Low-temperature Bose-Einstein condensates in time-dependent traps: Beyond the $U(1)$ symmetry-breaking approach

Y. Castin and R. Dum
Ecole Normale Supérieure, Laboratoire Kastler Brossel, 24, Rue Lhomond, F-75231 Paris Cedex 05, France
(Received 25 February 1997; revised manuscript received 7 October 1997)

We present a method to calculate the dynamics of very-low-temperature Bose-Einstein condensates in time-dependent traps. We consider a system with a well-defined number of particles, rather than a system in a coherent state with a well-defined phase. This preserves the $U(1)$ symmetry of the problem. We use a systematic asymptotic expansion in the square root of the fraction of noncondensed particles. In lowest order we recover the time-dependent Gross-Pitaevskii equation for the condensate wave function. The next order gives the linear dynamics of noncondensed particles. The higher order gives corrections to the time-dependent Gross-Pitaevskii equation including the effects of noncondensed particles on the condensate. We compare this method with the Bogoliubov–de Gennes approach.
[S1050-2947(98)00604-0]

PACS number(s): 03.75.Fi, 05.30.Jp

I. INTRODUCTION

Recently dramatic progress has been made in the experimental demonstration of Bose-Einstein condensation in dilute gases [1–3]. The fact that these condensates are obtained for a relatively small number of atoms (less than 10^7) that are trapped in harmonic potentials leads to new physical properties. The interaction between the atoms makes, however, a theoretical treatment nontrivial. An exact although purely numerical approach to study systems in thermal equilibrium is the quantum Monte Carlo method recently put forward in [4]. The most widely used approach is a Hartree-Fock mean-field approach, which can be extended to nonequilibrium situations. In the case of zero temperature it reduces to a description of the state of the condensate by the so-called Gross-Pitaevskii equation [5,6]. In the context of recent experiments this equation was studied initially by purely numerical means [7]. Recently analytical results have been obtained [8–11]. They allowed in [11] an easy quantitative study of the experimental results, such as ballistic expansion of the atomic cloud [12] and collective excitations of the condensate [13]. Although the Hartree-Fock approach leads to an intuitive understanding it does not lend itself to a systematic treatment and therefore no estimation of the range of validity of the time-dependent Gross-Pitaevskii equation is obtained. We provide one in the present paper, as we give the deviations of the state of the condensate from the predictions of the Gross-Pitaevskii equation.

Going beyond the Gross-Pitaevskii equation, Bogoliubov proposed a method to study how the condensed state of an interacting homogeneous gas differs from that of a noninteracting Bose gas; de Gennes gave an extension to inhomogeneous gases [5,14]. $U(1)$ symmetry breaking is an essential ingredient of the Bogoliubov–de Gennes approaches: the state of the system is described by a *coherent* state and therefore the atomic field operator has a nonzero expectation value. This mean value is a classical field characterizing the condensate; it constitutes an explicit $U(1)$ symmetry breaking as the condensate has a well-defined phase. The atomic field operator has quantum fluctuations around this mean value; the basic idea of Bogoliubov is to treat the quantum fluctuations in a linear approximation.

Any consistent way of applying the symmetry breaking approach has to reveal the fact that a *coherent* state is not a stationary state of the system, because it has not a well-defined number of particles. The Bogoliubov approach is applied in a careful manner in [15]; a time divergence of quantum fluctuations is then predicted, and interpreted as a quantum phase spreading of the condensate. This spreading invalidates the linearization around a classical field very soon in the trapped atomic gases because the number of particles is small. A similar conclusion is reached in [16] by explicitly calculating how an initial coherent state is deformed by the atomic interaction; due to this deformation the mean value of the field operator undergoes collapses and revivals (see our Sec. V).

In this paper we develop an approach based on a systematic expansion of the evolution equations for the atomic field operator in a system with exactly N particles. We do not rely on symmetry breaking and therefore we avoid the pathologies associated with phase fluctuations of the condensate. We split the atomic field operator into an operator with macroscopic matrix elements, which describes the condensate, and the remainder, which describes the non-condensed particles and has matrix elements smaller by a factor $\sim\sqrt{N}$. This motivates an expansion in powers of $1/\sqrt{N}$ [17]. We thereby give a justification for the prediction of the Gross-Pitaevskii equation for the condensate wave function. By including higher-order terms in our expansion we also derive deviations of the condensate wave function from the solution of the Gross-Pitaevskii equation. For a steady state we find that the predictions of the Gross-Pitaevskii equation are remarkably accurate at low temperatures for typical experimental parameters. For time-dependent systems, however, this conclusion is no longer true: the number of noncondensed particles may diverge in time and the predictions of the time-dependent Gross-Pitaevskii equation may eventually fail [18].

In Sec. II we define the condensate wave function and identify the square root of the fraction of noncondensed particles as the small physical parameter of our expansion. We also give a summary of the main results of the paper. In Sec. III we proceed explicitly with the expansion; this section may be skipped by readers not interested in a thorough derivation. To lowest order we recover the Gross-Pitaevskii equation for the condensate wave function; the next order gives the nonsymmetry breaking version of the Bogoliubov–de Gennes equations for the linearized quantum fluctuations. In Sec. IV we analyze the time evolution of the quantum fluctuations; we establish a remarkably simple link between the dynamics of the noncondensed particles and the linearization of the time-dependent Gross-Pitaevskii equation. We extend the concept of a modal decomposition of the quantum fluctuations to the explicitly time-dependent case. The dynamics is completely contained in the time evolution of the mode functions of the system, the operators corresponding to these mode functions are time independent. In Sec. V we compare our approach to the symmetry-breaking one and we interpret the collapse of the classical atomic field as the collapse of the correlation function of the atomic field operator due to fluctuations in the number of particles. In Sec. VI we give a correction to the Gross-Pitaevskii equation for the condensate wave function. We conclude in Sec. VII and indicate future applications of the general method presented in this paper.

II. BASIC EQUATIONS AND ASSUMPTIONS

A. The effective Hamiltonian

In our model we consider N scalar bosons in a time-dependent trapping potential $U(\vec{r},t)$. Those bosons undergo pair interactions, and as usual in theoretical treatments, we replace the true interaction potential by the local pseudopotential

$$V(\vec{r}_2-\vec{r}_1)=g\,\delta(\vec{r}_2-\vec{r}_1). \tag{1}$$

In this expression the coupling constant g between the particles is given by

$$g=4\pi\hbar^2 a_s/m, \tag{2}$$

where a_s is the s-wave scattering length for the true interaction potential and where m is the mass of the boson. The pseudopotential has to be regularized to be meaningful [19].

In second quantized form the model Hamiltonian is given by

$$\hat{H}=\int d\vec{r}\hat{\Psi}^\dagger(\vec{r})\left[\mathcal{H}(t)+\frac{1}{2}g\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})\right]\hat{\Psi}(\vec{r}), \tag{3}$$

where $\hat{\Psi}$ is the particle field operator (we always use $\hat{}$ to refer to operators acting in the N-body Fock space). The one-particle Hamiltonian $\mathcal{H}(t)$ includes the kinetic energy of the particle and the time-dependent trapping potential $U(\vec{r},t)$:

$$\mathcal{H}(t)=\frac{p^2}{2m}+U(\vec{r},t). \tag{4}$$

The Hamiltonian in Eq. (3) is invariant under a global phase change of $\hat{\Psi}$ referred to as the $U(1)$ symmetry. An atomic state with a nonvanishing mean value of $\hat{\Psi}$ would break this symmetry; it would necessarily involve a coherent superposition of states with different total number of particles.

B. Definition of the condensate wave function

In this section we define the notion of a condensate [20]. To this end we introduce the one-body density operator ρ_1 of the particles by

$$\langle\vec{r}'|\rho_1(t)|\vec{r}\rangle\equiv\langle\hat{\Psi}^\dagger(\vec{r},t)\hat{\Psi}(\vec{r}',t)\rangle, \tag{5}$$

where the $\hat{\Psi}$'s are taken in the Heisenberg picture and the expectation $\langle\cdots\rangle$ is taken in the initial state at $t=0$. We assume in this paper that the number of particles is well defined and equal to N (so that $\mathrm{Tr}[\rho_1]=N$) and we suppose that the N-particle system is initially in thermal equilibrium at temperature T.

A condensate is present if ρ_1 has an eigenvector $|\Phi_{\mathrm{ex}}\rangle$ with eigenvalue N_{ex} of the order of N much larger than all other eigenvalues,

$$\rho_1|\Phi_{\mathrm{ex}}\rangle=N_{\mathrm{ex}}|\Phi_{\mathrm{ex}}\rangle. \tag{6}$$

The condensate wave function $|\Phi_{\mathrm{ex}}\rangle$ is the *exact* state in which a macroscopic number N_{ex} of particles is condensed. In what follows it will be normalized to unity:

$$\langle\Phi_{\mathrm{ex}}|\Phi_{\mathrm{ex}}\rangle=1. \tag{7}$$

The existence of a macroscopically populated state Φ_{ex} motivates splitting the field operator into a part with macroscopic matrix elements and a remainder, which accounts for noncondensed particles:

$$\hat{\Psi}(\vec{r},t)=\Phi_{\mathrm{ex}}(\vec{r},t)\hat{a}_{\Phi_{\mathrm{ex}}}(t)+\delta\hat{\Psi}(\vec{r},t). \tag{8}$$

The mode operator $\hat{a}_{\Phi_{\mathrm{ex}}}$ is given by

$$\hat{a}_{\Phi_{\mathrm{ex}}}=\int d\vec{r}\Phi^*_{\mathrm{ex}}(\vec{r},t)\hat{\Psi}(\vec{r},t). \tag{9}$$

In the Schrödinger picture $\hat{a}_{\Phi_{\mathrm{ex}}}(t)$ annihilates a particle in the condensate wave function $\Phi_{\mathrm{ex}}(\vec{r},t)$. It has matrix elements on the order of $\sqrt{N_{\mathrm{ex}}}$ since the expectation value $\langle\hat{a}^\dagger_{\Phi_{\mathrm{ex}}}(t)\hat{a}_{\Phi_{\mathrm{ex}}}(t)\rangle$ is N_{ex}. The remainder $\delta\hat{\Psi}$ is obtained by projection of the field operator $\hat{\Psi}(\vec{r})$ orthogonally to Φ_{ex}:

$$\delta\hat{\Psi}(\vec{r},t)=\int d\vec{r}'\langle\vec{r}|Q_{\mathrm{ex}}(t)|\vec{r}'\rangle\hat{\Psi}(\vec{r}',t). \tag{10}$$

$Q_{\mathrm{ex}}(t)=\mathbb{1}-|\Phi_{\mathrm{ex}}\rangle\langle\Phi_{\mathrm{ex}}|$ projects onto the one-particle states orthogonal to the condensate wave function Φ_{ex}. To simplify the notation we introduce the operand $\circ$, which describes the action of a one-body operator O onto a field operator depending parametrically on $\vec{r}$, such as $\hat{\Psi}(\vec{r})$:

$$O\circ\hat{\Psi}\equiv\int d\vec{s}O|\vec{s}\rangle\hat{\Psi}(\vec{s}). \tag{11}$$

With this notation Eq. (10) reads

$$\delta\hat{\Psi}(t) = Q_{\rm ex}(t) \circ \hat{\Psi}(t). \tag{12}$$

This relation implies that $\delta\hat{\Psi}$ is orthogonal to $\Phi_{\rm ex}$:

$$\langle \Phi_{\rm ex}| \circ \delta\hat{\Psi} = \int d\vec{r} \Phi^*_{\rm ex}(\vec{r},t)\, \delta\hat{\Psi}(\vec{r},t) = 0. \tag{13}$$

It satisfies quasibosonic commutation relations

$$[\delta\hat{\Psi}(\vec{r},t), \delta\hat{\Psi}^\dagger(\vec{r}',t)] = \langle \vec{r}| Q_{\rm ex}(t) |\vec{r}'\rangle$$

and it commutes with $\hat{a}^\dagger_{\Phi_{\rm ex}}$.

