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Variational Thomas-Fermi theory of a nonuniform Bose condensate at zero temperature

Eddy Timmermans and Paolo Tommasini
Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics,
Cambridge, Massachusetts 02138

Kerson Huang
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology,
Cambridge, Massachuetts 02139

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We derive a description of the spatially inhomogeneous Bose-Einstein condensate, treating the system locally as a homogeneous Bose gas. This approach, similar to the Thomas-Fermi model for the inhomogeneous many-particle fermion system, is well suited to describe the atomic Bose-Einstein condensates that have recently been obtained experimentally through atomic trapping and cooling. In this paper, we confine our attention to the zero-temperature case, although the treatment can be generalized to finite temperatures, as we shall discuss elsewhere. Several features of this approach, which we shall call the Thomas-Fermi-Bogoliubov description, are very attractive. (i) It is simpler than the Hartree-Fock-Bogoliubov technique. We can obtain analytical results in the case of weakly interacting bosons for quantities such as the chemical potential, the local depletion, pairing, pressure, and density of states. (ii) The method provides an estimate for the error due to the inhomogeneity of the Bose-condensed system. This error is a local quantity so that the validity of the description for a given trap and a given number of trapped atoms can be tested as a function of position. We see, for example, that at the edge of the condensate the Thomas-Fermi-Bogoliubov theory always breaks down. (iii) The Thomas-Fermi-Bogoliubov description can be generalized to treat the statistical mechanics of the Bose gas at finite temperatures. [S1050-2947(97)01305-X]

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I. INTRODUCTION

The recently reported Bose-Einstein condensates (BECs) of trapped neutral atoms [1–3] represent unambiguous observations of a weakly interacting Bose-condensed gas. Quantitatively, we can characterize the strength of the interaction by the expansion parameter in the perturbation treatment of the homogeneous Bose gas, $\sqrt{na^3}$, where n is the density and a the scattering length of the interatomic potential. In the atomic-trap experiments, typically n $\sim 10^{12}$–10^{14} cm^{-3} and $a\sim 1$–5 nm, so that $\sqrt{na^3}\sim 10^{-2}$–3×10^{-5}. Thus, in the sense of perturbation theory, the observed condensates are indeed textbook examples of weakly interacting systems. For the uniform Bose gas, perturbation theory leads to simple analytical results. Although the trapped condensates can be described by means of the Hartree-Fock-Bogoliubov equations [4,5], the latter approach does not lend itself to an analytical perturbation treatment.

Intuitively, one expects that a many-body system whose density varies slowly in space can be described locally as a homogeneous system. Based on this picture, the Thomas-Fermi method [6,7] was proposed for the calculation of the electron density in a heavy atom. Lieb and Simon [8] showed that the treatment is exact in the limit when the atomic number goes to infinity. Application to a confined Bose condensate was pioneered by Goldman, Silvera, and Legget [9] and recently reconsidered by Chou, Yang, and Yu [10,11] for a system of noninteracting bosons. Recently, Wu and Griffin [12] applied the Thomas-Fermi approach to a hydrodynamic description of the BEC. As pointed out by Kagan, Shlyapnikov, and Walraven [13], the local-density description is valid when

$$\mu/\hbar\omega \gg 1, \tag{1}$$

where μ is the mean-field energy per particle, or chemical potential, and $\hbar\omega$ is the zero-point energy in the trap. A detailed discussion of where the Thomas-Fermi description for the condensate wave function breaks down was given by Dalfovo, Pitaevskii, and Stringari [15].

In this paper, we derive a Thomas-Fermi description of the condensate *and the fluctuations* from first principles within the framework of the variational technique. We emphasize that, unlike the practice of neglecting the kinetic-energy term in the Gross-Pitaevskii equation, which in the recent literature is sometimes called the Thomas-Fermi approximation, the resulting variational description is not limited to the condensate, but describes the depletion, pressure, and all other thermodynamic quantities. Furthermore, like the uniform gas, the Thomas-Fermi theory leads to a perturbation treatment of the weakly interacting condensates, giving simple analytical expressions for these quantities. Another important advantage of the Thomas-Fermi treatment is that it can be generalized to describe finite-temperature systems, as we plan to discuss in future work. In this paper we focus on the Bose gas at zero temperature.

The paper is organized as follows. In Sec. II, we generalize the usual Bogoliubov transformation to describe spatially inhomogeneous condensates. In Sec. III, we introduce the Wigner representation and gradient expansion, which provide the tools to describe the nearly homogeneous systems and make the Thomas-Fermi approximation. The advantage of this systematic approach to the Thomas-Fermi approximation is that it provides an estimate of the error incurred by the inhomogeneity of the condensate, allowing one to estimate the accuracy of the Thomas-Fermi results. We consider this point to be very important in view of the fact that some traps, depending on the potential and the number of trapped atoms, are too far from homogeneity to be described by a Thomas-Fermi description. In addition, even if the Thomas-Fermi description is valid in the middle of the trap, it breaks down at the edge of the condensate. In Secs. IV and V, we obtain the mean-field description of the Bose system in the Thomas-Fermi approximation. The equations, derived within the framework of the variational principle, provide a fully self-consistent description, indicating that the Thomas-Fermi description is by no means limited to weakly interacting systems. This remark can be expected to be of future importance in the light of recent experimental efforts to obtain condensates of higher density. Nonetheless, because of the special interest in the weakly interacting systems, we proceed in Sec. VI to derive a perturbation treatment and obtain analytical results for quantities such as the chemical potential, the local depletion, pairing, and pressure. With the experimental atomic traps in mind, we apply the results of the general theory to the special case of a trapping potential that is of the type of a simple spherically symmetric harmonic oscillator in Sec. VII. Finally, in Sec. VIII, we derive a density of states of the trapped weakly interacting condensate within the spirit of the Thomas-Fermi approximation.

