)\Phi^*(\mathbf{r},t)]\phi_i(\mathbf{r},t) \\ &\quad - \Omega^{-1/2}\int d\mathbf{r}\,\Big\{-\nabla^2\phi_i(\mathbf{r},t) + \Big[V_e(\mathbf{r},t) - \bar{\zeta}(t) - \zeta_e(t) \\ &\quad - 8\pi a N\xi\,\zeta(t)\Omega^{-1} + 16\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2 + 16\pi a A(\mathbf{r},t) \\ &\quad - 16\pi a\Omega^{-1}\int d\mathbf{r}'\,|\Phi(\mathbf{r}',t)|^2 A(\mathbf{r}',t)\Big]\,\phi_i(\mathbf{r},t)\Big\}\,\psi_1^*(\mathbf{r},t). \end{aligned} \tag{3.10}$$

In terms of $b_0^*(t)$ and $b_i^*(t)$, the Schrödinger equation (3.5) is

$$\theta'(t)\Psi(t) + b_0^*(t)\Psi_0(t) + \sum_{i=1}^{\infty} b_i^*(t)\Psi_i(t) = H^{(0)}\Psi(t), \tag{3.11}$$

with $H^{(0)}$ given by Eq. (2.44). From Eqs. (3.4), (3.6), and (3.7), the equality (3.11) is satisfied only if

$$b_0^*(t) = \bar{c}_0(t)a_0^*(t) \quad \text{and} \quad b_i^*(t) = \bar{c}_i(t)a_i^*(t), \tag{3.12}$$

where $\bar{c}_0(t)$ and $\bar{c}_i(t)$ are c-numbers such that

$$\theta'(t) + N\xi\bar{c}_0(t) + \sum_{i=1}^{\infty} n_i^0\bar{c}_i(t) = H^{(0)}. \tag{3.13}$$

From the mathematical point of view, this is the only condition that $\theta'(t)$, $\bar{c}_0(t)$, and $\bar{c}_i(t)$ must satisfy.

With $b_0^*(t)$ and $b_i^*(t)$ given by Eqs. (3.12), the equations of motion for $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$ follow from Eqs. (3.9) and (3.10), respectively. By virtue of the definitions (2.11) and (2.12) for $a_0^*(t)$ and $\psi_1^*(\mathbf{r},t)$, Eq. (3.9) with Eqs. (3.12) can be cast in the form

$$\begin{aligned} &\int d\mathbf{r}\,\psi^*(\mathbf{r})\Big\{-i(\partial/\partial t)\Phi(\mathbf{r},t) + \bar{c}_0(t)\Phi(\mathbf{r},t) \\ &\quad + \int d\mathbf{r}'\,[-\nabla'^2\Phi(\mathbf{r}',t) + V_e(\mathbf{r}',t)\Phi(\mathbf{r}',t) + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r}',t)|^2\Phi(\mathbf{r}',t) \\ &\quad + 16\pi a A(\mathbf{r}',t)\Phi(\mathbf{r}',t)][\delta(\mathbf{r}-\mathbf{r}') - \Omega^{-1}\Phi(\mathbf{r},t)\Phi^*(\mathbf{r}',t)]\Big\} = 0. \end{aligned} \tag{3.14}$$

Thus, the quantity in the braces must itself be zero, leading to

$$
\begin{aligned}
i(\partial/\partial t)\Phi(\mathbf{r},t) \;=\; & -\nabla^2\Phi(\mathbf{r},t) + V_e(\mathbf{r},t)\Phi(\mathbf{r},t) + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2\Phi(\mathbf{r},t) \\
& + 16\pi a A(\mathbf{r},t)\Phi(\mathbf{r},t) - \Bigg[\bar{\zeta}(t) + \zeta_e(t) + 8\pi a N\xi\Omega^{-1}\zeta(t) \\
& + 16\pi a\Omega^{-1}\int d\mathbf{r}'\, A(\mathbf{r}',t)|\Phi(\mathbf{r}',t)|^2\Bigg]\Phi(\mathbf{r},t) + \bar{c}_0(t)\Phi(\mathbf{r},t). \qquad (3.15)
\end{aligned}
$$

In the same vein, it follows from Eq. (3.10) with Eqs. (3.12) that, for $i = 1, 2, 3, \ldots,$

$$
\begin{aligned}
i(\partial/\partial t)\phi_i(\mathbf{r},t) \;=\; & \Bigg[-\nabla^2 + V_e(\mathbf{r},t) + 16\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2 + 16\pi a A(\mathbf{r},t) - \bar{\zeta}(t) - \zeta_e(t) \\
& - 8\pi a N\xi\Omega^{-1}\zeta(t) - 16\pi a\Omega^{-1}\int d\mathbf{r}'\, A(\mathbf{r}',t)|\Phi(\mathbf{r}',t)|^2 + \bar{c}_i(t)\Bigg]\phi_i(\mathbf{r},t) \\
& - \Omega^{-1}\Phi(\mathbf{r},t)\int d\mathbf{r}'\, \Phi^*(\mathbf{r}',t)8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r}',t)|^2\phi_i(\mathbf{r}',t). \qquad (3.16)
\end{aligned}
$$

These are the desired equations of motion for $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$.

Emphasis should be placed on the importance of the last term on the right-hand side of Eq. (3.16). This term is related to the fact that the coefficient of the third term on the right-hand side of Eq. (3.15) is 8 while that of Eq. (3.16) is 16. The latter is needed in order for the equations of motion to be consistent with the orthonormality as expressed by Eqs. (2.26). More precisely, the conditions (2.26) imply that

$$
\int d\mathbf{r}\,\{\Phi^*(\mathbf{r},t)i(\partial/\partial t)\phi_i(\mathbf{r},t) - \phi_i(\mathbf{r},t)[i(\partial/\partial t)\Phi(\mathbf{r},t)]^*\} \;=\; 0 \qquad (3.17)
$$

and

$$
\int d\mathbf{r}\,\{\phi_i^*(\mathbf{r},t)i(\partial/\partial t)\phi_j(\mathbf{r},t) - \phi_j(\mathbf{r},t)[i(\partial/\partial t)\phi_i(\mathbf{r},t)]^*\} \;=\; 0, \qquad (3.18)
$$

which are satisfied by Eqs. (3.15) and (3.16) provided $\bar{c}_0(t)$ and $\bar{c}_i(t)$ are real, as they should be.