C. Identification of a small parameter

A first approach to analyze the properties of the Bose-Einstein condensate would be to use standard perturbation theory to treat the effect of the interactions. As shown in [5,21] in the spatially homogeneous case one has to resum an infinite number of terms in the expansion because the total interaction energy ($\sim N\rho g$, ρ is the spatial density) is much larger than the splitting between the energy levels in the trap.

We prefer to use here a different approach, initiated by Bogoliubov [21] and generalized by de Gennes to the inhomogeneous case [14], that does not require any explicit resummation. We consider the regime where the mean number of noncondensed particles is much smaller than the number of condensed particles:

$$\langle \delta\hat{N}\rangle \equiv \int d\vec{r} \langle \delta\hat{\Psi}^\dagger(\vec{r},t)\, \delta\hat{\Psi}(\vec{r},t)\rangle \ll N_{\rm ex} \simeq N. \tag{14}$$

From the fact that $\delta\hat{\Psi}$ in Eq. (8) has matrix elements scaling as $\sqrt{\langle \delta\hat{N}\rangle}$ whereas those of $\hat{a}_{\Phi_{ex}}$ are of order $\sqrt{N}$ we conclude that the small expansion parameter under consideration is the square root of the noncondensed fraction $\sqrt{\langle \delta\hat{N}\rangle/N}$ [17].

A small value of $\langle \delta\hat{N}\rangle/N$ requires that the temperature T be low enough, in particular $T \ll T_c$ where T_c is the critical temperature for Bose-Einstein condensation, to avoid depletion of the condensate by thermal excitations. This condition on the temperature, however, is not sufficient as even at zero temperature not all the particles are condensed because of their interactions; for a homogeneous condensate the noncondensed fraction scales as $\sqrt{a_s^3\rho}$ for $\rho a_s^3 \ll 1$ [21], a result that approximately extends to the case of a condensate in a harmonic trap as we have shown by numerical calculations [22]. In the experimental conditions of [2] we have $\rho \sim 10^{14}$ cm^{-3} and $a_s \sim 25$ Å, which leads to a small noncondensed fraction $\sqrt{a_s^3\rho} \sim 10^{-3}$.

D. Practical implementation of the expansion procedure

In the calculations to come we will use a characterization of $|\Phi_{\rm ex}\rangle$ that turns out to be more operational than Eq. (6). Using Eq. (6) projected onto $\langle \vec{r}|$, and Eqs. (5), (8), and (9) we get

$$\langle \hat{a}^\dagger_{\Phi_{\rm ex}}(t)\, \delta\hat{\Psi}(\vec{r},t)\rangle = 0. \tag{15}$$

This means physically that there is no one-particle coherence, that is, no off-diagonal matrix elements of the one-body density operator, between the condensate and any state orthogonal to $|\Phi_{\rm ex}\rangle$.

Inspired by Eq. (15) we introduce the operator $\hat{\Lambda}_{\rm ex}$:

$$\hat{\Lambda}_{\rm ex}(\vec{r},t) = \frac{1}{\sqrt{\hat{N}}} \hat{a}^\dagger_{\Phi_{\rm ex}}(t)\, \delta\hat{\Psi}(\vec{r},t), \tag{16}$$

where $\hat{N}$ is the total number operator. The operator $\hat{\Lambda}_{\rm ex}$ commutes with $\hat{N}$ and therefore conserves the number of particles. The matrix elements of $\hat{\Lambda}_{\rm ex}$ are of order one and the expectation value of $\hat{\Lambda}_{\rm ex}$ vanishes exactly

$$\langle \hat{\Lambda}_{\rm ex}(\vec{r},t)\rangle = 0. \tag{17}$$

Equation (17) ensures that $\Phi_{\rm ex}$ is an eigenstate of the one-body density operator.

As stated before our expansion requires that the gas be in a weakly interactive regime ($\rho a_s^3 \ll 1$). We now identify a limit where this condition is automatically satisfied and that we shall use to perform our asymptotic expansion: This limit corresponds formally to

$$\begin{aligned} &N \to +\infty, \\ &Ng = \text{const} \equiv g_N, \end{aligned} \tag{18}$$

which amounts to the limit $a_s \to 0$ for $N \to \infty$. As we shall see in this limit $\langle \delta\hat{N}\rangle$ converges to a finite value so that the small formal parameter of the expansion is

$$\sqrt{\langle \delta\hat{N}\rangle/\hat{N}} \propto 1/\sqrt{\hat{N}}. \tag{19}$$

Whether we are allowed to use predictions resulting from the limit in Eq. (18) has to be checked for a given experimental situation at hand, that is, one has to compare the order of magnitude of the successive terms in the expansion.

A physical way to implement this limit without putting a_s to zero is to open the trap as the number of particles increases. More precisely we consider the limit

$$\begin{aligned} &N \to +\infty, \\ &\frac{Na_s}{L} = \text{const}, \\ &\frac{k_B T}{\hbar\omega} = \text{const} \end{aligned} \tag{20}$$

for a isotropic harmonic trap with frequency ω where $L = \sqrt{\hbar/2m\omega}$ is the spatial extension of the ground state of the trap. We thereby keep the interaction energy per particle constant in units of $\hbar\omega$. The critical number of particles for the formation of the condensate $N_c \sim (k_B T/\hbar\omega)^3$ is also kept constant, so that $N_c \ll N$. In this limit we expect the state of the condensate to become independent of N when the length is measured in units of L.

Assuming the limit of Eq. (18) we expand $\hat{\Lambda}_{\rm ex}$ and $\Phi_{\rm ex}$ in powers of $1/\sqrt{N}$:

$$\hat{\Lambda}_{\rm ex}=\hat{\Lambda}+\frac{1}{\sqrt{\hat{N}}}\hat{\Lambda}^{(1)}+\frac{1}{\hat{N}}\hat{\Lambda}^{(2)}+\cdots,$$
$$\Phi_{\rm ex}=\Phi+\frac{1}{\sqrt{\hat{N}}}\Phi^{(1)}+\frac{1}{\hat{N}}\Phi^{(2)}+\cdots. \tag{21}$$

From the normalization condition Eq. (7) we find that $|\Phi\rangle$ is normalized to unity. From Eq. (17) we find that the expectation value of $\hat{\Lambda}$ vanishes, which will determine Φ. From Eq. (14) we note also that $\hat{\Lambda}$ obeys the commutation relation

$$[\hat{\Lambda}(\vec{r},t),\hat{\Lambda}^{\dagger}(\vec{r}',t)]=\langle\vec{r}|Q(t)|\vec{r}'\rangle, \tag{22}$$

where Q projects onto the space orthogonal to Φ:

$$Q=\mathbb{1}-|\Phi\rangle\langle\Phi|. \tag{23}$$

This expansion puts rather stringent limits on the temperature, as the requirement $\langle\delta\hat{N}\rangle\ll N$ imposes that T be much smaller than the critical temperature T_c. An expansion based on the ratio of the density of noncondensed particles to the density of the condensate would have a broader range of application. Due to the presence of a trap the condensed particles form indeed a high-density cloud with a low-density background of noncondensed particles. So even with a significant fraction of noncondensed particles an expansion with this ratio as small parameter might work. At thermal equilibrium the numerical calculations of [4] confirm this expectation.

E. Summary of results

Imagine that a one-particle observable $\hat{X}=\Sigma_{i=1}^{N}X(i)$ of the system is measured, $X(i)$ acting on the state of particle i. An ensemble average over many experimental realizations with a fixed number N of particles will lead to the expectation value

$$\langle X(t)\rangle=\int d\vec{r}\int d\vec{r}'\langle\vec{r}|X(1)|\vec{r}'\rangle\langle\hat{\Psi}^{\dagger}(\vec{r},t)\hat{\Psi}(\vec{r}',t)\rangle. \tag{24}$$

The splitting Eq. (8) allows one to distinguish the contributions of the condensed and the noncondensed particles:

$$\langle X\rangle=\langle\hat{a}^{\dagger}_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}\rangle\langle\Phi_{\rm ex}|X(1)|\Phi_{\rm ex}\rangle+\int d\vec{r}\int d\vec{r}'\langle\vec{r}|X(1)|\vec{r}'\rangle \times\langle\delta\hat{\Psi}^{\dagger}(\vec{r},t)\,\delta\hat{\Psi}(\vec{r}',t)\rangle. \tag{25}$$

Note that there is no crossed term between the condensed and noncondensed particles in this expression, a consequence of Eq. (17). The expansion Eq. (21) allows the calculation of this expectation value with an error scaling as $\sqrt{\langle\delta\hat{N}\rangle/\hat{N}}$, where $\langle\delta\hat{N}\rangle$ is the number of noncondensed particles defined in Eq. (14):

$$\langle X\rangle\simeq(N-\langle\delta\hat{N}\rangle)\langle\Phi|X(1)|\Phi\rangle +\langle\Phi|X(1)|\Phi^{(2)}\rangle+\langle\Phi^{(2)}|X(1)|\Phi\rangle +\int d\vec{r}\int d\vec{r}'\langle\vec{r}|X(1)|\vec{r}'\rangle\langle\hat{\Lambda}^{\dagger}(\vec{r})\hat{\Lambda}(\vec{r}')\rangle. \tag{26}$$

The first line in Eq. (26) contains the leading contribution to $\langle X\rangle$, scaling as N. It involves the contribution of the lowest-order approximation Φ to the condensate wave function; Φ is always normalized to unity and is obtained from the Gross-Pitaevskii equation:

$$i\hbar\partial_t\Phi(\vec{r},t)=-\frac{\hbar^2}{2m}\Delta\Phi(\vec{r},t)+[U(\vec{r},t) +Ng|\Phi(\vec{r},t)|^2]\Phi(\vec{r},t), \tag{27}$$

where $U(\vec{r},t)$ is the trapping potential of Eq. (4). The factor $N-\langle\delta\hat{N}\rangle$ in Eq. (26) is the number of particles in the condensate, which is less than the total number of particles N in the system.

The second line of Eq. (26) is of order N^0; it is also a contribution of the condensed particles. It originates from the fact that the exact condensate wave function differs from the prediction Φ of the Gross-Pitaevskii equation by a term of order $1/N$, giving rise to a contribution to $\langle X\rangle$ of order N^0. To our knowledge this correction was not systematically taken into account before in the literature. The derivation of this correction is presented in Sec. VI; it accounts for the action of noncondensed particles onto the particles in the condensate.

The third line in Eq. (26), also of order N^0, corresponds to the direct contribution of the noncondensed particles. It involves the field operator $\hat{\Lambda}(\vec{r},t)$, defined by Eqs. (16) and (21), which describes the dynamics of the noncondensed particles to lowest order. For example, the leading order approximation for the mean number of noncondensed particles is

$$\langle\delta\hat{N}\rangle\simeq\int d\vec{r}\langle\hat{\Lambda}^{\dagger}(\vec{r},t)\hat{\Lambda}(\vec{r},t)\rangle. \tag{28}$$

As we show in Sec. III, the field operator $\hat{\Lambda}(\vec{r},t)$ fulfills partial differential equations reminiscent of the Bogoliubov–de Gennes equations [5]:

$$i\hbar\partial_t\begin{pmatrix}\hat{\Lambda}(\vec{r},t)\\ \hat{\Lambda}^{\dagger}(\vec{r},t)\end{pmatrix}=\mathcal{L}(t)\begin{pmatrix}\hat{\Lambda}(\vec{r},t)\\ \hat{\Lambda}^{\dagger}(\vec{r},t)\end{pmatrix}. \tag{29}$$

The partial differential operator $\mathcal{L}(t)$, given explicitly in Eq. (46), has a very simple physical interpretation, as shown in Sec. IV: consider a solution of the Gross-Pitaevskii equation arbitrarily close to Φ; its deviation from Φ will evolve according to the linearized Gross-Pitaevskii equation. The part $\delta\Phi_{\perp}$ of this deviation orthogonal to Φ evolves then exactly as $\hat{\Lambda},\hat{\Lambda}^{\dagger}$ in Eq. (29):

$$i\hbar\partial_t\begin{pmatrix}\delta\Phi_{\perp}(\vec{r},t)\\ \delta\Phi^{*}_{\perp}(\vec{r},t)\end{pmatrix}=\mathcal{L}(t)\begin{pmatrix}\delta\Phi_{\perp}(\vec{r},t)\\ \delta\Phi^{*}_{\perp}(\vec{r},t)\end{pmatrix}. \tag{30}$$

One can therefore determine the dynamics of the noncondensed particles from a linear stability analysis of the GPE.