II. GENERALIZED BOGOLIUBOV TRANSFORMATION

The Bogolubov quasiparticle concept [14] provides a very elegant description of the interacting Bose-Einstein condensate. The quasiparticles are represented by creation ($\eta^\dagger$) and annihilation (η) operators that are linear combinations of regular single-particle creation ($a^\dagger$) and annihilation (a) operators. In treating a homogeneous system, for which we can work in a basis of single-particle plane-wave states of momentum **k**, the Bogoliubov transformation that relates the quasiparticle and regular particle operators takes on a particularly simple form

$$\eta^\dagger_{\mathbf{k}} = x_{\mathbf{k}} a^\dagger_{\mathbf{k}} + y_{\mathbf{k}} a_{-\mathbf{k}}, \quad \eta_{\mathbf{k}} = x_{\mathbf{k}} a_{\mathbf{k}} + y_{\mathbf{k}} a^\dagger_{-\mathbf{k}}, \tag{2}$$

where, for the purpose of describing the static properties of a condensate in equilibrium, we can limit the transformation parameters $x_{\mathbf{k}}, y_{\mathbf{k}}$ to real numbers. Furthermore, the isotropy of the many-body system suggests that the transformation parameters depend only on the magnitude of the momentum $x_{\mathbf{k}} = x_k$ and $y_{\mathbf{k}} = y_k$. Requiring the quasiparticle operators to be canonical, $[\eta_{\mathbf{k}}, \eta^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}, [\eta_{\mathbf{k}}, \eta_{\mathbf{k}'}] = [\eta^\dagger_{\mathbf{k}}, \eta^\dagger_{\mathbf{k}'}] = 0$, gives an additional constraint to $x_{\mathbf{k}}$ and $y_{\mathbf{k}}$,

$$x_k^2 - y_k^2 = 1, \tag{3}$$

from which we can see that a single parameter σ_k, with $x_k = \cosh\sigma_k$ and $y_k = \sinh\sigma_k$, suffices to parametrize the Bogoliubov transformation (2). In addition, with Eq. (3), we can also write the Bogoliubov transformation as

$$a^\dagger_{\mathbf{k}} = x_k \eta^\dagger_{\mathbf{k}} - y_k \eta_{-\mathbf{k}}, \quad a_{\mathbf{k}} = x_k \eta_{\mathbf{k}} - y_k \eta^\dagger_{-\mathbf{k}}, \tag{4}$$

which is the inverse transformation of Eqs. (2).

It is useful to define the following quantities: the ''distribution function'' ρ and the ''pairing function'' Δ,

$$\rho_{\mathbf{k}} = \langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \rangle = \frac{1}{2}[\cosh 2\sigma_{\mathbf{k}} - 1],$$

$$\Delta_{\mathbf{k}} = -\langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle = \frac{1}{2}\sinh 2\sigma_{\mathbf{k}}, \tag{5}$$

where the angular brackets represent the ground-state expectation value. The best values for x_k and y_k are obtained variationally by minimizing the ground-state free energy.

As stated, the above description (1)–(3) applies only to homogeneous systems, whereas the treatment of a general (inhomogeneous) condensate, as we shall show below, involves a Bogoliubov transformation that is quite different in appearance from the homogeneous case. However, we can expect the results of the homogeneous treatment to describe the ''local'' behavior of an inhomogeneous condensate, provided the spatial variations of the condensate are sufficiently slow. In describing many-particle fermion systems, this intuitive picture forms one of the key ingredients of the well-known Thomas-Fermi description of slowly varying many-particle systems.

To arrive at a general treatment, we choose to work with boson-field operators $\hat{\Psi}(\mathbf{x})$ and $\hat{\Psi}^\dagger(\mathbf{x})$, an approach that offers the advantage of not having to specify a basis *a priori*. Furthermore, in the presence of a condensate, it is convenient to work with the fields $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}^\dagger(\mathbf{x})$, which are displaced from the original fields $\hat{\Psi}(\mathbf{x})$ and $\hat{\Psi}^\dagger(\mathbf{x})$ by the expectation value $\phi(\mathbf{x})$ of $\hat{\Psi}(\mathbf{x})$,

$$\hat{\Psi}(\mathbf{x}) = \hat{\psi}(\mathbf{x}) + \phi(\mathbf{x}), \quad \hat{\Psi}^\dagger(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x}) + \phi^*(\mathbf{x}), \tag{6}$$

where, for the purpose of describing the static properties of a condensate in equilibrium, ϕ can be taken to be real and $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}^\dagger(\mathbf{x})$ are the displaced field operators that satisfy the canonical commutation relation $[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}')$ and, furthermore,

$$\langle \hat{\psi}(\mathbf{x}) \rangle = \langle \hat{\psi}^\dagger(\mathbf{x}) \rangle = 0. \tag{7}$$

We introduce the Bogoliubov transformation as a general linear transformation relating the displaced fields to the quasiparticle fields $\hat{\xi}(\mathbf{x})$ and $\hat{\xi}^\dagger(\mathbf{x})$,

$$\hat{\psi}(\mathbf{x}) = \int d^3z [X(\mathbf{x},\mathbf{z}) \hat{\xi}(\mathbf{z}) - Y(\mathbf{x},\mathbf{z}) \hat{\xi}^\dagger(\mathbf{z})],$$

$$\hat{\psi}^\dagger(\mathbf{x}) = \int d^3z [X^*(\mathbf{x},\mathbf{z}) \hat{\xi}^\dagger(\mathbf{z}) - Y^*(\mathbf{x},\mathbf{z}) \hat{\xi}(\mathbf{z})], \tag{8}$$

which is the generalization of Eq. (3). The nonlocal nature of the generalized Bogoliubov transformation (8) should not be surprising: the ''homogeneous'' Bogoliubov transformation (2) can be written in the same form with the special feature, due to the homogeneity of the system, that $X(\mathbf{x},\mathbf{y})$ and $Y(\mathbf{x},\mathbf{y})$ depend only on $\mathbf{x}-\mathbf{y}$. Requiring the quasiparticle fields to be canonical leads to

$$\int d^3z[X(\mathbf{x},\mathbf{z})X(\mathbf{z},\mathbf{y})-Y(\mathbf{x},\mathbf{z})Y(\mathbf{z},\mathbf{y})]=\delta(\mathbf{x}-\mathbf{y}), \quad (9)$$

which is the generalization of Eq. (3).