These equations of motion can be simplified slightly as follows. The relation (3.13) is explicitly

$$
\begin{aligned}
& \theta'(t) + N\xi\bar{c}_0(t) + \sum_{i=1}^{\infty} n_i^0\bar{c}_i(t) \\
& \;=\; N[\bar{\zeta}(t) + \zeta_e(t)] + 4\pi a N^2\Omega^{-1}\zeta(t)[1-(1-\xi)^2] \\
& \quad + 16\pi a N\Omega^{-1}(1-\xi)\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2 A(\mathbf{r},t) - 8\pi a\int d\mathbf{r}\,[A(\mathbf{r},t)]^2. \qquad (3.19)
\end{aligned}
$$

A comparison of Eq. (3.19) with Eqs. (3.15) and (3.16) shows that it is desirable to introduce $c_0(t)$ and $c_i(t)$ according to the equations

$$\begin{aligned} \bar{c}_0(t) - c_0(t) &= \bar{c}_i(t) - c_i(t) \\ &= \bar{\zeta}(t) + \zeta_e(t) + 4\pi a N \Omega^{-1} \zeta(t)[1 - (1-\xi)^2] \\ &\quad + 16\pi a \Omega^{-1} \int d\mathbf{r}\, |\Phi(\mathbf{r}, t)|^2 A(\mathbf{r}, t). \end{aligned} \tag{3.20}$$

Then, $c_0(t)$ and $c_i(t)$ satisfy

$$\begin{aligned} &\theta'(t) + N\xi c_0(t) + \sum_{i=1}^{\infty} n_i^0 c_i(t) \\ &= -16\pi a N \xi \Omega^{-1} \int d\mathbf{r}\, |\Phi(\mathbf{r}, t)|^2 A(\mathbf{r}, t) - 8\pi a \int d\mathbf{r}\, [A(\mathbf{r}, t)]^2, \end{aligned} \tag{3.21}$$

and the equations of motion take the form

$$\begin{aligned} &i(\partial/\partial t)\Phi(\mathbf{r}, t) \\ &\quad = [-\nabla^2 + V_e(\mathbf{r}, t) + 8\pi a N \xi \Omega^{-1} |\Phi(\mathbf{r}, t)|^2 \\ &\qquad - 4\pi a N \xi^2 \Omega^{-1} \zeta(t) + 16\pi a A(\mathbf{r}, t) + c_0(t)]\Phi(\mathbf{r}, t) \end{aligned} \tag{3.22}$$

and, for $i = 1, 2, 3, \ldots,$

$$\begin{aligned} &i(\partial/\partial t)\phi_i(\mathbf{r}, t) \\ &\quad = [-\nabla^2 + V_e(\mathbf{r}, t) + 16\pi a N \xi \Omega^{-1} |\Phi(\mathbf{r}, t)|^2 - 4\pi a N \xi^2 \Omega^{-1} \zeta(t) + 16\pi a A(\mathbf{r}, t) \\ &\qquad + c_i(t)]\phi_i(\mathbf{r}, t) - \Omega^{-1}\Phi(\mathbf{r}, t) \int d\mathbf{r}'\, \Phi^*(\mathbf{r}', t) 8\pi a N \xi \Omega^{-1} |\Phi(\mathbf{r}', t)|^2 \phi_i(\mathbf{r}', t). \end{aligned} \tag{3.23}$$

Mathematically, Eqs. (3.21)–(3.23) are the only consequences of the N-body Schrödinger equation (3.5) with the state vector in the form of Eq. (3.4), i.e., Eqs. (3.21)–(3.23) together with Eq. (3.4) imply Eq. (3.5). However, physically it does not make sense to have equations of motion (3.23) for the single-particle wave functions $\phi_i(\mathbf{r}, t)$ with $c_i(t)$ that *depend* on the index i, because each $\phi_i(\mathbf{r}, t)$ should satisfy the same equation of motion. Therefore, the conclusion is reached that

$$\text{each } c_i(t) \text{ is independent of the index } i. \tag{3.24}$$

Although not compelling, it is natural to make the choice

$$c_0(t) = c_i(t) = 0. \tag{3.25}$$

With this choice, the final result reads

$$\theta'(t) = -16\pi a N\xi\Omega^{-1}\int d\mathbf{r}\,|\Phi(\mathbf{r},t)|^2 A(\mathbf{r},t) - 8\pi a\int d\mathbf{r}\,[A(\mathbf{r},t)]^2, \tag{3.26}$$

$$\begin{aligned} i(\partial/\partial t)\Phi(\mathbf{r},t) &= [-\nabla^2 + V_e(\mathbf{r},t) + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2 \\ &\quad - 4\pi a N\xi^2\Omega^{-1}\zeta(t) + 16\pi a A(\mathbf{r},t)]\Phi(\mathbf{r},t), \end{aligned} \tag{3.27}$$

and, for $i = 1, 2, 3, \ldots,$

$$\begin{aligned} &i(\partial/\partial t)\phi_i(\mathbf{r},t) \\ &\quad= [-\nabla^2 + V_e(\mathbf{r},t) + 16\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r},t)|^2 - 4\pi a N\xi^2\Omega^{-1}\zeta(t) + 16\pi a A(\mathbf{r},t)]\phi_i(\mathbf{r},t) \\ &\qquad - \Omega^{-1}\Phi(\mathbf{r},t)\int d\mathbf{r}'\,\Phi^*(\mathbf{r}',t) 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r}',t)|^2\phi_i(\mathbf{r}',t). \end{aligned} \tag{3.28}$$

Alternatively, both $c_0(t)$ and $c_i(t)$ can be chosen to be N^{-1} times the right-hand side of Eq. (3.26), leading to $\theta(t) = 0$. With both choices, the equation of motion for $\Phi(\mathbf{r},t)$ at zero temperature is trivially recovered when $\xi = 1$ and $A(\mathbf{r},t) = 0$.