As we do not break the $U(1)$ symmetry in this paper we find that our equation Eq. (29) differs from the Bogoliubov–de Gennes equations usually found in the literature. In the time-independent case the predictions for the excitation spectra coincide but the mode functions of the excitations and their population differ: as shown in Sec. V, in our treatment the excitations are produced only in states orthogonal to the condensate wave function Φ. The phase spreading predicted in the $U(1)$ symmetry-breaking approach is obtained in our approach for a system being in statistical mixtures of stationary states with different number of particles (see Sec. V).

III. ASYMPTOTIC EXPANSION IN THE LIMIT OF LARGE N

We now work out explicitly the $1/\hat{N}^{1/2}$ expansion outlined in the previous section. In this way we give a rigorous derivation to the time-dependent Gross-Pitaevskii equation, which determines Φ, the lowest-order approximation to $\Phi_{\rm ex}$. We also derive the evolution equations for $\hat{\Lambda},\hat{\Lambda}^\dagger$, the lowest-order approximation to $\hat{\Lambda}_{\rm ex},\hat{\Lambda}_{\rm ex}^\dagger$; those equations are similar to the Bogoliubov–de Gennes equations [14]. We finally show that the first-order correction to the Gross-Pitaevskii approximation Φ for the condensate wave function is of order $1/N$, to be calculated explicitly in Sec. VI.

In this section we proceed as follows: (1) We calculate the terms in $(d/dt)\hat{\Lambda}_{\rm ex}$ of order k in $1/\sqrt{N}$, where $k=-1,0,\ldots$ successively. (2) We take the mean value of the expression obtained in point 1. This mean value has to vanish exactly, as $\langle\hat{\Lambda}_{\rm ex}\rangle$ is zero to all order; this gives an equation for $\Phi^{(k+1)}$, the term of the condensate wave function of order $k+1$. The remainder of the expression obtained in point 1 is exactly $(d/dt)\hat{\Lambda}^{(k)}$.

A. Order $\hat{N}^{1/2}$: Gross-Pitaevskii equation

We now calculate the time derivative of $\hat{\Lambda}_{\rm ex}$ keeping only the leading terms. We show that this time derivative contains terms of order $\sqrt{\hat{N}}$, which at first sight contradicts the expansion chosen in Eq. (21). In fact these terms will be shown to depend on $\Phi_{\rm ex}$ only and vanish for an appropriate definition of Φ.

From the definitions Eq. (16) and Eq. (12) we get

$$\frac{d}{dt}\hat{\Lambda}_{\rm ex}=\frac{1}{\sqrt{\hat{N}}}\hat{a}_{\Phi_{\rm ex}}^\dagger\left[\left(\frac{d}{dt}Q_{\rm ex}\right)\circ\hat{\Psi}+Q_{\rm ex}\circ\left(\frac{d}{dt}\hat{\Psi}\right)\right]+\frac{1}{\sqrt{\hat{N}}}\left(\frac{d}{dt}\hat{a}_{\Phi_{\rm ex}}^\dagger\right)Q_{\rm ex}\circ\hat{\Psi}. \tag{31}$$

In this expression the first term in the right-hand side is *a priori* of order $\sqrt{\hat{N}}$, which we therefore take here as the leading order. This is apparent from the following rewriting of the first term inside the brackets:

$$\left(\frac{d}{dt}Q_{\rm ex}\right)\circ\hat{\Psi}=-Q_{\rm ex}\left(\frac{d}{dt}|\Phi_{\rm ex}\rangle\right)\hat{a}_{\Phi_{\rm ex}}-|\Phi_{\rm ex}\rangle\left(\frac{d}{dt}\langle\Phi_{\rm ex}|\right)\circ\delta\hat{\Psi} \tag{32}$$

resulting from Eq. (8) and from the time derivative of Eq. (7).

To calculate the second term inside the brackets of Eq. (31) we determine the time evolution of $\hat{\Psi}$ from the Hamiltonian and keep the pertinent order:

$$i\hbar\frac{d}{dt}\hat{\Psi}(\vec{r},t)=\mathcal{H}(t)\hat{\Psi}(\vec{r},t)+g\hat{\Psi}^\dagger(\vec{r},t)\hat{\Psi}(\vec{r},t)\hat{\Psi}(\vec{r},t) \tag{33}$$

$$=\mathcal{H}(t)\Phi_{\rm ex}(\vec{r},t)\hat{a}_{\Phi_{\rm ex}}(t)+g|\Phi_{\rm ex}(\vec{r},t)|^2\Phi_{\rm ex}(\vec{r},t)\times\hat{a}_{\Phi_{\rm ex}}^\dagger(t)\hat{a}_{\Phi_{\rm ex}}(t)\hat{a}_{\Phi_{\rm ex}}(t)+O(\hat{N}^0). \tag{34}$$

We turn to the last term in the right-hand side of Eq. (31): taking the time derivative of Eq. (9) we find that

$$\frac{1}{\sqrt{\hat{N}}}\frac{d}{dt}\hat{a}_{\Phi_{\rm ex}}=\frac{(d/dt\,\langle\Phi_{\rm ex}|)|\Phi_{\rm ex}\rangle}{\sqrt{\hat{N}}}\hat{a}_{\Phi_{\rm ex}}+\frac{1}{\sqrt{\hat{N}}}\left(\frac{d}{dt}\langle\Phi_{\rm ex}|\right)\circ\delta\hat{\Psi}+\frac{1}{\sqrt{\hat{N}}}\langle\Phi_{\rm ex}|\circ\frac{d}{dt}\hat{\Psi}. \tag{35}$$

This is of order $\hat{N}^0$ so that this last term does not contribute to the present order $\sqrt{\hat{N}}$.

Further reductions consistent with the leading order are obtained by replacing $\Phi_{\rm ex}$ by its lowest order Φ, and by identifying $\hat{a}_{\Phi_{\rm ex}}^\dagger\hat{a}_{\Phi_{\rm ex}}$ with $\hat{N}$:

$$\hat{a}_{\Phi_{\rm ex}}^\dagger\hat{a}_{\Phi_{\rm ex}}=\hat{N}-\int d\vec{r}\,\delta\hat{\Psi}^\dagger(\vec{r})\,\delta\hat{\Psi}(\vec{r})=\hat{N}+O(\hat{N}^0). \tag{36}$$

We finally get

$$i\hbar\frac{d}{dt}\hat{\Lambda}_{\rm ex}(\vec{r},t)=\sqrt{\hat{N}}\langle\vec{r}|Q(t)\left[\mathcal{H}_{\rm GP}(t)-i\hbar\frac{d}{dt}\right]|\Phi\rangle+O(\hat{N}^0), \tag{37}$$

where Q defined in Eq. (23) projects orthogonally to Φ. The operator $\mathcal{H}_{\rm GP}$ is given by

$$\mathcal{H}_{\rm GP}(t)=\frac{p^2}{2m}+U(\vec{r},t)+g_N|\Phi(\vec{r},t)|^2. \tag{38}$$

From the requirement Eq. (17), $(d/dt)\,\langle\hat{\Lambda}_{\rm ex}\rangle=0$, and the expectation value of Eq. (37) determines the lowest-order approximation to $\Phi_{\rm ex}$:

$$Q(t)\left[-i\hbar\frac{d}{dt}+\mathcal{H}_{\rm GP}(t)\right]|\Phi(t)\rangle=0. \tag{39}$$

Therefore we have

$$\left[-i\hbar\frac{d}{dt}+\mathcal{H}_{\rm GP}(t)\right]|\Phi(t)\rangle=\xi(t)|\Phi(t)\rangle, \tag{40}$$

where the arbitrary real function $\xi(t)$ corresponds to an arbitrary global phase of the wave function Φ. We recover the time-dependent Gross-Pitaevskii equation [5], which is usually written with the choice $\xi(t)\equiv 0$. The last term in the one-particle Hamiltonian $\mathcal{H}_{\rm GP}(t)$ describes an effective mean-field potential due to particle interactions.

When the system is in a steady state, the one-body density matrix ρ_1 is time independent and Φ can be chosen time independent as well; Eq. (40) then reduces to

$$\mathcal{H}_{\rm GP}|\Phi\rangle=\mu|\Phi\rangle, \tag{41}$$

where $\xi(t)\equiv\mu$ is a constant determined from the normalization of Φ to unity. It is known that μ corresponds to the lowest-order approximation to the chemical potential of the system [5]. In what follows we take the solution of Eq. (41) as the initial condition for the time evolution of $\Phi(t)$, in particular we set

$$\xi(t=0)=\mu. \tag{42}$$

B. Order $\hat{N}^0$: Time-dependent Bogoliubov–de Gennes equations

In this subsection we collect the terms of order $\hat{N}^0$ in $(d/dt)\hat{\Lambda}_{\rm ex}$ to derive the time evolution of $\hat{\Lambda}$. The correction $\Phi^{(1)}$ is obtained by a calculation to the same order; it is shown in the next subsection that $\Phi^{(1)}$ is in fact zero, and we directly use this result here.

We take again the exact Eq. (31). The terms of order $\hat{N}^{1/2}$ vanish due to our choice of Φ so we are left with terms of order $\hat{N}^0$. The first term inside the brackets is already given by Eq. (32); as $\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}=\hat{N}+O(\hat{N}^0)$, only the last term of Eq. (32) contributes to Eq. (31).

The second term inside the brackets of Eq. (31) is obtained to order $\hat{N}^0$ by substituting Eq. (8) into Eq. (33) and keeping only terms linear in $\delta\hat{\Psi}$; the terms involving only $\hat{a}_{\Phi_{\rm ex}}$ have already contributed indeed to the previous order $\sqrt{N}$ and their next-order contribution to Eq. (31) is found to be of order $\hat{N}^{-1/2}$ rather than $\hat{N}^0$ because $\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}=\hat{N}+O(\hat{N}^0)$. One is left with

$$\begin{aligned} i\hbar\frac{d}{dt}\delta\hat{\Psi}=&-i\hbar|\Phi_{\rm ex}\rangle\left(\frac{d}{dt}\langle\Phi_{\rm ex}|\right)\circ\delta\hat{\Psi}\\ &+Q\circ\{[\mathcal{H}+2g\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}|\Phi_{\rm ex}(\vec{r},t)|^2]\delta\hat{\Psi}\\ &+g_N\Phi_{\rm ex}(\vec{r},t)^2\hat{a}^2_{\Phi_{\rm ex}}\delta\hat{\Psi}^\dagger\}+O(1/\sqrt{\hat{N}}). \end{aligned} \tag{43}$$

Finally the last term on the right hand side of Eq. (31) is obtained from Eq. (35); in this last equation $(d/dt)\hat{\Psi}$ is correctly replaced by its approximation of order $\sqrt{\hat{N}}$ [Eq. (34)], so that

$$\begin{aligned} i\hbar\frac{1}{\sqrt{\hat{N}}}\frac{d}{dt}\hat{a}_{\Phi_{\rm ex}}=&\frac{1}{\sqrt{\hat{N}}}\langle\Phi_{\rm ex}|\left[\mathcal{H}_{\rm GP}(t)-i\hbar\frac{d}{dt}\right]|\Phi_{\rm ex}\rangle\hat{a}_{\Phi_{\rm ex}}\\ &+O(1/\sqrt{\hat{N}})\\ =&\,\xi(t)\frac{1}{\sqrt{\hat{N}}}\hat{a}_{\Phi_{\rm ex}}+O(1/\sqrt{\hat{N}}). \end{aligned} \tag{44}$$

The reader interested in obtaining a more global point of view on the derivation is referred to our Appendix A; the exact value of $(d/dt)\hat{\Lambda}_{\rm ex}$ is given in this appendix; from this expression one can straightforwardly identify the terms order by order.