It is possible to derive equations for the inhomogeneous Bose systems by variationally determining the best transformations X and Y, minimizing the free energy. This, however, is not the path we choose to follow here. Instead, we manipulate the generalized Bogoliubov transformations in a manner similar to the procedure to obtain the Wigner distribution from the off-diagonal single-particle density function. Once this is achieved, the steps that lead to a Thomas-Fermi description are known from quantum transport theory. One interesting aspect of this treatment is that the central object of the theory is not a distribution function, which in some sense can still be regarded as an observable, but a transformation. Although this transformation determines the value of all observables, it is clearly not an observable quantity by itself.

III. WIGNER REPRESENTATION AND GRADIENT EXPANSION

Wigner showed that a quantum-mechanical single-particle system, customarily characterized by its wave function $\Psi(\mathbf{x})$, can alternatively be fully characterized by a different function

$$\rho_W(\mathbf{R},\mathbf{p})=\int d^3r\ \Psi^*(\mathbf{R}+\mathbf{r}/2)\Psi(\mathbf{R}-\mathbf{r}/2)\exp(i\mathbf{p}\cdot\mathbf{r}), \quad (10)$$

where here, as in the rest of the paper, we work in units in which $\hbar=1$. This function (10), known as the Wigner distribution function, can be interpreted as a phase-space distribution function [16] and leads to a description that is remarkably close to classical mechanics. The analogy with a classical phase-space distribution function is not complete (for example, ρ_W can take on negative values), but can be justified by the fact that the quantum-mechanical expectation value of observables are equal to the "phase-space integrals" of the corresponding classical quantities, weighted by $(2\pi)^{-3}\rho_W$,

$$\langle\Psi|f|\Psi\rangle=\int d^3x\ \Psi^*(\mathbf{x})f(\mathbf{x})\Psi(\mathbf{x})$$
$$=(2\pi)^{-3}\int d^3p\int d^3R\ f(\mathbf{R})\rho_W(\mathbf{R},\mathbf{p}),$$

$$\langle\Psi|\hat{\mathbf{p}}|\Psi\rangle=\int d^3x\ \Psi^*(\mathbf{x})\hat{\mathbf{p}}\Psi(\mathbf{x})$$
$$=(2\pi)^{-3}\int d^3p\int d^3R\ \ \mathbf{p}\ \rho_W(\mathbf{R},\mathbf{p}), \quad (11)$$

etc. More recently, the many-particle generalization of the Wigner distribution has found many important applications in diverse areas such as nuclear [17] and solid-state physics [18].

An important motivation to work in the transformed representation of Eq. (10), $(\mathbf{x},\mathbf{x}')\to(\mathbf{R},\mathbf{p})$,

$$A_W(\mathbf{R},\mathbf{p})=\int d^3r\ A(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)\exp(i\mathbf{p}\cdot\mathbf{r}), \quad (12)$$

and its inverse

$$A(\mathbf{x},\mathbf{x}')=(2\pi)^{-3}\int d^3p\ A_W([\mathbf{x}+\mathbf{x}']/2,\mathbf{p})$$
$$\times\exp(-i\mathbf{p}\cdot[\mathbf{x}-\mathbf{x}']), \quad (13)$$

which shall henceforth be referred to as the Wigner representation, is that it is extraordinarily well suited to describe nearly homogeneous systems. This convenient feature follows from the gradient expansion [17,18]. The gradient expansion shows that, to first order, a "product" operator $C(\mathbf{x},\mathbf{x}')=\int d^3z\ A(\mathbf{x},\mathbf{z})B(\mathbf{z},\mathbf{x}')$ in the Wigner representation simply gives the algebraic product of A and B, $C_W(\mathbf{R},\mathbf{p})\approx A_W(\mathbf{R},\mathbf{p})B_W(\mathbf{R},\mathbf{p})$. The higher-order corrections to this approximation can be written as a series of terms containing successively higher-order derivatives in the $(\mathbf{R},\mathbf{p})$ coordinates,

$$C_W(\mathbf{R},\mathbf{p})\approx A_W(\mathbf{R},\mathbf{p})B_W(\mathbf{R},\mathbf{p})+\frac{1}{2\mathrm{i}}\sum_{j=1}^{3}\left[\frac{\partial A_W}{\partial R_j}\frac{\partial B_W}{\partial p_j}-\frac{\partial A_W}{\partial p_j}\frac{\partial B_W}{\partial R_j}\right]-\frac{1}{8}\sum_{j=1}^{3}\left[\frac{\partial^2 A_W}{\partial R_j^2}\frac{\partial^2 B_W}{\partial p_j^2}+\frac{\partial^2 A_W}{\partial p_j^2}\frac{\partial^2 B_W}{\partial R_j^2}-2\frac{\partial^2 A_W}{\partial R_j\partial p_j}\frac{\partial^2 B_W}{\partial R_j\partial p_j}\right]+\cdots. \quad (14)$$

The first-order correction in the gradient expansion (14) is $\{A_W,B_W\}_{\mathrm{PB}}$, the Poisson bracket of A_W and B_W. If we know that the range of A_W and B_W in $\mathbf{p}$ space is of the order of p_c, then the magnitude of the derivatives $\partial B_W/\partial p$ and $\partial^2 B_W/\partial p^2$ in (14) can be estimated to be of the order of B_W/p_c and B_W/p_c^2, respectively. This approximation will allow us to obtain a very simple estimate of the "inhomogeneity" error.