IV. PAIR PRODUCTION

The pair production becomes manifest by retaining terms proportional to $\psi_1^*(\mathbf{r},t)^2 a_0(t)^2$ and $a_0^*(t)^2\psi_1(\mathbf{r},t)^2$ in the approximate Hamiltonian of Eq. (2.43). In the time-independent case at zero temperature, the N-body Schrödinger state vector assumes the following form [2, 3]:

$$\Psi = \mathcal{N} e^P (N!)^{-1/2} a_0^{*N}|\text{vac}\rangle, \tag{4.1}$$

where

$$P = (2N)^{-1}\int d\mathbf{r}\,d\mathbf{r}'\,\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')K_0(\mathbf{r},\mathbf{r}')a_0^2 \tag{4.2}$$

describes the scattering of pairs of atoms from the condensate to other states, $K_0(\mathbf{r},\mathbf{r}')$ is the pair-excitation function, and $\mathcal{N}$ is a normalization constant. Of course, the external potential is also assumed to be independent of time. As is discussed in Ref. [2], this assumption on the form of the Schrödinger wave function amounts to a definitive prescription of how to approximate the many-particle Green's functions.

At finite temperatures, the inclusion of pair creation in the case with translational invariance has been recognized to enable a systematic treatment of physical effects such as first and second sound [8]. In the presence of an external potential the role of pair excitation is equally important. Except for a complication concerning the N-body Schrödinger state vector, the analysis of the pair-excitation function for nonzero temperatures is quite similar to that for zero temperature. Following the procedure presented in Sec. 3 of Ref. [3], consider the time-independent case; by neglecting a constant, the relevant terms from H_2 are just those from $H^{(2)}$. Similar to Eq. (3.5) in Ref. [3],

$$\begin{aligned} H_2 &= H^{(2)} \\ &= \int d\mathbf{r} \left\{ |\nabla\psi_1(\mathbf{r})|^2 + \left[-\bar{\zeta} - \zeta_e - \frac{8\pi a N\xi}{\Omega}\,\zeta + V_e(\mathbf{r}) + \frac{16\pi a N\xi}{\Omega}\,|\Phi(\mathbf{r})|^2 \right.\right. \\ &\quad \left. + 16\pi a A(\mathbf{r}) - \frac{16\pi a}{\Omega} \int d\mathbf{r}'\, |\Phi(\mathbf{r}')|^2 A(\mathbf{r}') \right] \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) \\ &\quad \left. + \frac{4\pi a}{\Omega}\, a_0^2 \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 + \frac{4\pi a}{\Omega}\, a_0^{*2} \Phi^*(\mathbf{r})^2 \psi_1(\mathbf{r})^2 \right\}. \end{aligned} \tag{4.3}$$

Note the appearance of N here only in the combination $N\xi$.

Define

$$H_2' = e^{-P} H_2 e^{P}, \tag{4.4}$$

where

$$P = (2N\xi)^{-1} \int d\mathbf{r}\, d\mathbf{r}'\, \psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') K_0(\mathbf{r},\mathbf{r}') a_0^2, \tag{4.5}$$

which results from Eq. (4.2) by replacing N by $N\xi$. Without loss of generality, this pair-excitation function $K_0(\mathbf{r},\mathbf{r}')$ is chosen to satisfy

$$K_0(\mathbf{r},\mathbf{r}') = K_0(\mathbf{r}',\mathbf{r}) \tag{4.6}$$

and

$$\int d\mathbf{r}'\, \Phi^*(\mathbf{r}') K_0(\mathbf{r},\mathbf{r}') = 0. \tag{4.7}$$

The calculation of H_2' introduced by Eq. (4.4) is carried out in some detail in Appendix B. H_2' can be written as

$$H_2' \sim H_2'' + H_{2c}', \tag{4.8}$$

where

$$\begin{aligned} H_2'' &= \int d\mathbf{r} \left\{ |\nabla\psi_1(\mathbf{r})|^2 + \left[-\bar{\zeta} - \zeta_e - \frac{8\pi a N\xi}{\Omega}\,\zeta + V_e(\mathbf{r}) + \frac{16\pi a N\xi}{\Omega}\,|\Phi(\mathbf{r})|^2 + 16\pi a A(\mathbf{r}) \right.\right. \\ &\quad \left. - \frac{16\pi a}{\Omega} \int d\mathbf{r}'\, |\Phi(\mathbf{r}')|^2 A(\mathbf{r}') \right] \psi_1^*(\mathbf{r})\psi_1(\mathbf{r}) + \frac{4\pi a}{\Omega}\, \Phi^*(\mathbf{r})^2 a_0^{*2} \psi_1(\mathbf{r})^2 \\ &\quad \left. + \Phi^*(\mathbf{r})^2 \frac{4\pi a N\xi}{\Omega} \left[K_0(\mathbf{r},\mathbf{r}) + 2\int d\mathbf{r}'\, K_0(\mathbf{r},\mathbf{r}')\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r}) \right] \right\}, \end{aligned} \tag{4.9}$$

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

$$\begin{aligned} H'_{2c} \;=\; & \int d\mathbf{r} \left\{ \frac{4\pi a}{\Omega}\, \Phi(\mathbf{r})^2 \psi_1^*(\mathbf{r})^2 - (N\xi)^{-1} \int d\mathbf{r}' \, [\nabla_{\mathbf{r}}^2 K_0(\mathbf{r},\mathbf{r}')] \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') \right. \\ & + \left[-\bar{\zeta} - \zeta_e - \frac{8\pi a N\xi}{\Omega}\, \zeta + V_e(\mathbf{r}) + \frac{16\pi a N\xi}{\Omega}\, |\Phi(\mathbf{r})|^2 + 16\pi a A(\mathbf{r}) \right. \\ & \left. - \frac{16\pi a}{\Omega} \int d\mathbf{r}''\, |\Phi(\mathbf{r}'')|^2 A(\mathbf{r}'') \right] (N\xi)^{-1} \int d\mathbf{r}' \, K_0(\mathbf{r},\mathbf{r}') \psi_1^*(\mathbf{r}) \psi_1^*(\mathbf{r}') \\ & \left. + \Phi^*(\mathbf{r})^2 \frac{4\pi a}{\Omega} \int d\mathbf{r}' \, d\mathbf{r}'' \, K_0(\mathbf{r},\mathbf{r}') K_0(\mathbf{r},\mathbf{r}'') \psi_1^*(\mathbf{r}') \psi_1^*(\mathbf{r}'') \right\} a_0^2. \end{aligned} \tag{4.10}$$