We collect the previous results and identify $\Phi_{\rm ex}$ and $g\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}$ with Φ and $g\hat{N}$, respectively, in a manner consistent with the order $\hat{N}^0$ of the calculation, keeping in mind the asymptotic expansion Eq. (18), that is, $g=O(1/N)$. We obtain the time evolution of the operators $\hat{\Lambda},\hat{\Lambda}^\dagger$ of Eq. (21):

$$i\hbar\frac{d}{dt}\begin{pmatrix}\hat{\Lambda}(t)\\ \hat{\Lambda}^\dagger(t)\end{pmatrix}=\mathcal{L}(t)\circ\begin{pmatrix}\hat{\Lambda}(t)\\ \hat{\Lambda}^\dagger(t)\end{pmatrix} \tag{45}$$

with

$$\mathcal{L}(t)=\begin{pmatrix}\mathcal{H}_{\rm GP}(t)+g_NQ(t)|\Phi(\vec{r},t)|^2Q(t)-\xi(t) & g_NQ(t)\Phi^2(\vec{r},t)Q^*(t)\\ -g_NQ^*(t)\Phi^{*2}(\vec{r},t)Q(t) & -\mathcal{H}_{\rm GP}(t)-g_NQ^*(t)|\Phi(\vec{r},t)|^2Q^*(t)+\xi(t)\end{pmatrix}. \tag{46}$$

In this expression the complex conjugate of any one-body operator η is defined in the basis of the localized states $|\vec{r}\rangle$, that is

$$\langle\vec{r}|X^*|\vec{r}\rangle\equiv(\langle\vec{r}|X|\vec{r}\rangle) \tag{47}$$

For example, $Q^*(t)$ projects orthogonally to the state $|\Phi^*\rangle$ whose wave function is $\Phi^*(\vec{r},t)$.

When the system is in a steady state $\zeta(t)=\mu$, as discussed in the previous section, and our equations (45) become very similar to the Bogoliubov–de Gennes equations [5]; the only difference is the emergence of the projectors Q,Q^*. This difference is due to the fact that we are considering states of the total system with a fixed number of particles, whereas the standard treatments in the literature introduce states with ''broken symmetry.'' The physical consequences of the presence of the projectors will be discussed in Sec. V.

C. Order $\hat{N}^{-1/2}$: Corrections to the Gross-Pitaevskii equation

Neglecting terms of order $O(1/\sqrt{\hat{N}})$ in $(d/dt)\hat{\Lambda}_{\rm ex}$ in Eq. (A3) given in Appendix A, we get from the requirement Eq. (17) that $(d/dt)\langle\hat{\Lambda}\rangle=0$ and therefore

$$Q_{\rm ex}\left[-i\hbar\frac{d}{dt}+\mathcal{H}+g_N|\Phi_{\rm ex}|^2\right]|\Phi_{\rm ex}\rangle=O(1/\sqrt{\hat{N}}). \quad (48)$$

Consistently we replace $Q_{\rm ex}$ and $\Phi_{\rm ex}$ by their expansion up to order $1/\sqrt{\hat{N}}$; this leads to

$$\begin{pmatrix} Q(t) & 0 \\ 0 & Q^*(t)\end{pmatrix}\left(i\hbar\frac{d}{dt}-\mathcal{L}_{\rm GP}(t)\right)\begin{pmatrix}\Phi^{(1)}(t)\\ \Phi^{(1)*}(t)\end{pmatrix}=0, \quad (49)$$

where

$$\mathcal{L}_{\rm GP}=\begin{pmatrix}\mathcal{H}+2g_N|\Phi(\vec{r})|^2-\xi & g_N\Phi^2(\vec{r})\\ -g_N\Phi^{*2}(\vec{r}) & -\mathcal{H}-2g_N|\Phi(\vec{r})|^2+\xi\end{pmatrix}. \quad (50)$$

We have used the fact that $\langle\Phi^{(1)}|\Phi\rangle+\langle\Phi|\Phi^{(1)}\rangle=0$ from the normalization condition Eq. (7). The operator $\mathcal{L}_{\rm GP}$ corresponds to the linear evolution of small deviations from the solution $\Phi(t)$ in the Gross-Pitaevskii equation (40) as shown in the next section. Equation (49) for $\Phi^{(1)}$ is linear and homogeneous so that

$$\Phi^{(1)}(t)\equiv 0 \quad (51)$$

$\forall t$ if $\Phi^{(1)}(t=0)\equiv 0$.

The system is initially in thermal equilibrium; in this case, from a time-reversal symmetry argument, the N-particle wave function is real and therefore $\Phi_{\rm ex}(\vec{r},t=0),\Phi(\vec{r},t=0)$, and $\Phi^{(1)}(\vec{r},t=0)$ can be chosen real. From the normalization condition Eq. (7) we find that $|\Phi^{(1)}(t=0)\rangle$ is orthogonal to $|\Phi(t=0)\rangle$. We project Eq. (49) for $t=0$ onto $|\Phi^{(1)}(t=0)\rangle$:

$$\langle\Phi^{(1)}|[\mathcal{H}+3g_N\Phi(\vec{r})^2-\mu]|\Phi^{(1)}\rangle=0, \quad (52)$$

which imposes

$$\Phi^{(1)}\equiv 0 \quad (53)$$

as the operator in the above equation is strictly positive because Φ is the ground state of $\mathcal{H}_{\rm GP}$ (at least for $g>0$).

The first correction to Φ is therefore of $O(1/N)$. It will be discussed in Sec. VI.

IV. TIME EVOLUTION OF $\hat{\Lambda}$

We show that the time evolution of the operators $\hat{\Lambda}$, that is, the dynamics of the noncondensed particles, amounts to propagating orthogonal perturbations to Φ.

The time evolution of $\hat{\Lambda}$ is performed most conveniently by choosing a basis which diagonalizes $\mathcal{L}$ at $t=0$. At $t=0$ we expand $\hat{\Lambda}$ in this eigenbasis of modal functions with coefficients that are operator valued. We give an interpretation of these operators as annihilation operators of elementary excitations of the system. For time-dependent problems the evolution of $\hat{\Lambda}$ is totally contained in the time dependence of the modal functions and the operator-valued coefficients are constants of motion.

A. Physical interpretation of the time evolution operator

In this section we show the equivalence of the time evolution of the quantum fluctuations described by $\hat{\Lambda}$ and the time evolution of small perturbations $\delta\Phi$ of the time-dependent solution Φ of the Gross-Pitaevskii equation. Linearizing the time-dependent Gross-Pitaevskii equation around the solution Φ, we obtain

$$i\hbar\frac{d}{dt}\begin{pmatrix}\delta\Phi(t)\\ \delta\Phi^*(t)\end{pmatrix}=\mathcal{L}_{\rm GP}(t)\begin{pmatrix}\delta\Phi(t)\\ \delta\Phi^*(t)\end{pmatrix}, \quad (54)$$

where $\mathcal{L}_{\rm GP}(t)$ has already been introduced in Eq. (50).

$\mathcal{L}_{\rm GP}(t)$ is different from $\mathcal{L}$ because of the presence of projectors Q,Q^* in $\mathcal{L}$. Physically this results from the orthogonality to Φ of the quantum fluctuations described by $\hat{\Lambda}$ [see Eq. (13)]. We therefore consider the evolution of the components of the perturbations $\delta\Phi(t)$ orthogonal to Φ, that is, of $|\delta\Phi_\perp(t)\rangle=Q(t)|\delta\Phi(t)\rangle$. We take the time derivative of this relation and split $|\delta\Phi\rangle$ into $|\delta\Phi_\perp\rangle$ and a part proportional to $|\Phi\rangle$:

$$\begin{aligned}i\hbar\frac{d}{dt}\begin{pmatrix}\delta\Phi_\perp(t)\\ \delta\Phi_\perp^*(t)\end{pmatrix}=&\left[\begin{pmatrix}Q(t)&0\\0&Q^*(t)\end{pmatrix}\mathcal{L}_{\rm GP}(t)\right.\\ &\left.+i\hbar\frac{d}{dt}\begin{pmatrix}Q(t)&0\\0&Q^*(t)\end{pmatrix}\right]\begin{pmatrix}\delta\Phi_\perp(t)\\ \delta\Phi_\perp^*(t)\end{pmatrix}\\ &+g_N(\langle\Phi|\delta\Phi\rangle+\langle\delta\Phi|\Phi\rangle)\\ &\times\begin{pmatrix}Q|\Phi|^2|\Phi\rangle\\ -Q^*|\Phi|^2|\Phi^*\rangle\end{pmatrix}, \quad (55)\end{aligned}$$

where we used $|\Phi|^2|\Phi\rangle=\Phi^2|\Phi^*\rangle$ and $\dot{Q}\Phi=-Q\dot{\Phi}$. The source term that couples $\delta\Phi_\perp$ to the component of $\delta\Phi$ proportional to Φ vanishes due to the normalization condition $\langle\Phi|\Phi\rangle=(\langle\Phi|+\langle\delta\Phi|)(|\Phi\rangle+|\delta\Phi\rangle)=1$ obeyed to first order in $\delta\Phi$. The homogeneous term can be identified with $\mathcal{L}$ defined in Eq. (46) using the identity $i\hbar\,(d/dt)\,Q=[\mathcal{H}_{\rm GP},Q]$:

$$i\hbar\frac{d}{dt}\begin{pmatrix}\delta\Phi_\perp(t)\\ \delta\Phi_\perp^*(t)\end{pmatrix}=\mathcal{L}(t)\begin{pmatrix}\delta\Phi_\perp(t)\\ \delta\Phi_\perp^*(t)\end{pmatrix}. \quad (56)$$

Remarkably this shows that, in the linear response regime, the quantum fluctuations associated with $\hat{\Lambda}$ evolve in exactly the same way as the classical orthogonal perturbation $\delta\Phi_\perp$.

We can restate the same conclusion in terms of the time evolution operators. Let $U_{\rm GP}(t)$ be the evolution operator corresponding to $\mathcal{L}_{\rm GP}$. Let $U(t)$ be the evolution operator corresponding to $\mathcal{L}$ and restricted to the space orthogonal to $[\Phi(t=0),0]$ and $[0,\Phi^*(t=0)]$. From Eqs. (54) and (56) we get, as shown explicitly in Appendix B,

$$U(t)=\begin{pmatrix}Q(t)&0\\0&Q^*(t)\end{pmatrix}U_{\rm GP}(t)\begin{pmatrix}Q(0)&0\\0&Q^*(0)\end{pmatrix}. \quad (57)$$

This result shows that propagating with $\mathcal{L}$ amounts to propagating with $\mathcal{L}_{\rm GP}$ and projecting the result with $Q(t), Q^*(t)$. If one can determine how a small deviation from a given solution $\Phi(t)$ of the Gross-Pitaevskii equation evolves in time one can from that immediately derive the dynamics of the noncondensed particles.