At this point, we return to the generalized Bogoliubov transformation, $X(\mathbf{x},\mathbf{y}),Y(\mathbf{x},\mathbf{y})$ of Sec. II. Working in the Wigner representation and expanding the "canonicity" relation (9) between X and Y in the manner of the gradient expansion, we find up to first order in the spatial derivatives a relation that is similar to the constraint equation (3) of the homogeneous Bogoliubov transformation,

$$X_W^2(\mathbf{R},\mathbf{p})-Y_W^2(\mathbf{R},\mathbf{p})\approx 1. \quad (15)$$

Consequently, the general Bogoliubov transform can be parametrized in the same way as the Bogoliubov transform for the homogeneous Bose gas, $X_W(\mathbf{R},\mathbf{p})=\cosh[\sigma(\mathbf{R},\mathbf{p})]$, $Y_W(\mathbf{R},\mathbf{p})=\sinh[\sigma(\mathbf{R},\mathbf{p})]$, where for the slowly varying condensate, the σ parameters depend on the momentum *and* position: $\sigma(\mathbf{R},\mathbf{p})$. The distribution and pairing functions $\rho(\mathbf{x},\mathbf{x}')=\langle\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x}')\rangle$ and $\Delta(\mathbf{x},\mathbf{x}')=-\langle\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}')\rangle$ take on the following form in the Wigner representation:

$$\rho_W(\mathbf{R},\mathbf{p})=\frac{1}{2}\{\cosh[2\sigma(\mathbf{R},\mathbf{p})]-1\},$$

$$\Delta_W(\mathbf{R},\mathbf{p})=\frac{1}{2}\sinh[2\sigma(\mathbf{R},\mathbf{p})]. \tag{16}$$

The local σ parametrization of the Bogoliubov transformation is crucial to the Thomas-Fermi description and it is upon the validity of Eq. (15) that the Thomas-Fermi theory rests. The error introduced to Eq. (15) due to the inhomogeneity of the system can be estimated by the lowest-order nonvanishing term in the gradient expansion (14). Notice that the first-order term in the gradient expansion of Eq. (15) vanishes since it is the sum of Poisson brackets of quantities with themselves. Consequently, the error has to be estimated from the second-order term.

IV. ENERGY DENSITY

In the variational method, the quantity to minimize is F, the ground-state free energy, which we can put in a local form $F=\int d^3R\, f(\mathbf{R})$, where $f(\mathbf{R})$ is the energy density. We achieve this result in two steps. In the first step, we shift to the Wigner representation in the integrand for the mean-field expression for the ground-state energy. In the second step, we notice that the short-range nature of the interatomic interaction renders the resulting integrand essentially local i.e., the integrand contains only *single* (not double) integrals over the position variables.

The ground-state free energy is the expectation value of $\hat{H}-\mu\hat{N}$, where $\hat{H}$ is the many-body Hamiltonian of the boson system, $\hat{N}$ the number operator, and μ the chemical potential:

$$\begin{aligned}\hat{H}-\mu\hat{N}=&\int d^3x\;\hat{\Psi}(\mathbf{x})^{\dagger}\hat{h}(\mathbf{x})\hat{\Psi}(\mathbf{x})\\&+\frac{1}{2}\int d^3x\; d^3y\;\hat{\Psi}(\mathbf{y})^{\dagger}\hat{\Psi}(\mathbf{x})^{\dagger}\\&\times V(|\mathbf{x}-\mathbf{y}|)\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{y}),\end{aligned} \tag{17}$$

where $V(|\mathbf{x}-\mathbf{y}|)$ represents the interatomic potential and $\hat{h}(\mathbf{x})$ is the one-body part of the free energy,

$$\hat{h}(\mathbf{x})=-\frac{\nabla^2}{2m}+V_{\text{ext}}(\mathbf{x})-\mu, \tag{18}$$

where $V_{\text{ext}}(\mathbf{x})$ is the external potential.

The presence of a condensate displaces the field operators $\hat{\Psi}(\mathbf{x})$ by their expectation value $\phi(\mathbf{x})$. To generate the variational free energy, we shall use the mean-field approximation, in which terms of first and third order in $\hat{\psi}$ and $\hat{\psi}^{\dagger}$ vanish [Eq. (7)] and the fourth-order term factorizes as

$$\begin{aligned}\langle\hat{\psi}(\mathbf{y})^{\dagger}\hat{\psi}(\mathbf{x})^{\dagger}\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{y})\rangle\approx&\,\Delta^*(\mathbf{x},\mathbf{y})\Delta(\mathbf{x},\mathbf{y})+\rho(\mathbf{y},\mathbf{x})\rho(\mathbf{x},\mathbf{y})\\&+\rho(\mathbf{x},\mathbf{x})\rho(\mathbf{y},\mathbf{y}).\end{aligned} \tag{19}$$

The variational nature of this procedure is ensured by the existence of a variational ground state that gives this type of factorization. In fact, the variational ground state corresponds to the choice of the Gaussian wave functional [5].

The displacement of the fields and the factorization of the expectation values, although straightforward, gives rise to a somewhat lengthy expression for the free energy. It is then convenient to classify the different contributions by their order in ϕ and their functional dependence on ρ and Δ. (i) h_1 is the one-body contribution of zeroth order in ϕ to the ground-state energy,

$$h_1=\int d^3x\; d^3y\;\hat{h}(\mathbf{x})\rho(\mathbf{y},\mathbf{x})\delta(\mathbf{x}-\mathbf{y}). \tag{20}$$

(ii) In analogy with the Hartree-Fock theory, we call V_{dir}, given below, the direct energy contribution to the energy,

$$V_{\text{dir}}=\frac{1}{2}\int d^3x\; d^3y\;\rho(\mathbf{y},\mathbf{y})\rho(\mathbf{x},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{21}$$

(iii) Using the same analogy to the Hartree-Fock treatment, the exchange energy V_{exch} is equal to

$$V_{\text{exch}}=\frac{1}{2}\int d^3x\; d^3y\;\rho(\mathbf{x},\mathbf{y})\rho(\mathbf{y},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{22}$$