Without further ado, the integro-differential equation for $K_0(\mathbf{r},\mathbf{r}')$ is found to be (see Appendix B)

$$\begin{aligned} & -\nabla_{\mathbf{r}}^2 K_0(\mathbf{r},\mathbf{r}') - \nabla_{\mathbf{r}'}^2 K_0(\mathbf{r},\mathbf{r}') + \frac{8\pi a N\xi}{\Omega}\, \Phi(\mathbf{r})^2 \delta(\mathbf{r}-\mathbf{r}') \\ & + \left\{ -2\bar{\zeta} - 2\zeta_e - \frac{16\pi a N\xi}{\Omega}\, \zeta + V_e(\mathbf{r}) + V_e(\mathbf{r}') + \frac{16\pi a N\xi}{\Omega}\, [|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2] \right. \\ & \left. + 16\pi a [A(\mathbf{r}) + A(\mathbf{r}')] - \frac{32\pi a}{\Omega} \int d\mathbf{r}'' \, |\Phi(\mathbf{r}'')|^2 A(\mathbf{r}'') \right\} K_0(\mathbf{r},\mathbf{r}') \\ & + \frac{8\pi a N\xi}{\Omega} \int d\mathbf{r}'' \, \Phi^*(\mathbf{r}'')^2 K_0(\mathbf{r},\mathbf{r}'') K_0(\mathbf{r}',\mathbf{r}'') \\ & \quad = \frac{8\pi a N\xi}{\Omega^2} \left\{ \Phi(\mathbf{r})\Phi(\mathbf{r}') [|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2 - \zeta] + \Phi(\mathbf{r}) \int d\mathbf{r}'' \, K_0(\mathbf{r}',\mathbf{r}'') |\Phi(\mathbf{r}'')|^2 \Phi^*(\mathbf{r}'') \right. \\ & \qquad \left. + \Phi(\mathbf{r}') \int d\mathbf{r}'' \, K_0(\mathbf{r},\mathbf{r}'') |\Phi(\mathbf{r}'')|^2 \Phi^*(\mathbf{r}'') \right\}. \end{aligned} \tag{4.11}$$

A comparison with the corresponding Eq. (3.25) of Ref. [3] for the zero-temperature case shows that Eq. (4.11) can be obtained under the replacements

$$N \to N\xi$$

and

$$V_e(\mathbf{r}) \;\to\; V_e(\mathbf{r}) + 16\pi a A(\mathbf{r}) - \frac{16\pi a}{\Omega} \int d\mathbf{r}'' \, |\Phi(\mathbf{r}'')|^2 A(\mathbf{r}''). \tag{4.12}$$

For zero external potential ($V_e = 0$) and periodic boundary conditions, Eq. (4.9) with Eq. (4.11) yield the phonon spectrum to the lowest order in the particle density, in agreement with the results of Lee and Yang (Eq. (18) in Ref. [7]). Notably, in the case of zero temperature, the phonon spectrum has been found to remain gapless in the sense of Hohenberg and Martin [19] and Griffin [20] even to higher orders in the particle density [26].

V. DISCUSSION AND CONCLUSION

In Sec. 3, the lowest-order equations of motion are obtained for the condensate wave function $\Phi(\mathbf{r},t)$ and single-particle excitation wave functions $\phi_i(\mathbf{r},t)$. In some correspondence with recent experimental situations, the following steps can be taken to simplify these equations:

(i) The external potential is assumed to be independent of time t, i.e., $V_e(\mathbf{r},t) = V_e(\mathbf{r})$.

(ii) The Bose-Einstein system is considered to be in equilibrium. $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$ are written as

$$\Phi(\mathbf{r},t) \;=\; e^{-iEt}\Phi(\mathbf{r}), \tag{5.1}$$

$$\phi_j(\mathbf{r},t) \;=\; e^{-iE_jt}\phi_j(\mathbf{r}) \quad (j = 1,\, 2,\, 3,\, \ldots), \tag{5.2}$$

where E is the lowest energy per particle in the condensate and E_j is the energy of the jth state. Equations (3.27) and (3.28) then become

$$\begin{aligned}&[-\nabla^2 + V_e(\mathbf{r}) + 8\pi aN\xi\Omega^{-1}|\Phi(\mathbf{r})|^2 - 4\pi aN\xi^2\Omega^{-1}\zeta \\ &\quad + 16\pi aA(\mathbf{r}) - E]\Phi(\mathbf{r}) = 0\end{aligned} \tag{5.3}$$

and, for $i = 1,\, 2,\, 3,\, \ldots,$

$$\begin{aligned}&[-\nabla^2 + V_e(\mathbf{r}) + 16\pi aN\xi\Omega^{-1}|\Phi(\mathbf{r})|^2 - 4\pi aN\xi^2\Omega^{-1}\zeta + 16\pi aA(\mathbf{r}) - E_i]\phi_i(\mathbf{r}) \\ &\quad - \Omega^{-1}\Phi(\mathbf{r})\int d\mathbf{r}\,\Phi^*(\mathbf{r}')8\pi aN\xi\Omega^{-1}|\Phi(\mathbf{r}')|^2\phi_i(\mathbf{r}') = 0,\end{aligned} \tag{5.4}$$

while the total energy of the system is

$$\mathcal{E} \;=\; N\xi E + \sum_{i=1}^{\infty} n_i^0 E_i - 16\pi aN\xi\Omega^{-1}\int d\mathbf{r}\,|\Phi(\mathbf{r})|^2 A(\mathbf{r}) - 8\pi a\int d\mathbf{r}\,[A(\mathbf{r})]^2, \tag{5.5}$$

with

$$A(\mathbf{r}) = \Omega^{-1}\sum_{i=1}^{\infty} |\phi_i(\mathbf{r})|^2 n_i^0. \tag{5.6}$$

Note that the equation for $\Phi(\mathbf{r})$ is coupled with the equations for the $\phi_i(\mathbf{r})$'s through the density $A(\mathbf{r})$.