In a recent work [18] we have identified physical situations where the wave function $\Phi(t)$ is an unstable solution of the Gross-Pitaevskii equation, i.e., a small initial deviation from $\Phi(0)$ will be amplified exponentially with time. From the above discussion we conclude that the same property holds for the field operator $\hat{\Lambda}$; the density of noncondensed particles, $\langle \hat{\Lambda}^\dagger \hat{\Lambda} \rangle$, will then diverge exponentially with time, until the Bogoliubov approximation fails.

B. Time-dependent modal decomposition

To study the dynamics of the noncondensed particles we have to solve Eq. (45) for $\hat{\Lambda}, \hat{\Lambda}^\dagger$. We obtain in this section a solution to this equation in terms of an infinite sum of time independent operators with time-dependent coefficients. Those coefficients correspond to the time propagation by $U(t)$ of the eigenmodes of $\mathcal{L}$ at $t=0$. The time-independent operators constitute a complete set of ''constants of motion'' for Eq. (45).

1. Spectral decomposition of $\mathcal{L}(t=0)$

We consider first the case of the system being in a steady state. The operator $\mathcal{L}$ in Eq. (45) is time independent with ξ given by Eq. (42) and we diagonalize it. We start by exploring the symmetries of $\mathcal{L}$. The first one corresponds to a time reversal spin-flip symmetry:

$$\sigma_1 \mathcal{L} \sigma_1 = -\mathcal{L}^*, \tag{58}$$

where $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ is the first Pauli matrix. The second one expresses the fact that $\mathcal{L}$ is Hermitian for the spinorial scalar product of signature $(1,-1)$:

$$\sigma_3 \mathcal{L} \sigma_3 = \mathcal{L}^\dagger, \tag{59}$$

where $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is the third Pauli matrix. This has the following consequences for the eigenvectors of $\mathcal{L}$. If (u,v) is an eigenvector with eigenvalue E, (v^*,u^*) is an eigenvector of $\mathcal{L}$ with the eigenvalue $-E^*$ and $(u,-v)$ is an eigenvector of $\mathcal{L}^\dagger$ with the eigenvalue E.

We assume that $\mathcal{L}(t=0)$ is diagonalizable and that all eigenvalues are real [23]. In this case if $\{(u_k,v_k), E_k>0, k=1,\ldots\}$ is the set of eigenvectors with *strictly positive* eigenvalues E_k, we can write the eigenbasis of $\mathcal{L}(t=0)$ as $\{(u_k,v_k),(\Phi,0),(0,\Phi^*),(v_k^*,u_k^*), k=1,\ldots\}$. We have embodied the fact that $(\Phi,0)$ and $(0,\Phi^*)$ span the zero eigenvalue subspace of $\mathcal{L}$.

With Eq. (59) we get an eigenbasis of $\mathcal{L}^\dagger$ (left eigenvectors of $\mathcal{L}$) from the one of $\mathcal{L}$ by action of σ_3: $\{(u_k,-v_k), (\Phi,0),(0,\Phi^*),(-v_k^*,u_k^*), k=1,\ldots\}$ (where we choose the signs for convenience). The vectors (u_k,v_k) and $(u_{k'}, -v_{k'})$ $(k \neq k')$ are orthogonal because they correspond to different eigenvalues for $\mathcal{L}$ and $\mathcal{L}^\dagger$. For the same reason (u_k,v_k) and $(-v_{k'}^*, u_{k'}^*)$ $(\forall k,k')$ are orthogonal and as well $|u_k\rangle$ and $|v_k\rangle$ are orthogonal to $|\Phi\rangle$ and $|\Phi^*\rangle$, respectively. The eigenbasis can be normalized so that [24]

$$\begin{aligned} \langle u_k | u_{k'} \rangle - \langle v_k | v_{k'} \rangle &= \delta_{kk'}, \\ \langle v_k | u_{k'}^* \rangle - \langle u_k | v_{k'}^* \rangle &= 0. \end{aligned} \tag{60}$$

With this normalization we get the decomposition of unity

$$\begin{aligned} \mathbb{1} = &\begin{pmatrix} |\Phi\rangle \\ 0 \end{pmatrix} (\langle \Phi|, 0) + \begin{pmatrix} 0 \\ |\Phi^*\rangle \end{pmatrix} (0, \langle \Phi^*|) + \sum_{k>0} \begin{pmatrix} |u_k\rangle \\ |v_k\rangle \end{pmatrix} \\ &\times (\langle u_k|, -\langle v_k|) + \begin{pmatrix} |v_k^*\rangle \\ |u_k^*\rangle \end{pmatrix} (-\langle v_k^*|, \langle u_k^*|) \end{aligned} \tag{61}$$

and of the operator $\mathcal{L}$

$$\mathcal{L} = \sum_{k>0} E_k \begin{pmatrix} |u_k\rangle \\ |v_k\rangle \end{pmatrix} (\langle u_k|, -\langle v_k|) - E_k \begin{pmatrix} |v_k^*\rangle \\ |u_k^*\rangle \end{pmatrix} (-\langle v_k^*|, \langle u_k^*|). \tag{62}$$

We finally expand $(\hat{\Lambda}, \hat{\Lambda}^\dagger)$ at time $t=0$ in the eigenbasis of $\mathcal{L}(t=0)$:

$$\begin{pmatrix} \hat{\Lambda}(\vec{r}, t=0) \\ \hat{\Lambda}^\dagger(\vec{r}, t=0) \end{pmatrix} = \sum_{k=1}^{\infty} \hat{b}_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + \hat{b}_k^\dagger \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix}. \tag{63}$$

The coefficients $\hat{b}_k$ are obtained by projection on the eigenvector (u_k, v_k) using the adjoint vector $(u_k, -v_k)$:

$$\hat{b}_k = \int d\vec{r} u_k^*(\vec{r}) \hat{\Lambda}(\vec{r}) - v_k^*(\vec{r}) \hat{\Lambda}^\dagger(\vec{r}). \tag{64}$$

They are in fact operators, and they form a bosonic algebra as a consequence of Eq. (60):

$$[\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{kk'}, \tag{65}$$

$$[\hat{b}_k, \hat{b}_{k'}] = 0. \tag{66}$$

2. Time evolution of the modes

To get $(\hat{\Lambda}, \hat{\Lambda}^\dagger)$ at any later time t we have to evolve the decomposition Eq. (63) by action of $U(t)$ onto the vectors (u_k, v_k); this simply means that they satisfy

$$i\hbar \frac{d}{dt} \begin{pmatrix} |u_k(t)\rangle \\ |v_k(t)\rangle \end{pmatrix} = \mathcal{L}(t) \begin{pmatrix} |u_k(t)\rangle \\ |v_k(t)\rangle \end{pmatrix} \tag{67}$$

for all modes k. The $\hat{b}_k$'s have the desired property of being time independent:

$$\frac{d}{dt} \hat{b}_k = 0. \tag{68}$$

The decomposition Eq. (63) extends to $t>0$ as

$$\begin{pmatrix} \hat{\Lambda}(\vec{r}, t) \\ \hat{\Lambda}^\dagger(\vec{r}, t) \end{pmatrix} = \sum_{k=1}^{\infty} \hat{b}_k \begin{pmatrix} u_k(\vec{r}, t) \\ v_k(\vec{r}, t) \end{pmatrix} + \hat{b}_k^\dagger \begin{pmatrix} v_k^*(\vec{r}, t) \\ u_k^*(\vec{r}, t) \end{pmatrix} \tag{69}$$

which shows explicitly that the time evolution of $\hat{\Lambda}(\vec{r},t)$ is contained in the time dependence of the mode functions $u_k(\vec{r},t), v_k(\vec{r},t)$. Such an expression is very convenient, because one has to deal only with the evolution of regular functions rather than with operators to calculate the evolution of $\hat{\Lambda}$. Note that this time evolution conserves the decomposition of unity of Eq. (61).

C. Physics contained in the $\hat{b}_k$'s: Elementary excitations

We express the Hamiltonian Eq. (3) up to $O(\hat{N}^0)$ in terms of Φ and $\hat{\Lambda},\hat{\Lambda}^\dagger$, specializing for simplicity to the time independent case where $\xi(t)\equiv\mu, (d/dt)\,|\Phi(t)\rangle\equiv 0$. We find that terms linear in $\delta\hat{\Psi}$ disappear because of Eqs. (41), (13). We get [25]

$$\hat{H}=\hat{N}\langle\Phi|\mathcal{H}+\frac{(N-1)g}{2}|\Phi(\vec{r})|^2|\Phi\rangle-\frac{1}{2}\mathrm{Tr}[Q(\mathcal{H}_{\mathrm{GP}}-\mu+g_N|\Phi|^2)]+\frac{1}{2}(\hat{\Lambda}^\dagger,-\hat{\Lambda})\circ\mathcal{L}\circ\begin{pmatrix}\hat{\Lambda}\\ \hat{\Lambda}^\dagger\end{pmatrix}+O(1/\sqrt{\hat{N}}). \tag{70}$$

The first line contains two terms depending on N only; the first term is the mean energy one would get if all the N particles were in the same quantum state $|\Phi\rangle$. The second line is quadratic in the field operator $\hat{\Lambda}$ and is at the origin of the dynamics of the noncondensed particles described by Eq. (46).

We now insert in Eq. (70) the modal expansion of $\hat{\Lambda},\hat{\Lambda}^\dagger$ [Eq. (63)]. Since these modes are eigenvectors of $\mathcal{L}$, Eq. (70) simply reads as

$$\hat{H}=E_0(\hat{N})+\sum_{k>0}E_k\hat{b}_k^\dagger\hat{b}_k+O(1/\sqrt{\hat{N}}),$$
$$E_0(\hat{N})=\hat{N}\langle\Phi|\mathcal{H}+\frac{(N-1)g}{2}|\Phi(\vec{r})|^2|\Phi\rangle-\sum_{k>0}E_k\langle v_k|v_k\rangle. \tag{71}$$

This corresponds to a set of uncoupled harmonic oscillators [26]. The ground state of the N-particle system is given by the vacuum of the $\hat{b}_k$'s. The excited states are obtained by successively applying the operators $\hat{b}_k^\dagger$ on the vacuum. The excitation operator $\hat{b}_k^\dagger$ is a superposition of a transfer of a particle out of the condensate into the state u_k ($u_k\hat{\Lambda}^\dagger$) and a transfer of a particle from state v_k^* into the condensate ($v_k\hat{\Lambda}$). One recovers the same algebra as for the usual Bogoliubov–de Gennes equations; as shown in Sec. V A, the spectrum E_k coincides with the well-known Bogoliubov one, whereas the modes functions are different. Another difference is that our excitation operators $b_k^\dagger$ conserve the total number of particles in the system.

Note that even for a time-dependent problem the number of excitations $\Sigma_{k>0}\langle\hat{b}_k^\dagger\hat{b}_k\rangle$ is preserved by the time evolution because of Eq. (68). This conclusion, however, does not hold for the mean number $\langle\delta\hat{N}\rangle$ of noncondensed particles, which depends explicitly on the mode functions; e.g., for a system initially prepared at temperature T we get at any later time

$$\langle\delta\hat{N}(t)\rangle=\sum_k\langle\hat{b}_k^\dagger\hat{b}_k\rangle\langle u_k(t)|u_k(t)\rangle+\langle\hat{b}_k^\dagger\hat{b}_k+1\rangle\times\langle v_k(t)|v_k(t)\rangle, \tag{72}$$

where $\langle\hat{b}_k^\dagger\hat{b}_k\rangle=[\exp(E_k/k_BT)-1]^{-1}$.

Two different types of excitations of the system are considered in the literature. A state with a time-dependent condensate wave function $\Phi(t)$ constitutes a collective excitation of the system. Such a collective excitation can be produced, e.g., by a time modulation of the trapping potential. This is distinct from the one-particle excitation created by $\hat{b}_k^\dagger$ even though, as a consequence of Eq. (57), the spectrum of the collective excitations (defined as the eigenfrequencies of the linearized Gross-Pitaevskii equation around time independent solution) coincide with the spectrum formed by the $E_k/\hbar$'s.