(iv) Standard Hartree-Fock theory does not describe pairing and the pairing energy V_{pair},

$$V_{\text{pair}}=\frac{1}{2}\int d^3x\; d^3y\;\Delta^*(\mathbf{y},\mathbf{x})\Delta(\mathbf{y},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|), \tag{23}$$

is consequently absent from the Hartree-Fock expressions. In second order in ϕ, we find contributions that can be obtained from the above terms by replacing either $\Delta(\mathbf{x},\mathbf{y})$ or $\rho(\mathbf{x},\mathbf{y})$ by $\phi(\mathbf{x})\phi(\mathbf{y})$. (v) For example, the one-body contribution due to the kinetic and potential energy of the condensate is h_1^{ϕ}, where

$$h_1^{\phi}=\int d^3x\;\phi(\mathbf{x})\hat{h}(\mathbf{x})\phi(\mathbf{x}). \tag{24}$$

(vi) V_{dir}^{ϕ} is the direct contribution to the interaction energy, stemming from the interaction of the condensate with the particles that have been ‘‘forced’’ out of the condensate (depletion),

$$V_{\text{dir}}^{\phi}=\frac{1}{2}\int d^3x\; d^3y\;\phi(\mathbf{y})\phi(\mathbf{y})\rho(\mathbf{x},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{25}$$

(vii) Similarly, V_{exch}^{ϕ} is the exchange contribution of second order in ϕ,

$$V_{\text{exch}}^{\phi}=\frac{1}{2}\int d^3x\; d^3y\;\phi(\mathbf{y})\phi(\mathbf{x})\rho(\mathbf{y},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{26}$$

(viii) We represent the pairing energy of the condensate with the particles out of the condensate by $V^{\phi}_{\rm pair}$,

$$V^{\phi}_{\rm pair}=\frac{1}{2}\int d^3x\ d^3y\ \phi(\mathbf{y})\phi(\mathbf{x})\Delta(\mathbf{y},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{27}$$

(ix) Finally, we denote the contribution of fourth order in ϕ, representing the interaction energy of the condensate with itself by $V^{\phi\phi}$,

$$V^{\phi\phi}=\frac{1}{2}\int d^3x\ d^3y\ \phi^2(\mathbf{y})\phi^2(\mathbf{x})V(|\mathbf{x}-\mathbf{y}|). \tag{28}$$

With this notation, the mean-field expression for the ground-state energy reads

$$\begin{aligned}F=\langle\hat{H}-\mu\hat{N}\rangle={}&h_1+V_{\rm dir}+V_{\rm exch}+V_{\rm pair}+h_1^{\phi}+2V^{\phi}_{\rm dir}+2V^{\phi}_{\rm exch}\\&-2V^{\phi}_{\rm pair}+V^{\phi\phi},\end{aligned} \tag{29}$$

where the minus sign of the $V^{\phi}_{\rm pair}$ term stems from the definition of $\Delta=-\langle\hat{\psi}\hat{\psi}\rangle$.

At this point, we introduce the Wigner representation into the integrands of the above contributions to the mean-field expressions for the ground-state free energy. The resulting expressions resemble the corresponding terms for the homogeneous gas, with an additional label $\mathbf{R}$ over which is integrated. For the sake of notational convenience we introduce the following integration symbol $\int_{\mathbf{R}}$ or $\int_{\mathbf{p}}$, which represents the usual integral over all of space $\int d^3\mathbf{R}$ if $\mathbf{R}$ is a position variable or $(2\pi)^{-3}\int d^3p$ if $\mathbf{p}$ is a momentum variable:

$$\int_{\mathbf{p}}\equiv(2\pi)^{-3}\int d^3p, \qquad \int_{\mathbf{R}}\equiv\int d^3R. \tag{30}$$

The terms of zeroth order in ϕ then give

$$h_1=\int_{\mathbf{R}}\int_{\mathbf{p}}\left[\frac{p^2}{2m}+V(\mathbf{R})-\mu\right]\rho_W(\mathbf{R},\mathbf{p}),$$

$$V_{\rm exch}=\frac{1}{2}\int_{\mathbf{R}}\int_{\mathbf{p}}\int_{\mathbf{p}'}\rho_W(\mathbf{R},\mathbf{p})v(\mathbf{p}-\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}'),$$

$$V_{\rm pair}=\frac{1}{2}\int_{\mathbf{R}}\int_{\mathbf{p}}\int_{\mathbf{p}'}\Delta_W(\mathbf{R},\mathbf{p})v(\mathbf{p}-\mathbf{p}')\Delta_W(\mathbf{R},\mathbf{p}'),$$

$$\begin{aligned}V_{\rm dir}=\frac{1}{2}\int_{\mathbf{R}}\int_{\mathbf{r}}\int_{\mathbf{p}}\int_{\mathbf{p}'}\int_{\mathbf{q}}&\rho_W(\mathbf{R}-\mathbf{r}/2,\mathbf{p})\rho_W\\&\times(\mathbf{R}+\mathbf{r}/2,\mathbf{p}')\exp(i\mathbf{q}\cdot\mathbf{r})v(\mathbf{q}),\end{aligned} \tag{31}$$

where v is the Fourier transform of the interaction potential $v(\mathbf{q})=\int d^3r\ V(\mathbf{r})\exp(-i\mathbf{q}\cdot\mathbf{r})$.