(iii) The numbers n_i^0 are assumed to obey the Bose-Einstein distribution

$$n_i^0 = [z^{-1}e^{E_i/(k_{\mathrm{B}}T)} - 1]^{-1}, \qquad i = 1,\, 2,\, 3,\, \ldots, \tag{5.7}$$

where z is a suitable Lagrange multiplier or 'fugacity' subject to condition (2.33), k_B is Boltzmann's constant, and the temperature T is below the Bose-Einstein transition point. Once $\Phi(\mathbf{r})$ and $A(\mathbf{r})$ are determined, the pair-excitation function $K_0(\mathbf{r},\mathbf{r}')$ satisfies the integro-differential equation (4.11). Note also that, with Eq. (5.7), $A(\mathbf{r})$ is identified with the density of the normal fluid in the language of superfluid He^4.

The paper can be summarized as follows. The theoretical approach of Refs. [2] and [3] is extended to the case where the superfluid coexists with the normal fluid. Accordingly, the many-body Hamiltonian is approximated for finite temperatures below the transition point by retaining interaction terms that describe pair excitation from the condensate into other states. In the spirit of Lee and Yang [7], the occupation numbers of these states are assumed not to differ drastically from their equilibrium values. The occupation number for the condensate is assumed to be $N\xi$, where ξ is treated as a fixed number. The density of the thermal component, $A(\mathbf{r},t)$, is introduced explicitly and $\psi_1^*(\mathbf{r},t)\psi_1(\mathbf{r},t)-A(\mathbf{r},t)$ is considered as small. In the first-order theory, terms of the approximate Hamiltonian proportional to $a_0(t)^2$ and $a_0^*(t)^2$ are neglected, while a suitable choice for an N-body Schrödinger state vector leads to lowest-order equations of motion for $\Phi(\mathbf{r},t)$ and $\phi_i(\mathbf{r},t)$. With the purpose of studying systematically effects of pair excitation, such as corrections to the total energy and sound vibrations, a next step is to introduce the pair-excitation function $K_0(\mathbf{r},\mathbf{r}';t)$. A lowest-order equation of motion is given for the time-independent $K_0(\mathbf{r},\mathbf{r}')$. Except for a complication involving the N-body state vector, the derivation is similar to the case of zero temperature [3], with an effective potential accounting for the presence of the normal component.

Equations (5.3)–(5.5) and (4.11) are believed to be new. A previous attempt to obtain some of these equations is due to Goldman, Silvera, and Leggett [13], who had referred to [2]. These are all lowest-order equations that may acquire corrections in the particle density. For instance, in order to get the first correction for the condensate wave function, the pair excitation needs to act back on it, modifying its equation of motion beyond the Popov approximation [17]. The present approach is sufficiently general to calculate the first corrections to Eqs. (5.3) and (5.4). More demanding is the derivation of higher-order corrections, where logarithms of the expansion parameter may appear, as in the known case with zero temperature and periodic boundary conditions [26, 27].

The approximate Hamiltonian of Sec. 4 does not include, for example, the decay of a phonon. This fact implies that the equations of motion obtained in this paper hold only over a moderate time scale. The analysis should necessarily be modified for shorter or longer time scales.

Acknowledgments

DM wishes to thank Professor Bertrand Halperin for a useful discussion. TTW is greatly indebted to Professor Chen Ning Yang for numerous discussions.

APPENDIX A: CASE WITH TRANSLATIONAL INVARIANCE AND PERIODIC BOUNDARY CONDITIONS

In this appendix, the approximations applied to the five pieces of V as given by Eqs. (2.15)–(2.19) are considered for the translationally invariant case of Lee and Yang [7], when the free-particle representation with periodic boundary conditions is conveniently chosen. In particular, the total number N of particles is given by

$$N = a_0^* a_0 + \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^* a_{\mathbf{k}}, \tag{A1}$$

where the subscript $\mathbf{k}$ refers to the momentum of the particle. It follows from

$$\Phi(\mathbf{r}) = 1 \tag{A2}$$

and the definition (2.20) that

$$\zeta = 1. \tag{A3}$$

Because of momentum conservation, Eqs. (2.16) and (2.18) give

$$V_1 = 0 \tag{A4}$$

and

$$V_3 = \frac{8\pi a}{\Omega} \sum_{\substack{\mathbf{k}\neq 0\\ \mathbf{k}'\neq 0\\ \mathbf{k}+\mathbf{k}'\neq 0}} (a_0^* a_{\mathbf{k}+\mathbf{k}'}^* a_{\mathbf{k}} a_{\mathbf{k}'} + a_{\mathbf{k}}^* a_{\mathbf{k}'}^* a_{\mathbf{k}+\mathbf{k}'} a_0). \tag{A5}$$

Every term on the right-hand side of Eq. (A5) involves at least three distinct momenta, only one of them being zero. Following Refs. [6] and [7], all such terms are neglected when the density is low, i.e., such terms are of higher order in $(Na^3/\Omega)^{1/2}$. Therefore, Eq. (A5) is replaced by

$$V_3 \sim 0. \tag{A6}$$

With (A4) and (A6), the only surviving pieces are V_0, V_2, and V_4. In terms of $a_{\mathbf{k}}^*$ and $a_{\mathbf{k}}$, they are explicitly

$$V_0 = \frac{4\pi a}{\Omega}\, a_0^{*2} a_0^2, \tag{A7}$$

$$V_2 = \frac{4\pi a}{\Omega} \sum_{\mathbf{k}\neq 0} (a_0^{*2} a_{\mathbf{k}} a_{-\mathbf{k}} + a_{\mathbf{k}}^* a_{-\mathbf{k}}^* a_0^2 + 4 a_0^* a_{\mathbf{k}}^* a_{\mathbf{k}} a_0), \tag{A8}$$

and

$$V_4 = \frac{4\pi a}{\Omega} \sum_{\substack{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4 \\ \mathbf{k}_i \neq 0}} a_{\mathbf{k}_1}^* a_{\mathbf{k}_2}^* a_{\mathbf{k}_3} a_{\mathbf{k}_4}. \tag{A9}$$