V. COMPARISON WITH THE SYMMETRY-BREAKING APPROACH

In the approach used in the literature up to now [5] the $U(1)$ symmetry is broken by splitting the field operator $\hat{\Psi}(\vec{r})$ into a classical field $\sqrt{N}\Phi(\vec{r})$ and a part describing quantum fluctuations. These quantum fluctuations can be shown [5] to have a time evolution similar to that of $\hat{\Lambda},\hat{\Lambda}^\dagger$ [Eq. (45)] with $\mathcal{L}$ replaced by $\mathcal{L}_{\mathrm{GP}}$ given by Eq. (50). In this section we investigate the physical differences in the dynamics induced by $\mathcal{L}$ and $\mathcal{L}_{\mathrm{GP}}$, restricting for simplicity to a time independent condensate wave function [with the convention $\xi(t)\equiv\mu$ and $\Phi(t)\equiv\Phi(0)$].

Mathematically $\mathcal{L}_{\mathrm{GP}}$ contrarily to $\mathcal{L}$ does not involve the projector Q orthogonally to Φ. $\mathcal{L}$ and $\mathcal{L}_{\mathrm{GP}}$ still have the same spectrum, leading to identical elementary excitation spectra for the $U(1)$ symmetry-conserving and $U(1)$ symmetry-breaking approaches. However, the eigenvectors of $\mathcal{L}_{\mathrm{GP}}$ do not form a complete basis: there is a ''missing eigenvector,'' which is at the origin of the ''momentum'' operator of the condensate introduced in [15]. In the $U(1)$ symmetry-breaking approach this ''missing eigenvector'' is responsible for a divergence linear in time of the quantum fluctuations, resulting in a phase spreading of the condensate. We show how this phase spreading emerges in the $U(1)$ symmetry-preserving approach.

A. Comparison of the spectral properties: The ''missing eigenvector''

Even though the symmetries for $\mathcal{L}_{\mathrm{GP}}$ are the same as those mentioned for $\mathcal{L}$, the modal decomposition performed in Sec. IV B has to be adapted. A remarkable property is that the eigenvalues of $\mathcal{L}$ and of $\mathcal{L}_{\mathrm{GP}}$ are the same; for eigenvalues $E\neq 0$ we find indeed a one-to-one correspondence between the eigenvectors (u,v) for $\mathcal{L}$ and the eigenvectors (U,V) of $\mathcal{L}_{\mathrm{GP}}$:

$$|u\rangle = Q|U\rangle,$$

$$|v\rangle = Q^*|V\rangle$$

[$\langle u|u\rangle - \langle v|v\rangle = \langle U|U\rangle - \langle V|V\rangle = 1$ and Q is given by Eq. (23)].

For the eigenvalue $E=0$, however, we find as the only eigenvector for $\mathcal{L}_{\rm GP}$: $(\Phi, -\Phi^*)$. One vector is therefore missing in order to form a basis. This missing vector will be obtained as an eigenvector (u_a, v_a) of $\mathcal{L}_{\rm GP}^2$ with eigenvalue zero. As a consequence the action of $\mathcal{L}_{\rm GP}$ on (u_a, v_a) gives an eigenvector of $\mathcal{L}_{\rm GP}$ with eigenvalue zero, so that

$$\mathcal{L}_{\rm GP}\begin{pmatrix} |u_a\rangle \\ |v_a\rangle \end{pmatrix} = \alpha \begin{pmatrix} |\Phi\rangle \\ -|\Phi\rangle \end{pmatrix}. \tag{73}$$

Here α is a complex number and without loss of generality we assume that Φ is real. By adding and/or subtracting the two lines in Eq. (73) we get

$$\begin{aligned} &(\mathcal{H}_{\rm GP} - \mu)(|u_a\rangle - |v_a\rangle) = 0, \\ &(\mathcal{H}_{\rm GP} + 2g_N|\Phi(\vec{r})|^2 - \mu)(|u_a\rangle + |v_a\rangle) = 2\alpha|\Phi\rangle. \end{aligned} \tag{74}$$

The first line imposes $|u_a\rangle - |v_a\rangle \propto |\Phi\rangle$. We wish to have (u_a, v_a) orthogonal to the only eigenvector of $\mathcal{L}_{\rm GP}$ with $E=0$, which imposes $|u_a\rangle = |v_a\rangle = |\Phi_a\rangle$. The second line [Eq. (74)] determines uniquely $|\Phi_a\rangle$. We construct the adjoint basis as done in Sec. IV B (this is possible due to the fact that $\mathcal{L}_{\rm GP}$ and $\mathcal{L}$ have the same symmetries). By choosing α such that (Φ, Φ) is the adjoint vector of (Φ_a, Φ_a), we have

$$\langle \Phi | \Phi_a \rangle = 1/2 \tag{75}$$

and we get the decomposition of unity

$$\begin{aligned} 1 = &\begin{pmatrix} |\Phi\rangle \\ -|\Phi^*\rangle \end{pmatrix}(\langle\Phi_a|, -\langle\Phi_a^*|) + \begin{pmatrix} |\Phi_a\rangle \\ |\Phi_a^*\rangle \end{pmatrix}(\langle\Phi|, \langle\Phi^*|) \\ &+ \sum_{k>0} \begin{pmatrix} |U_k\rangle \\ |V_k\rangle \end{pmatrix}(\langle U_k|, -\langle V_k|) + \begin{pmatrix} |V_k^*\rangle \\ |U_k^*\rangle \end{pmatrix}(-\langle V_k^*|, \langle U_k^*|) \end{aligned} \tag{76}$$

and of the operator $\mathcal{L}_{\rm GP}$

$$\begin{aligned} \mathcal{L}_{\rm GP} = &\alpha \begin{pmatrix} |\Phi\rangle \\ -|\Phi^*\rangle \end{pmatrix}(\langle\Phi|, \langle\Phi^*|) + \sum_{k>0} E_k \begin{pmatrix} |U_k\rangle \\ |V_k\rangle \end{pmatrix} \\ &\times (\langle U_k|, -\langle V_k|) - E_k \begin{pmatrix} |V_k^*\rangle \\ |U_k^*\rangle \end{pmatrix}(-\langle V_k^*|, \langle U_k^*|). \end{aligned} \tag{77}$$

Comparing this with the expansion Eq. (62) for $\mathcal{L}$ we see that there is an extra term in the expansion of $\mathcal{L}_{\rm GP}$. The physical implications for the Bogoliubov Hamiltonian are discussed now, and the implications for the dynamics of the quantum fluctuations are the subject of the next section.

In the symmetry-breaking point of view, the quantum field operator is split as $\hat{\Psi} = \sqrt{N}\Phi + \hat{\tilde{\Psi}}$, where $\sqrt{N}\Phi$ is the classical field. Reproducing the analysis of Sec. IV C, we find that the Bogoliubov Hamiltonian is now

$$\hat{H}_{U(1)} = (\text{function}(N)) + \frac{1}{2}(\hat{\tilde{\Psi}}^\dagger, -\hat{\tilde{\Psi}})\mathcal{L}_{\rm GP}\begin{pmatrix} \hat{\tilde{\Psi}} \\ \hat{\tilde{\Psi}}^\dagger \end{pmatrix}. \tag{78}$$

Inserting the spectral decomposition Eq. (77) in this expression, we recover the form obtained in [15]:

$$\hat{H}_{U(1)} = E_{U(1)}(N) + \frac{1}{2}\alpha \hat{P}_{U(1)}^2 + \sum_{k>0} E_k \hat{B}_k^\dagger \hat{B}_k, \tag{79}$$

with

$$\begin{aligned} \begin{pmatrix} \hat{\tilde{\Psi}}(\vec{r}) \\ \hat{\tilde{\Psi}}^\dagger(\vec{r}) \end{pmatrix} = &\frac{1}{i\hbar}\hat{Q}_{U(1)}\begin{pmatrix} \Phi(\vec{r}) \\ -\Phi^*(\vec{r}) \end{pmatrix} + \hat{P}_{U(1)}\begin{pmatrix} \Phi_a(\vec{r}) \\ \Phi_a^*(\vec{r}) \end{pmatrix} \\ &+ \sum_{k>0} \hat{B}_k \begin{pmatrix} U_k(\vec{r}) \\ V_k(\vec{r}) \end{pmatrix} + \hat{B}_k^\dagger \begin{pmatrix} V_k^*(\vec{r}) \\ U_k^*(\vec{r}) \end{pmatrix}, \end{aligned} \tag{80}$$

$$\hat{Q}_{U(1)} = i\hbar(\langle\Phi_a|\circ\hat{\tilde{\Psi}} - \langle\Phi_a^*|\circ\hat{\tilde{\Psi}}^\dagger), \tag{81}$$

$$\hat{P}_{U(1)} = \langle\Phi|\circ\hat{\tilde{\Psi}} + \langle\Phi^*|\circ\hat{\tilde{\Psi}}^\dagger, \tag{82}$$

$$\hat{B}_k = \langle U_k|\circ\hat{\tilde{\Psi}} - \langle V_k|\circ\hat{\tilde{\Psi}}^\dagger. \tag{83}$$

As discussed in [15] $\hat{H}_{U(1)}$ corresponds to a set of uncoupled harmonic oscillators plus the ''kinetic'' energy of an unbound ''phase'' coordinate $\hat{Q}_{U(1)}$ conjugate to the ''momentum'' $\hat{P}_{U(1)}$.

The frequencies of the harmonic oscillators in $\hat{H}_{U(1)}$ constitute the spectrum of elementary excitations. They exactly coincide with the ones obtained in our $U(1)$ symmetry-preserving approach, as expected from the fact that $\mathcal{L}_{\rm GP}$ and $\mathcal{L}$ have the same spectrum. As a consequence the thermodynamical properties predicted from the two approaches are identical.

B. Phase spreading of the condensate

The state (Φ_a, Φ_a) introduced in the last subsection is not a regular mode of $\mathcal{L}_{\rm GP}$ and we will see now that it has a contribution to the dynamics of the quantum fluctuations linearly diverging in time.

The physical meaning of Φ_a and α is clarified by the following observation. Taking the derivative with respect to N of the time-independent Gross-Pitaevskii equation (41) for a fixed g ($\partial_N g_N = g$) and for a real Φ we obtain an equation similar to Eq. (74):

$$(\mathcal{H} + 3Ng\Phi^2 - \mu)\partial_N(\sqrt{N}|\Phi\rangle) = \mu'\sqrt{N}|\Phi\rangle \tag{84}$$

from which we conclude

$$\alpha = N\mu' \tag{85}$$

and

$$|\Phi_a\rangle = \sqrt{N}\partial_N(\sqrt{N}|\Phi\rangle), \tag{86}$$

where we use the normalization condition $\langle\Phi|\Phi_a\rangle=1/2$.