The terms that are of second order in ϕ can be obtained by replacing one ρ or Δ by $\phi\phi$. In the Wigner representation, this procedure yields expressions that are similar to the corresponding terms of zeroth order in ϕ with $\rho_W(\mathbf{R},\mathbf{p})$ or $\Delta_W(\mathbf{R},\mathbf{p})$ replaced by a function $Q_W(\mathbf{R},\mathbf{p})$, where

$$Q_W(\mathbf{R},\mathbf{p})=\int_{\mathbf{r}}\phi(\mathbf{R}+\mathbf{r}/2)\phi(\mathbf{R}-\mathbf{r}/2)\exp(i\mathbf{p}\cdot\mathbf{r}). \tag{32}$$

Notice that the contributions of second order in ϕ are nonlocal in the sense that their expressions contain integrals over more than one position variable. Nevertheless, if we consider the scale on which the physical quantities vary in space, or in momentum space, it becomes apparent that the nonlocal integrals can be approximated by local expressions. We illustrate this point by considering the exchange ($V^{\phi}_{\rm exch}$) and pairing ($V^{\phi}_{\rm pair}$) energies. The key to obtain local expressions is to notice that $Q_W(\mathbf{R},\mathbf{p})$ varies with respect to $\mathbf{p}$ on the scale of $\mathbf{R}_0^{-1}$, where $\mathbf{R}_0$ is the size of the condensate. On the other hand, $v(\mathbf{p}-\mathbf{p}')$ varies on the scale of l_r^{-1}, where l_r is the range of the atom-atom interaction. Typically $\mathbf{R}_0\gg l_r$ so that $Q_W(\mathbf{R},\mathbf{p})$ varies much more rapidly with respect to $\mathbf{p}$ than $v(\mathbf{p}-\mathbf{p}')$. In fact, when $\mathbf{p}$ is large enough to make $v(\mathbf{p}-\mathbf{p}')$ significantly different from $v(\mathbf{p}')$, $Q_W(\mathbf{R},\mathbf{p})\approx 0$. Thus we can replace $v(\mathbf{p}-\mathbf{p}')$ by $v(\mathbf{p}')$ in the integrands

$$\begin{aligned}V^{\phi}_{\rm exch}\approx{}&\frac{1}{2}\int_{\mathbf{R}}\int_{\mathbf{r}}\int_{\mathbf{p}}\int_{\mathbf{p}'}\phi(\mathbf{R}+\mathbf{r}/2)\phi(\mathbf{R}-\mathbf{r}/2)\\&\times\exp(i\mathbf{p}\cdot\mathbf{r})v(\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}')\\={}&\frac{1}{2}\phi^2(\mathbf{R})\int_{\mathbf{R}}\int_{\mathbf{p}'}v(\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}'),\end{aligned}$$

$$V^{\phi}_{\rm pair}\approx\frac{1}{2}\phi^2(\mathbf{R})\int_{\mathbf{R}}\int_{\mathbf{p}'}v(\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}'). \tag{33}$$

The same considerations regarding the relative magnitude of the relevant length scales show that we can similarly simplify the expression of the ϕ^4 interaction energy $V^{\phi\phi}$ and the direct interaction energies $V_{\rm dir}$ and $V^{\phi}_{\rm dir}$. The local expressions are most easily obtained by considering the difference in length scales before introducing the Wigner representation. In coordinate space, we notice that $\rho(\mathbf{x},\mathbf{x})\approx\rho(\mathbf{y},\mathbf{y})$ if $|\mathbf{x}-\mathbf{y}|\leqslant l_r$. Thus we can replace $\rho(\mathbf{x},\mathbf{x})$ by $\rho(\mathbf{y},\mathbf{y})$ in an integrand if it is accompanied by $V(|\mathbf{x}-\mathbf{y}|)$:

$$\begin{aligned}V_{\rm dir}\approx{}&\frac{1}{2}\int d^3x\ d^3y\ \rho^2(\mathbf{x},\mathbf{x})V(|\mathbf{x}-\mathbf{y}|)\\={}&\frac{1}{2}v(0)\int_{\mathbf{R}}\int_{\mathbf{p}}\int_{\mathbf{p}'}\rho_W(\mathbf{R},\mathbf{p})\rho_W(\mathbf{R},\mathbf{p}'),\end{aligned}$$

$$V^{\phi}_{\rm dir}\approx\frac{1}{2}v(0)\int_{\mathbf{R}}\int_{\mathbf{p}}\phi^2(\mathbf{R})\rho_W(\mathbf{R},\mathbf{p}),$$

$$V^{\phi\phi}\approx\frac{1}{2}v(0)\int_{\mathbf{R}}\phi^4(\mathbf{R}). \tag{34}$$

To conclude this section, we summarize the results by remarking that the Wigner representation and the length scale considerations bring the free energy in an almost-local form. We need to qualify that statement because of the appearance of the Laplacian, a nonlocal operator, in the h^{ϕ} contribution to the energy. In fact, it is the nonlocality of this term that gives rise to a generalized Gross-Pitaevskii or nonlinear Schrödinger equation (NLSE). The resulting (almost-local) ground-state free energy is $F=\int d^3Rf(\mathbf{R})$, where

$$
\begin{aligned}
f(\mathbf{R}) = {} & \int_{\mathbf{p}} \left[\frac{p^2}{2m} + V_{\text{ext}}(\mathbf{R}) - \mu\right]\rho(\mathbf{R},\mathbf{p}) + v_{\text{exch}}(\mathbf{R}) + v_{\text{dir}}(\mathbf{R}) \\
& + v_{\text{pair}}(\mathbf{R}) + \phi(\mathbf{R})\left[\frac{-\nabla^2}{2m} + V_{\text{ext}}(\mathbf{R}) - \mu\right]\phi(\mathbf{R}) \\
& + 2v^{\phi}_{\text{exch}}(\mathbf{R}) + 2v^{\phi}_{\text{dir}}(\mathbf{R}) - 2v^{\phi}_{\text{pair}}(\mathbf{R}) + \frac{1}{2}v(0)\phi^4(\mathbf{R}),
\end{aligned}
\tag{35}
$$

where the exchange, direct, and pairing energy densities are the integrands of the corresponding interaction energy contributions to the free energy:

$$
\begin{aligned}
v_{\text{exch}}(\mathbf{R}) &= \frac{1}{2}\int_{\mathbf{p}}\int_{\mathbf{p}'} \rho(\mathbf{R},\mathbf{p})v(\mathbf{p}-\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}'), \\
v_{\text{pair}}(\mathbf{R}) &= \frac{1}{2}\int_{\mathbf{p}}\int_{\mathbf{p}'} \Delta_W(\mathbf{R},\mathbf{p})v(\mathbf{p}-\mathbf{p}')\Delta_W(\mathbf{R},\mathbf{p}'), \\
v_{\text{dir}}(\mathbf{R}) &= \frac{1}{2}v(0)\int_{\mathbf{p}}\int_{\mathbf{p}'} \rho_W(\mathbf{R},\mathbf{p})\rho_W(\mathbf{R},\mathbf{p}'), \\
v^{\phi}_{\text{exch}}(\mathbf{R}) &= \frac{1}{2}\phi^2(\mathbf{R})\int_{\mathbf{p}} \rho_W(\mathbf{R},\mathbf{p})v(\mathbf{p}), \\
v^{\phi}_{\text{pair}}(\mathbf{R}) &= \frac{1}{2}\phi^2(\mathbf{R})\int_{\mathbf{p}} \Delta_W(\mathbf{R},\mathbf{p})v(\mathbf{p}), \\
v^{\phi}_{\text{dir}}(\mathbf{R}) &= \frac{1}{2}\phi^2(\mathbf{R})v(0)\int_{\mathbf{p}} \rho_W(\mathbf{R},\mathbf{p}).
\end{aligned}
\tag{36}
$$

Notice that the free energy and free-energy density are functionals of $\Delta(\mathbf{R},\mathbf{p})$, $\rho(\mathbf{R},\mathbf{p})$, and $\phi(\mathbf{R})$. In the next section we determine the equilibrium values of $\Delta(\mathbf{R},\mathbf{p})$, $\rho(\mathbf{R},\mathbf{p})$ and $\phi(\mathbf{R})$ by minimizing $F[\rho,\Delta,\phi;\mu]$.

V. SELF-CONSISTENT MEAN-FIELD THEORY

In this section we derive the self-consistent mean-field equations that describe the nearly uniform Bose condensate at zero temperature. In the variational method, one minimizes the mean-field ground-state free energy $F[\rho,\Delta,\phi;\mu]$. Writing the integrands of the different contributions to the mean-field free energy in the Wigner representation, followed by the length scale arguments of the preceding section, showed that $F[\rho_W,\Delta_W,\phi;\mu]$ is essentially a local quantity. Finally, in the Thomas-Fermi limit of a nearly homogeneous system, $\rho_W(\mathbf{R},\mathbf{p})$ and $\Delta_W(\mathbf{R},\mathbf{p})$ are parametrized by a single Bogoliubov transformation parameter $\sigma(\mathbf{R},\mathbf{p})$ in the manner of Eq. (16). Thus, to describe a nearly homogeneous system, we minimize the Thomas-Fermi ground-state free energy, which is obtained from the mean-field free energy, assuming that ρ_W and Δ_W are parametrized by σ [Eq. (16)], $F[\sigma,\phi;\mu] = F[\rho_W(\sigma),\Delta_W(\sigma),\phi;\mu]$. We obtain the condensate wave function $\phi_0(\mathbf{R})$ and Bogoliubov parameter $\sigma_0(\mathbf{R},\mathbf{p})$ that describe the condensate by varying σ and ϕ independently to get a minimum in F:

$$
\left.\frac{\delta F}{\delta\phi(\mathbf{R})}\right|_{\sigma=\sigma_0,\phi=\phi_0} = 0 \quad (\text{NLSE}),
$$

$$
\left.\frac{\delta F}{\delta\sigma(\mathbf{R},\mathbf{p})}\right|_{\sigma=\sigma_0,\phi=\phi_0} = 0. \tag{37}
$$

The ϕ variation $\delta F/\delta\phi = 0$ gives the NLSE. The σ variation $\delta F/\delta\sigma = 0$ gives an equation for $\sigma_0(\mathbf{R},\mathbf{p})$. From $\rho = \frac{1}{2}[\cosh(2\sigma) - 1]$ and $\Delta = \frac{1}{2}\sinh(2\sigma)$ [Eq. (16)], we find that $\partial\rho/\partial\sigma = \sinh(2\sigma)$ and $\partial\Delta/\partial\sigma = \cosh(2\sigma)$, so that $\delta F/\delta\sigma = 0$ is equivalent to

$$
\tanh(2\sigma_0) = \frac{-\delta F/\delta\Delta_W}{\delta F/\delta\rho_W}. \tag{38}
$$

Now, several terms of the NLSE, as well as the functional derivatives $\delta F/\delta\Delta$, and $\delta F/\delta\rho$ in Eq. (38), depend on σ_0 and ϕ_0 so that the resulting equations have to be solved self-consistently. To make the self-consistent nature of the equations more explicit, we consider the σ-dependent contributions to the functional derivatives $\delta V_{\text{exch}}/\delta\rho$, $\delta V_{\text{dir}}/\delta\rho$, and $\delta V_{\text{pair}}/\delta\Delta$, which we shall call the generalized potentials

$$
\begin{aligned}
U_{\text{exch}}(\mathbf{R},\mathbf{p}) &= \delta V_{\text{exch}}/\delta\rho_W(\mathbf{R},\mathbf{p}) = \int_{\mathbf{p}'} v(\mathbf{p}-\mathbf{p}')\rho_W(\mathbf{R},\mathbf{p}'), \\
U_{\text{dir}}(\mathbf{R}) &= \delta V_{\text{dir}}/\delta\rho_W(\mathbf{R},\mathbf{p}) = v(0)\int_{\mathbf{p}'} \rho_W(\mathbf{R},\mathbf{p}'), \\
U_{\text{pair}}(\mathbf{R},\mathbf{p}) &= \delta V_{\text{pair}}/\delta\Delta_W(\mathbf{R},\mathbf{p}) = \int_{\mathbf{p}'} v(\mathbf{p}-\mathbf{p}')\Delta_W(\mathbf{R},\mathbf{p}'),
\end{aligned}
\tag{39}
$$