There are two distinct types of terms in V_2, namely, off-diagonal and diagonal terms in the momentum representation. Let

$$V_2 = V_{21} + V_{22}, \tag{A10}$$

where

$$V_{21} = \frac{4\pi a}{\Omega} \sum_{\mathbf{k}\neq 0} (a_0^{*2} a_{\mathbf{k}} a_{-\mathbf{k}} + a_{\mathbf{k}}^* a_{-\mathbf{k}}^* a_0^2) \tag{A11}$$

and

$$V_{22} = \frac{16\pi a}{\Omega} \sum_{\mathbf{k}\neq 0} a_0^* a_{\mathbf{k}}^* a_{\mathbf{k}} a_0. \tag{A12}$$

Since V_{21} is already in the desired form, it only remains to find the appropriate approximations to V_0, V_{22}, and V_4.

These approximations are to be carried out using $a_0^* a_0 \sim N\xi$ and the relation (A1). Thus, for V_0 the procedure is

$$\begin{aligned} V_0 &\sim 4\pi a \Omega^{-1} (a_0^* a_0)^2 \\ &= 4\pi a \Omega^{-1} \left\{ N\xi + \left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^* a_{\mathbf{k}} \right] \right\}^2 \\ &\sim 4\pi a \Omega^{-1} \left\{ N^2\xi^2 + 2N\xi \left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^* a_{\mathbf{k}} \right] \right\} \\ &= 4\pi a \Omega^{-1} \left[N^2 \xi(2-\xi) - 2N\xi \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^* a_{\mathbf{k}} \right]. \end{aligned} \tag{A13}$$

Similarly, the approximation to V_{22} of Eq. (A12) is obtained by

$$\begin{aligned} V_{22} &= 16\pi a\Omega^{-1}\left\{N\xi + \left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right]\right\} \\ &\quad \times \left\{N(1-\xi) - \left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right]\right\} \\ &\sim 16\pi a\Omega^{-1}\left\{N^2\xi(1-\xi) + N(1-2\xi)\left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right]\right\} \\ &= 16\pi a\Omega^{-1}\left\{N^2(1-\xi)^2 - N(1-2\xi)\sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right\}. \end{aligned} \tag{A14}$$

In the same spirit as the approximation of (A5) by (A6), the only terms kept for the right-hand side of (A9) are those where

$$\mathbf{k}_1 = \mathbf{k}_3 \quad \text{and} \quad \mathbf{k}_2 = \mathbf{k}_4$$

or

$$\mathbf{k}_1 = \mathbf{k}_4 \quad \text{and} \quad \mathbf{k}_2 = \mathbf{k}_3. \tag{A15}$$

Therefore, the first step of approximating Eq. (A9) is

$$V_4 \sim \frac{8\pi a}{\Omega} \sum_{\substack{\mathbf{k}_1\neq 0 \\ \mathbf{k}_2\neq 0}} a^*_{\mathbf{k}_1} a^*_{\mathbf{k}_2} a_{\mathbf{k}_1} a_{\mathbf{k}_2}. \tag{A16}$$

Note that, in going from Eq. (A9) to (A16), the terms

$$\frac{4\pi a}{\Omega} \sum_{\substack{\mathbf{k}_1\neq 0 \\ \mathbf{k}_2\neq 0}} a^*_{\mathbf{k}_1} a^*_{-\mathbf{k}_1} a_{\mathbf{k}_2} a_{-\mathbf{k}_2}$$

have been neglected because they are of higher order in $(Na^3/\Omega)^{1/2}$. The treatment of this Eq. (A16) is similar to those that lead to the approximations (A13) and (A14), namely,

$$\begin{aligned} V_4 &\sim 8\pi a\Omega^{-1}\left\{N(1-\xi) - \left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right]\right\}^2 \\ &\sim 8\pi a\Omega^{-1}\left\{N^2(1-\xi)^2 - 2N(1-\xi)\left[N(1-\xi) - \sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right]\right\} \\ &= 8\pi a\Omega^{-1}\left\{-N^2(1-\xi)^2 + 2N(1-\xi)\sum_{\mathbf{k}\neq 0} a^*_{\mathbf{k}} a_{\mathbf{k}}\right\}. \end{aligned} \tag{A17}$$

It remains to sum up all contributions to the V_i's:

$$\begin{aligned} V &= V_0 + V_1 + V_2 + V_3 + V_4 \\ &\sim 4\pi a(N/\Omega)N[(1-\xi)^2+1] + 8\pi a(N/\Omega)\xi \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^* a_{\mathbf{k}} \\ &\quad + 4\pi a\Omega^{-1} \sum_{\mathbf{k}\neq 0} [a_0^{*2} a_{\mathbf{k}} a_{-\mathbf{k}} + a_{\mathbf{k}}^* a_{-\mathbf{k}}^* a_0^2]. \end{aligned} \tag{A18}$$

Compare with Eq. (14) in Sec. 3 of Ref. [7]. The corresponding V there is approximated by

$$4\pi a\rho_0 N[1+(1-\xi)^2] + 2\sum{}' \, 8\pi a\xi\rho_0 a_{\mathbf{k}}^* a_{\mathbf{k}} + \sum{}' \, 8\pi a\xi\rho_0 B_{S(\mathbf{k})}(\mathbf{k}),$$

where $\rho_0 = N/\Omega$, the sum $\sum{}'$ extends over the upper half of the $\mathbf{k}$ space by excluding $\mathbf{k} = 0$, and

$$B_{S(\mathbf{k})}(\mathbf{k}) = a_{\mathbf{k}} a_{-\mathbf{k}} + a_{\mathbf{k}}^* a_{-\mathbf{k}}^*.$$

APPENDIX B: DETAILED DERIVATION OF THE EQUATION FOR $K_0(\mathbf{r}, \mathbf{r}')$

In this appendix, the integro-differential equation (4.11) is derived in some detail. The starting point is the evaluation of H_2' of Eq. (4.4) according to the relation

$$H_2' = H_2 + e^{-P}[H_2, e^P], \tag{B1}$$

where P is provided by Eq. (4.5).