A crucial consequence of the fact that $\mathcal{L}_{\rm GP}$ is not diagonalizable is a linear divergence of the time evolution operator $U_{\rm GP}$:

$$U_{\rm GP}(t)\begin{pmatrix}|\Phi_a\rangle\\|\Phi_a\rangle\end{pmatrix}=(1-i\mathcal{L}_{\rm GP}t/\hbar)\begin{pmatrix}|\Phi_a\rangle\\|\Phi_a\rangle\end{pmatrix}$$

$$\underset{t\to\infty}{\sim}-iN\mu' t/\hbar\begin{pmatrix}|\Phi\rangle\\-|\Phi\rangle\end{pmatrix} \tag{87}$$

[since the series expansion of $\exp(-i\mathcal{L}_{\rm GP}t/\hbar)$ in this expression terminates]. As the eigenmodes of $\mathcal{L}_{\rm GP}$ are subject to a mere oscillation in time, according to Eq. (77), we can write more generally:

$$U_{\rm GP}(t)\underset{t\to\infty}{\sim}-iN\mu' t/\hbar\begin{pmatrix}|\Phi\rangle\\-|\Phi\rangle\end{pmatrix}(\langle\Phi|,\langle\Phi|). \tag{88}$$

We examine now the consequence of this divergence in the Bogoliubov approach with symmetry breaking. The quantum fluctuating part $\hat{\tilde{\Psi}}$ of the quantum atomic field evolves as

$$\begin{pmatrix}\hat{\tilde{\Psi}}(t)\\\hat{\tilde{\Psi}}^\dagger(t)\end{pmatrix}=U_{\rm GP}(t)\begin{pmatrix}\hat{\tilde{\Psi}}(0)\\\hat{\tilde{\Psi}}^\dagger(0)\end{pmatrix} \tag{89}$$

so that $(\hat{\tilde{\Psi}},\hat{\tilde{\Psi}}^\dagger)$ will diverge linearly with time:

$$\hat{\tilde{\Psi}}(\vec{r},t)\underset{t\to\infty}{\sim}-\frac{iN\mu' t}{\hbar}\Phi(\vec{r})\hat{P}_{U(1)}, \tag{90}$$

where the ''momentum'' $\hat{P}_{U(1)}$ defined in the previous subsection is a constant of motion. This divergence Eq. (90) renders the Bogoliubov approach with symmetry breaking invalid at times $t>t_c$ where

$$t_c=\frac{\hbar}{\mu'\sqrt{N}}. \tag{91}$$

For those times indeed quantum fluctuations $\hat{\tilde{\Psi}}$ become comparable to the classical field $\sqrt{N}\Phi$. This problem was identified already in [15] and interpreted as a quantum phase spreading of the condensate. In an alternative treatment t_c is identified with the collapse time [16] of the mean value of $\hat{\Psi}$ for an initial coherent state. In the asymptotic limit Eq. (18) we find that μ' scales as $1/N$ so that t_c diverges as $\sqrt{N}$. For typical experimental parameters ($N=10^6$ sodium atoms in a harmonic trap with a frequency 100 Hz) we find $t_c=0.2$ s.

This collapse time t_c can be justified in our $U(1)$ symmetry-preserving approach as follows. Since $\langle\hat{\Psi}\rangle=0$ the appropriate quantity to consider is the correlation function of the field operator $\hat{\Psi}(\vec{r},t)$

$$C(\vec{r},\vec{r}',t)=\langle\hat{\Psi}^\dagger(\vec{r},t)\hat{\Psi}(\vec{r}',0)\rangle. \tag{92}$$

For a fixed number of particles N we calculate $C(\vec{r},\vec{r}',t)$ in the steady state using Eq. (8). The main contribution stems from $\hat{a}_\Phi$; the contribution from $\delta\hat{\Psi}$ is smaller and vanishes in the long time limit. This can be seen from the modal decomposition Eq. (63): the different terms oscillate with different frequencies $E_k-E_{k'}(k\neq k')$ and interfere destructively. Finally we predict

$$C_N(\vec{r},\vec{r}',t)\underset{t\to\infty}{\sim}Ne^{i\mu t/\hbar}\Phi^*(\vec{r})\Phi(\vec{r}')+O(N^0). \tag{93}$$

No damping is observed for the correlation function of the condensed part.

If we allow a Poissonian distribution for the total number of particles the average of $C_N(\vec{r},\vec{r}',t)$ will result in a collapse (and subsequent revival) of the correlation function as μ and Φ depend on N. To get an estimate of the collapse time we neglect the N dependence of Φ and linearize $\mu(N)$ around the mean value $\overline{N}$:

$$\begin{aligned}C(\vec{r},\vec{r}',t)&=\sum_N\frac{\overline{N}^N}{N!}e^{-\overline{N}}C_N(\vec{r},\vec{r}',t)\\&\simeq\overline{N}e^{i\mu t/\hbar}\exp[\overline{N}(e^{i\mu' t/\hbar}-1-i\mu' t/\hbar)]\\&\quad\times\Phi^*(\vec{r})\Phi(\vec{r}')\\&\simeq_{\mu' t\ll 1}\overline{N}e^{i\mu t/\hbar}e^{-1/2\,(t/t_c)^2}\Phi^*(\vec{r})\Phi(\vec{r}')\end{aligned} \tag{94}$$

with t_c given by Eq. (91) with $N=\overline{N}$. This derivation seems more intuitive than the one based on the symmetry breaking approach.

VI. CORRECTIONS TO THE GROSS-PITAEVSKII EQUATION

The discussion presented in Sec. II E has shown that the calculation of the expectation value of atomic observables (such as the spatial density) to order N^0 includes, in addition to the intuitively expected contribution of the noncondensed particles, a term of the same order due to the deviation $\Phi^{(2)}/N$ of the exact condensate wave function from the Gross-Pitaevskii approximation Φ. This complication, absent from the homogeneous case (where the condensate wave function is exactly a plane wave), cannot be avoided in harmonic traps.

In order to get an equation for $\Phi^{(2)}$ we follow the general procedure outlined at the beginning of Sec. III; we calculate the terms of order $1/\sqrt{\hat{N}}$ in the exact Eq. (A3) of the Appendix and we use the requirement Eq. (17) on their mean value to get an equation for $\Phi^{(2)}$. In the term R_2 of Eq. (A3) we keep the lowest-order terms $(\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}\to\hat{N},\Phi_{\rm ex}\to\Phi,\hat{a}^\dagger_{\Phi_{\rm ex}}\delta\hat{\Psi}\to\sqrt{\hat{N}}\hat{\Lambda},\delta\hat{\Psi}^\dagger\delta\hat{\Psi}\to\hat{\Lambda}^\dagger\hat{\Lambda})$. The substitutions $\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}\to\hat{N}$ and $\Phi_{\rm ex}\to\Phi$ can also be effected in the term R_1, as the terms neglected in these substitutions are N times smaller than the leading terms. The mean value of R_1 in this order is therefore zero and does not contribute to Eq. (17). Finally in R_0 we make the substitution $\Phi_{\rm ex}\to\Phi+\Phi^{(2)}/\hat{N}$ and $\hat{a}^\dagger_{\Phi_{\rm ex}}\hat{a}_{\Phi_{\rm ex}}\to\hat{N}-\int d\vec{r}'\hat{\Lambda}^\dagger(\vec{r}')\hat{\Lambda}(\vec{r}')$. We collect all these

terms. With the same argument we used to identify $\mathcal{L}$ in Eq. (56), we get a linear inhomogeneous equation for the component $\Phi_\perp^{(2)}$ orthogonal to Φ:

$$\left(i\hbar\frac{d}{dt}-\mathcal{L}(t)\right)\begin{pmatrix}\Phi_\perp^{(2)}(t)\\ \Phi_\perp^{(2)*}(t)\end{pmatrix}=\begin{pmatrix}Q(t)S(t)\\ -Q^*(t)S^*(t)\end{pmatrix} \quad (95)$$

where $\mathcal{L}$ is given by Eq. (46) and

$$\begin{aligned}S(\vec{r})=&-g_N|\Phi(\vec{r})|^2\Phi(\vec{r})\left\langle 1+\int d\vec{s}\hat{\Lambda}^\dagger(\vec{s})\hat{\Lambda}(\vec{s})\right\rangle\\ &+2g_N\Phi(\vec{r})\langle\hat{\Lambda}^\dagger(\vec{r})\hat{\Lambda}(\vec{r})\rangle+g_N\Phi^*(\vec{r})\langle\hat{\Lambda}(\vec{r})\hat{\Lambda}(\vec{r})\rangle\\ &-g_N\int d\vec{s}|\Phi(\vec{s})|^2\langle[\hat{\Lambda}^\dagger(\vec{s})\Phi(\vec{s})+\hat{\Lambda}(\vec{s})\Phi^*(\vec{s})]\hat{\Lambda}(\vec{r})\rangle.\end{aligned} \quad (96)$$

The first term in Eq. (96) corrects the overestimation of the number of condensed particles in calculating their mutual interaction $(N\to N-[1+\langle\delta\hat{N}\rangle])$ in the Gross-Pitaevskii equation. The terms in the second line describe the interaction of the condensed particles and the noncondensed ones. The fact that the coupling constant is $2g_N$ rather than g_N in the term involving the density of noncondensed particles $\langle\hat{\Lambda}^\dagger\Lambda\rangle$ can be understood in a mean-field picture: for the noncondensed particles one has to apply the Hartree-Fock approximation, whereas for the condensed particles only the Hartree term is kept. For the zero range interaction potential Eq. (1) the Hartree and the Fock terms have identical contributions, hence the factor of two. The term in $\langle\hat{\Lambda}\hat{\Lambda}\rangle$ is obtained also in a Hartree-Fock-Bogoliubov mean-field treatment [27]. The terms in the last two lines of Eq. (96) involve the spatial correlation function of the noncondensed particles.

No explicit equation can be obtained for the component of $\Phi^{(2)}$ along Φ. One can in fact show that, apart from the normalization constraint Eq. (7) imposing that this component is purely imaginary, it can be chosen at will, using the arbitrariness of the global phase of $\Phi_{\rm ex}$. This is why, in particular, the expectation value in Eq. (26) is unaffected by the substitution $\Phi^{(2)}\to\Phi^{(2)}+i\gamma\Phi$, where γ is any real number.

VII. CONCLUSION AND OUTLOOK

We have presented a systematic expansion of the evolution equations of the field operator for a very-low-temperature Bose-Einstein condensed gas with a well-defined number of particles N. The expansion is valid if the fraction of noncondensed particles is small. It gives to lowest order the condensate wave function as a solution of the Gross-Pitaevskii equation and to next order the linear dynamics of the noncondensed particles. We can consistently include higher-order terms in the asymptotic expansion. This allows in particular to include the feedback of noncondensed particles on the condensate wave function resulting in a correction of order $1/N$ to the prediction of the Gross-Pitaevskii equation.

We have numerically shown [22] for an isotropic trap and for systems in a steady state at $T=0$ that the fraction of noncondensed particles is approximately given by $\langle\delta\hat{N}\rangle/N\simeq\sqrt{\rho a_s^3}$ where ρ is the density at the center of the trap. Applying this formula to the anisotropic traps used in recent experiments at MIT [2] we predict a fraction of noncondensed particles of the order 10^{-3}, which demonstrates the validity of the Gross-Pitaevskii equation at $T=0$ for a system in a steady state.

What happens to a condensate that is not in a steady state? This is a situation occurring in recent experiments. In a first type of experiment the trap was abruptly switched off and the expanding cloud monitored. We have analyzed this situation in [11] with the Gross-Pitaevskii equation. With the present theory we are able to show that the number of noncondensed particles is not increased by an abrupt opening of the trap.

In a second type of experiment the condensate is excited by a time modulation of the trap frequency and then oscillates in the unperturbed potential. At very low temperature (T much smaller than the critical temperature T_c) and for a strongly enough driven system we have shown in a recent paper [18] that the solution of the Gross-Pitaevskii equation approximating the condensate wave function is unstable. According to Sec. IV A the density of noncondensed particles will then increase exponentially with time. This exponential increase of course will saturate at some stage, when the interaction between the noncondensed particles has to be taken into account, an effect that would require the calculation of $\hat{\Lambda}^{(1)}$, the first-order correction to $\hat{\Lambda}$ [see Eq. (21)].

Note added in proof. Recently an article appeared that proposed an expansion of the evolution equations that is equivalent to our approach: C. W. Gardiner, Phys. Rev. A **56**, 1414 (1997).