For the purpose of calculating the commutator of the preceding equation, it is useful to bear in mind that

$$[\psi_1(\mathbf{r}), \psi_1^*(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}') - \Omega^{-1}\,\Phi(\mathbf{r})\Phi^*(\mathbf{r}'), \tag{B2}$$

which easily follows from Eqs. (2.12) (by eliminating the time t) and the usual commutation relations

$$[\psi(\mathbf{r}), \psi^*(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}')$$

and

$$[a_0, a_0^*] = 1.$$

All requisite commutators are now evaluated straightforwardly. Noting that

$$\begin{aligned}
[\psi_1(\mathbf{r}), P] &= (2N\xi)^{-1} \int d\mathbf{r}_1\, d\mathbf{r}'_1\, \{\delta(\mathbf{r}-\mathbf{r}_1)\psi_1^*(\mathbf{r}'_1) + \delta(\mathbf{r}-\mathbf{r}'_1)\psi_1^*(\mathbf{r}_1)\} K_0(\mathbf{r}_1, \mathbf{r}'_1) a_0^2 \\
&= (N\xi)^{-1} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') a_0^2, \qquad \text{(B3)}
\end{aligned}$$

$$\begin{aligned}
[\psi_1(\mathbf{r}), P^2] &= (2N\xi)^{-2} \int d\mathbf{r}_1\, d\mathbf{r}'_1\, d\mathbf{r}_2\, d\mathbf{r}'_2\, K_0(\mathbf{r}_1, \mathbf{r}'_1) K_0(\mathbf{r}_2, \mathbf{r}'_2) \\
&\quad \times \sum_{\substack{i,j=1 \\ i\neq j}}^{2} \psi_1^*(\mathbf{r}_i)\psi_1^*(\mathbf{r}'_i)\{\delta(\mathbf{r}-\mathbf{r}_j)\psi_1^*(\mathbf{r}'_j) + \delta(\mathbf{r}-\mathbf{r}'_j)\psi_1^*(\mathbf{r}_j)\} a_0^4 \\
&= 2(N\xi)^{-1} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') P a_0^2, \qquad \text{(B4)}
\end{aligned}$$

it is deduced by induction that

$$[\psi_1(\mathbf{r}), P^n] = n(N\xi)^{-1} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') P^{n-1} a_0^2, \qquad n = 1,\, 2,\, \ldots, \qquad \text{(B5)}$$

which is in turn used to furnish

$$[\psi_1(\mathbf{r}), e^P] = \sum_{n=1}^{\infty} \frac{1}{n!} [\psi_1(\mathbf{r}), P^n] = \frac{1}{N\xi} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') e^P a_0^2. \qquad \text{(B6)}$$

Likewise,

$$[\psi_1^*(\mathbf{r})\psi_1(\mathbf{r}), e^P] = (N\xi)^{-1} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}') e^P a_0^2, \qquad \text{(B7)}$$

$$[|\nabla\psi_1(\mathbf{r})|^2, e^P] = (N\xi)^{-1} \int d\mathbf{r}'\, \psi_1^*(\mathbf{r}')[\nabla\psi_1^*(\mathbf{r}) \cdot \nabla_{\mathbf{r}} K_0(\mathbf{r}, \mathbf{r}')] e^P a_0^2. \qquad \text{(B8)}$$

It remains to calculate $[a_0^{*2}\psi_1(\mathbf{r})^2, e^P]$. In view of the relation

$$[a_0^{*2}\psi_1(\mathbf{r})^2, P] = a_0^{*2}[\psi_1(\mathbf{r})^2, P] + [a_0^{*2}, P]\psi_1(\mathbf{r})^2, \qquad \text{(B9)}$$

where

$$\begin{aligned}
[a_0^{*2}, P] &= (2N\xi)^{-1} \int d\mathbf{r}\, d\mathbf{r}'\, \psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}')(-4a_0^* a_0 - 2) \\
&\sim -2 \int d\mathbf{r}\, d\mathbf{r}'\, \psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}') K_0(\mathbf{r}, \mathbf{r}'), \qquad \text{(B10)}
\end{aligned}$$

it is recognized that a_0^{*2} can be treated here approximately as commuting with P:

$$[a_0^{*2}\psi_1(\mathbf{r})^2, e^P] \sim a_0^{*2}[\psi_1(\mathbf{r})^2, e^P]. \qquad \text{(B11)}$$

With

$$[\psi_1(\mathbf{r})^2, P] \;=\; (N\xi)^{-1}\left\{K_0(\mathbf{r},\mathbf{r}) + 2\int d\mathbf{r}'\,\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')\right\} a_0^2, \tag{B12}$$

$$\begin{aligned}[\psi_1(\mathbf{r})^2, P^2] \;=\; & 2(N\xi)^{-1}\left\{K_0(\mathbf{r},\mathbf{r})P + P2\int d\mathbf{r}'\,\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')\right.\\ & \left. + (N\xi)^{-1}\int d\mathbf{r}'\,d\mathbf{r}''\,\psi_1^*(\mathbf{r}')\psi_1^*(\mathbf{r}'')K_0(\mathbf{r},\mathbf{r}')K_0(\mathbf{r},\mathbf{r}'')a_0^2\right\} a_0^2, \end{aligned} \tag{B13}$$

where use is made of Eq. (B3), it is deduced by induction that ($n = 2,\, 3,\, \ldots$)

$$\begin{aligned}[\psi_1(\mathbf{r})^2, P^n] \;=\; & n(N\xi)^{-1}\left\{K_0(\mathbf{r},\mathbf{r})P^{n-1} + P^{n-1}2\int d\mathbf{r}'\,\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')\right.\\ & \left. + (n-1)P^{n-2}(N\xi)^{-1}\int d\mathbf{r}'\,d\mathbf{r}''\,\psi_1^*(\mathbf{r}')\psi_1^*(\mathbf{r}'')K_0(\mathbf{r},\mathbf{r}')K_0(\mathbf{r},\mathbf{r}'')a_0^2\right\} a_0^2. \end{aligned} \tag{B14}$$

Accordingly,

$$\begin{aligned}[\psi_1(\mathbf{r})^2, e^P] \;=\; & (N\xi)^{-1}e^P\left\{K_0(\mathbf{r},\mathbf{r}) + 2\int d\mathbf{r}'\,\psi_1^*(\mathbf{r}')\psi_1(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')\right.\\ & \left. + (N\xi)^{-1}\int d\mathbf{r}'\,d\mathbf{r}''\,\psi_1^*(\mathbf{r}')\psi_1^*(\mathbf{r}'')K_0(\mathbf{r},\mathbf{r}')K_0(\mathbf{r},\mathbf{r}'')a_0^2\right\} a_0^2. \end{aligned} \tag{B15}$$

The combination of Eq. (4.3) with expressions (B1), (B7), (B8), (B11), and (B15), along with the approximation $a_0^{*2}a_0^2 \sim (N\xi)^2$ immediately yield (4.8)–(4.10).

In analogy with the case of zero temperature [3], the integro-differential equation for $K_0(\mathbf{r},\mathbf{r}')$ is obtained via the condition that H'_{2c} be zero. For this purpose, it is desirable to introduce a function $L(\mathbf{r},\mathbf{r}')$ such that

$$H'_{2c} = (2N\xi)^{-1}\int d\mathbf{r}\,d\mathbf{r}'\,\psi_1^*(\mathbf{r})\psi_1^*(\mathbf{r}')L(\mathbf{r},\mathbf{r}')\,a_0^2, \tag{B16}$$

$$L(\mathbf{r},\mathbf{r}') = L(\mathbf{r}',\mathbf{r}), \tag{B17}$$

and

$$\int d\mathbf{r}'\,\Phi^*(\mathbf{r}')L(\mathbf{r},\mathbf{r}') = 0 \tag{B18}$$

without loss of generality. The equation for $K_0(\mathbf{r},\mathbf{r}')$ then follows from

$$L(\mathbf{r},\mathbf{r}') = 0. \tag{B19}$$

By inspection of Eq. (4.10),

$$\begin{aligned} L(\mathbf{r},\mathbf{r}') \;=\; & -\nabla^2_{\mathbf{r}} K_0(\mathbf{r},\mathbf{r}') - \nabla^2_{\mathbf{r}'} K_0(\mathbf{r},\mathbf{r}') + 8\pi a N\xi\Omega^{-1}\,\Phi(\mathbf{r})^2\delta(\mathbf{r}-\mathbf{r}') \\ & + \Big\{ -2\bar{\zeta} - 2\zeta_e - 16\pi a\zeta N\xi\Omega^{-1} - 32\pi a\Omega^{-1}\int d\mathbf{r}''\,|\Phi(\mathbf{r}'')|^2 A(\mathbf{r}'') + V_e(\mathbf{r}) + V_e(\mathbf{r}') \\ & + 16\pi a N\xi\Omega^{-1}[|\Phi(\mathbf{r})|^2 + |\Phi(\mathbf{r}')|^2] + 16\pi a[A(\mathbf{r}) + A(\mathbf{r}')] \Big\} K_0(\mathbf{r},\mathbf{r}') \\ & + 8\pi a N\xi\Omega^{-1}\int d\mathbf{r}''\,K_0(\mathbf{r},\mathbf{r}'')K_0(\mathbf{r}'',\mathbf{r}')\Phi^*(\mathbf{r}'')^2 - \lambda(\mathbf{r})\Phi(\mathbf{r}') - \lambda(\mathbf{r}')\Phi(\mathbf{r}). \end{aligned} \tag{B20}$$

Clearly, $\lambda(\mathbf{r})$ is determined through multiplication of both sides of the preceding expression by $\Phi^*(\mathbf{r}')$ and subsequent integration over $\mathbf{r}'$ by taking into account Eqs. (B18) and (4.7). Integration by parts is performed with attention to $K_0(\mathbf{r},\mathbf{r}')$ and $\Phi(\mathbf{r}')$ that do not yield any surface terms:

$$\begin{aligned} & \lambda(\mathbf{r})\Omega + \Phi(\mathbf{r})\int d\mathbf{r}'\,\Phi^*(\mathbf{r}')\lambda(\mathbf{r}') \\ & = \int d\mathbf{r}'\,K_0(\mathbf{r},\mathbf{r}')[-\nabla^2_{\mathbf{r}'} + V_e(\mathbf{r}') + 16\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r}')|^2 + 16\pi a A(\mathbf{r}')]\Phi^*(\mathbf{r}') \\ & \quad + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}) \\ & = 8\pi a N\xi\Omega^{-1}\int d\mathbf{r}'\,K_0(\mathbf{r},\mathbf{r}')|\Phi(\mathbf{r}')|^2\Phi^*(\mathbf{r}') + 8\pi a N\xi\Omega^{-1}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}), \end{aligned} \tag{B21}$$

where use was made of the time-independent version of Eq. (3.27), given by Eq. (5.3). The unique solution of this trivial integral equation for $\lambda(\mathbf{r})$ is

$$\lambda(\mathbf{r}) = 8\pi a N\xi\Omega^{-2}\left\{[|\Phi(\mathbf{r})|^2 - \tfrac{1}{2}\zeta]\Phi(\mathbf{r}) + \int d\mathbf{r}'\,K_0(\mathbf{r},\mathbf{r}')|\Phi(\mathbf{r}')|^2\Phi^*(\mathbf{r}')\right\}. \tag{B22}$$

Substitution of this $\lambda(\mathbf{r})$ into Eq. (B20) and imposition of Eq. (B19) lead to Eq. (4.11).

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