ACKNOWLEDGMENTS

We thank Isabelle Bouchoule, Emmanuel Mandonnet, and Maxim Olshanii for their valuable contributions to this work. We are grateful to Alice Sinatra, Maciej Lewenstein, Franck Laloë, and Werner Krauth for discussions and comments on the manuscript. R.D. thanks the FWF of the Austrian government for financial spport. Laboratoire Kastler Brossel is a unité de recherche de l'Ecole Normale Supérieure et de l'Université Pierre et Marie Curie, associée au CNRS.

APPENDIX A

The equations of motions for $\hat{\Lambda}_{\rm ex}(\vec{r},t)$ follow from

$$\begin{aligned}i\hbar\frac{d}{dt}(\hat{a}^\dagger_{\Phi_{\rm ex}}(t)\,\delta\hat{\Psi}(\vec{r},t))=&\,i\hbar\,\partial_t(\hat{a}^\dagger_{\Phi_{\rm ex}}(t)\,\delta\hat{\Psi}(\vec{r},t))\\ &+[\hat{a}^\dagger_{\Phi_{\rm ex}}(t)\,\delta\hat{\Psi}(\vec{r},t),\hat{H}(t)]\end{aligned} \quad (A1)$$

and include an explicit time dependence due to $\Phi_{\rm ex}(t)$:

$$\begin{aligned}\partial_t\hat{a}^{(t)}_{\Phi_{\rm ex}}&=\int d\vec{s}(\partial_t\Phi^*_{\rm ex}(\vec{s},t))\hat{\Psi}(\vec{s}),\\ \partial_t\delta\hat{\Psi}(\vec{r},t)&=\int d\vec{s}(\partial_t Q_{\rm ex}(\vec{r},\vec{s},t))\hat{\Psi}(\vec{s}).\end{aligned} \quad (A2)$$

From this we get the exact Heisenberg equations

$$\frac{1}{\sqrt{\hat N}} i\hbar \frac{d}{dt}(\hat a^\dagger_{\Phi_{ex}} \delta\hat\Psi(\vec r)) = \frac{1}{\sqrt{\hat N}} \int d\vec s \sum_{k=0}^{4} R_k(\vec r,\vec s), \quad \text{(A3)}$$

where we collected terms in powers of $\delta\hat\Psi$

$$\begin{aligned}
R_0(\vec r,\vec s) &= \hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} Q_{ex}(\vec r,\vec s)[-i\hbar\partial_t + \mathcal{H} \\
&\quad + g(\hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} - 1)|\Phi_{ex}(\vec s)|^2]\Phi_{ex}(\vec s),
\end{aligned}$$

$$\begin{aligned}
R_1(\vec r,\vec s) &= Q_{ex}(\vec r,\vec s)[\mathcal{H} + 2g(\hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} - 1)|\Phi_{ex}(\vec s)|^2] \\
&\quad \times \hat a^\dagger_{\Phi_{ex}} \delta\hat\Psi(\vec s) - \Phi_{ex}(\vec r) \\
&\quad \times [i\hbar\partial_t \Phi^*_{ex}(\vec s)]\hat a^\dagger_{\Phi_{ex}} \delta\hat\Psi(\vec s) \\
&\quad + Q_{ex}(\vec r,\vec s) g \hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} \Phi^2_{ex}(\vec s)\, \delta\hat\Psi^\dagger(\vec s)\hat a_{\Phi_{ex}} \\
&\quad - \hat a^\dagger_{\Phi_{ex}} \delta\hat\Psi(\vec r)\Phi^*_{ex}(\vec s)[-i\hbar\partial_t + \mathcal{H} \\
&\quad + g\hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} |\Phi_{ex}(\vec s)|^2]\Phi_{ex}(\vec s),
\end{aligned}$$

$$\begin{aligned}
R_2(\vec r,\vec s) &= -\delta\hat\Psi(\vec s)^\dagger \delta\hat\Psi(\vec r)[-i\hbar\partial_t + \mathcal{H} \\
&\quad + 2g\hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} |\Phi_{ex}(\vec s)|^2]\Phi_{ex}(\vec s) + g Q_{ex}(\vec r,\vec s) \\
&\quad \times [\hat a^{\dagger 2}_{\Phi_{ex}} \delta\hat\Psi^2(\vec s)\Phi^*_{ex}(\vec s) \\
&\quad + 2g\hat a^\dagger_{\Phi_{ex}} \hat a_{\Phi_{ex}} \delta\hat\Psi^\dagger(\vec s)\,\delta\hat\Psi(\vec s)\Phi_{ex}(\vec s)] \\
&\quad - g\Phi^*_{ex}(\vec s)|\Phi_{ex}(\vec s)|^2 \hat a_{\Phi_{ex}}{}^{+2} \delta\hat\Psi(\vec s)\,\delta\hat\Psi(\vec r),
\end{aligned}$$

$$\begin{aligned}
R_3(\vec r,\vec s) &= g Q_{ex}(\vec r,\vec s)\hat a^\dagger_{\Phi_{ex}} \delta\hat\Psi(\vec s)^\dagger \delta\hat\Psi(\vec s)^2 \\
&\quad - g\,\delta\hat\Psi^\dagger(\vec s)\,\delta\hat\Psi^\dagger(\vec s)\hat a_{\Phi_{ex}} \Phi^2_{ex}(\vec s)\,\delta\hat\Psi(\vec r) \\
&\quad - 2g\,\delta\hat\Psi^\dagger(\vec s)\,\delta\hat\Psi(\vec s)\hat a^\dagger_{\Phi_{ex}} |\Phi_{ex}(\vec s)|^2 \delta\hat\Psi(\vec r),
\end{aligned}$$

$$R_4(\vec r,\vec s) = -g\,\delta\hat\Psi^{\dagger 2}(\vec s)\,\delta\hat\Psi(\vec s)\Phi_{ex}(\vec s)\,\delta\hat\Psi(\vec r). \quad \text{(A4)}$$

APPENDIX B

To prove theorem (57) we define the operator

$$X(t) = \mathcal{Q}(t) U_{GP}(t) \mathcal{Q}(0), \quad \text{(B1)}$$

where $\mathcal{Q}(t)$ is a generalized projector

$$\mathcal{Q}(t) = \begin{pmatrix} Q(t) & 0 \\ 0 & Q^*(t) \end{pmatrix}. \quad \text{(B2)}$$

At $t=0, X(0) = \mathcal{Q}(0) = U(0)$ since U is restricted to the states orthogonal to $[\Phi(0),0]$ and $[0,\Phi^*(0)]$. To determine the evolution of X we take the time derivative of Eq. (B1):

$$i\hbar \frac{d}{dt} X(t) = M_X(t) U_{GP}(t) \mathcal{Q}(0), \quad \text{(B3)}$$

$$\begin{aligned}
M_X(t) &= \mathcal{L}\mathcal{Q}(t) \\
&\quad + g_N \begin{pmatrix} Q|\Phi(\vec r,t)|^2 P & Q\Phi(\vec r,t)^2 P^* \\ -Q^*\Phi(\vec r,t)^{*2} P & -Q^*|\Phi(\vec r,t)|^2 P^* \end{pmatrix}
\end{aligned}$$

($P = |\Phi\rangle\langle\Phi|$). Using $|\Phi|^2 P = \Phi^2 |\Phi^*\rangle\langle\Phi|$ we rewrite $M_X(t)$ as

$$M_X(t) = \mathcal{L}\mathcal{Q}(t) + g_N \begin{pmatrix} Q|\Phi(\vec r,t)|^2|\Phi\rangle \\ -Q^*|\Phi(\vec r,t)|^2|\Phi^*\rangle \end{pmatrix} (\langle\Phi|, \langle\Phi^*|). \quad \text{(B4)}$$

The last step consists in proving that

$$[\langle\Phi(t)|, \langle\Phi^*(t)|]\, U_{GP}(t)\mathcal{Q}(0) \equiv 0. \quad \text{(B5)}$$

This relation holds at $t=0$; it holds at any later time t because its time derivative vanishes. Therefore

$$i\hbar \frac{d}{dt} X(t) = \mathcal{L}(t)\mathcal{Q}(t) U_{GP}(t)\mathcal{Q}(0) = \mathcal{L}(t) X(t) \quad \text{(B6)}$$

and $X(t) = U(t)$ Q.E.D.

[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).

[2] K. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[3] C. C. Bradley, C. A. Sackett, and R. G. Hulet, Phys. Rev. Lett. **78**, 985 (1997).

[4] W. Krauth, Phys. Rev. Lett. **77**, 3695 (1996).

[5] Ph. Nozières and D. Pines, *The Theory of Quantum Liquids* (Addison-Wesley, New York, 1990), Vol. II.

[6] G. Baym and C. Pethick, Phys. Rev. Lett. **76**, 6 (1996).

[7] P. A. Rupprecht, M. J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995); M. Edwards, P. A. Ruprecht, K. Burnett, R. J. Dodd, and C. W. Clark, *ibid.* Phys. Rev. A **53**, R1954 (1996).

[8] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).

[9] Y. Kagan, E. L. Surkov, and G. Shlyapnikov, Phys. Rev. A **54**, R1753 (1996).

[10] A. Garcia-Perez, R. Michinel, I. Cirac, M. Lewenstein, and P. Zoller, Phys. Rev. Lett. **77**, 5320 (1996).

[11] Y. Castin and R. Dum, Phys. Rev. Lett. **77**, 5315 (1996).

[12] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, and W. Ketterle, Phys. Rev. Lett. **77**, 416 (1996).

[13] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **77**, 420 (1996); M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G.

Townsend, and W. Ketterle, *ibid.* **77**, 988 (1996).
[14] P. G. de Gennes, *Superconductivity of Metals and Alloys* (W. A. Benjamin, New York, 1966); A. L. Fetter, Ann. Phys. (N.Y.) **70**, 67 (1972).
[15] M. Lewenstein and Li You, Phys. Rev. Lett. **77**, 3489 (1996).
[16] E. M. Wright, D. F. Walls, and J. C. Garrison, Phys. Rev. Lett. **77**, 2158 (1996).
[17] For a formally correct definition of this expansion see Eq. (20).
[18] Y. Castin and R. Dum, Phys. Rev. Lett. **79**, 3553 (1997).
[19] In fact the δ distribution in the pseudopotential does not lead to a well-defined scattering problem and has to be regularized as discussed in [21], that is, $\delta(\vec{r})\psi(\vec{r})$ has to be replaced by $\delta(\vec{r})\partial_r[r\psi(\vec{r})]$ for a wave function ψ. The corresponding scattering amplitude for a relative momentum $\hbar k$ between the particles is then $-a_s/(1+ika_s)$ for the s wave and vanishes for the other waves. The pseudopotential therefore has the same binary scattering properties as the true interaction potential in the limit $k\to 0$. Note that to the order of the calculations performed in this paper this regularization is not essential. The use of the pseudopotential is correct only in the dilute gas limit, where the three-body interactions are negligible (which imposes $\rho|a_s|^3 \ll 1$ on the spatial density ρ).
[20] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).
[21] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).
[22] Y. Castin and R. Dum (unpublished).
[23] We have to verify that numerically and find indeed for $g>0$ real eigenvalues. Physically this means that the condensate is stable with respect to quantum fluctuations.
[24] For a positive scattering length ($g>0$) one can prove indeed that $\langle u_k|u_k\rangle - \langle v_k|v_k\rangle$ is positive.
[25] As $\hat{H}$ is calculated up to order $\hat{N}^0$ a careful reader may argue that the contribution of $\Phi^{(2)}$ defined in Eq. (21) is relevant. In fact, it vanishes: as Φ solves Eq. (41), the quantity $\langle\Phi|\mathcal{H} + \frac{1}{2}g_N|\Phi(\vec{r})|^2|\Phi\rangle$ does not vary to first order in any norm-preserving change of Φ.
[26] The term with the trace in Eq. (70) and the sum in Eq. (71) are in fact infinite. They can be made finite using the regularization of [19].
[27] A. Griffin, Phys. Rev. B **53**, 9341 (1996).