where we name the generalized potentials after the respective interaction energies of which they are the functional derivatives: U_{exch} is the exchange potential, U_{dir} the direct potential, and U_{pair} the pairing potential. Writing the distribution and pairing function in the integrands of the generalized potentials in terms of 2σ, we find with Eq. (38) that the generalized potentials implicitly depend on the functional derivatives of F:

$$
\begin{aligned}
U_{\text{exch}}(\mathbf{R},\mathbf{p}) = {} & \int_{\mathbf{p}'} v(\mathbf{p}-\mathbf{p}') \\
& \times \frac{1}{2}\left[\frac{\delta F/\delta\rho}{\sqrt{(\delta F/\delta\rho)^2 - (\delta F/\delta\Delta)^2}} - 1\right],
\end{aligned}
$$

$$U_{\mathrm{dir}}(\mathbf{R})=v(0)\int_{\mathbf{p}'}\frac{1}{2}\left[\frac{\delta F/\delta\rho}{\sqrt{(\delta F/\delta\rho)^2-(\delta F/\delta\Delta)^2}}-1\right],$$

$$U_{\mathrm{pair}}(\mathbf{R},\mathbf{p})=\int_{\mathbf{p}'}v(\mathbf{p}-\mathbf{p}')\times\frac{1}{2}\left[\frac{-\delta F/\delta\Delta}{\sqrt{(\delta F/\delta\rho)^2-(\delta F/\delta\Delta)^2}}\right], \tag{40}$$

where it is understood that the functional derivatives in the integrands are evaluated at $\mathbf{R}$ and $\mathbf{p}'$. Functional differentiation shows that the functional derivatives of F in turn depend on the generalized potentials

$$\frac{\delta F}{\delta\Delta_W(\mathbf{R},\mathbf{p})}=U_{\mathrm{pair}}(\mathbf{R},\mathbf{p})-\phi^2(\mathbf{R})v(\mathbf{p}),$$

$$\frac{\delta F}{\delta\rho_W(\mathbf{R},\mathbf{p})}=\frac{p^2}{2m}+V_{\mathrm{ext}}(\mathbf{R})-\mu+U_{\mathrm{exch}}(\mathbf{R},\mathbf{p})+U_{\mathrm{dir}}(\mathbf{R},\mathbf{p})+\phi^2(\mathbf{R})[v(\mathbf{p})+v(0)]. \tag{41}$$

Thus Eqs. (40) and (41) self-consistently determine the generalized potentials. Furthermore, there is a dependence on the condensate wave function ϕ. The latter has to be obtained from the NLSE:

$$\left[-\frac{\nabla^2}{2m}+V_{\mathrm{ext}}(\mathbf{R})-\mu+U(\mathbf{R})+v(0)\phi^2(\mathbf{R})\right]\phi(\mathbf{R})=0, \tag{42}$$

where the potential $U(\mathbf{R})$ is equal to

$$U(\mathbf{R})=U_{\mathrm{dir}}(\mathbf{R})+U_{\mathrm{exch}}(\mathbf{R},0)-U_{\mathrm{pair}}(\mathbf{R},0). \tag{43}$$

This potential term stems from the interaction of the condensate with the particles out of the condensate.

Equations (40)–(42) and (43) are the full set of self-consistent mean-field equations that describe the condensate in the Thomas-Fermi approximation. The self-consistent equations for the homogeneous gas [19] are recovered by setting $V_{\mathrm{ext}}=0$ and by assuming that ϕ is independent of position so that the kinetic-energy contribution to the NLSE vanishes. Regarding the connection with the intuitive Thomas-Fermi model, we note that μ and V_{ext} in the self-consistent mean-field equations always appear as $\mu-V_{\mathrm{ext}}(\mathbf{R})$, so that it is natural to define a local effective chemical potential

$$\mu_{\mathrm{eff}}(\mathbf{R})=\mu-V_{\mathrm{ext}}(\mathbf{R}). \tag{44}$$

In fact, this is the essence of the Thomas-Fermi description: the system is described locally as a homogeneous system with a position-dependent effective chemical potential (44).

The solutions to the fully self-consistent equations determine the expectation value of all (static) physical observables as a function of the chemical potential μ. One observable we can obtain in this manner is N, the number of trapped particles,

$$N(\mu)=\frac{\partial F}{\partial\mu}=\int_{\mathbf{R}}\int_{\mathbf{p}}\rho(\mathbf{R},\mathbf{p})+\int_{\mathbf{R}}\phi^2(\mathbf{R}), \tag{45}$$

the inversion of which yields $\mu(N)$, from which we can cast the results for the thermodynamic quantities in terms of the parameter that is controlled or measured in the experiment: the number of atoms N.

VI. LOW-DENSITY LIMIT

The self-consistent equations (40)–(42) and (43) can be solved iteratively. In the low-density regime, where $\sqrt{na^3}\ll 1$, we approximate the result by the expressions obtained after a single iteration, starting from $\sigma_0^{(0)}=0$ ($U_{\mathrm{exch}}^{(0)}=U_{\mathrm{dir}}^{(0)}=U_{\mathrm{pair}}^{(0)}=0$, where the superscript indicates the order of the iteration). With this first guess we solve the NLSE and obtain the functional derivatives [Eq. (40)] $\delta F/\delta\rho$ and $\delta F/\delta\Delta$, yielding the first-order σ parameter [Eq. (38)] $\sigma^{(1)}$ and the generalized potentials [Eqs. (39)] $U_{\mathrm{dir}}^{(1)}$, $U_{\mathrm{exch}}^{(1)}$, and $U_{\mathrm{pair}}^{(1)}$. With $\sigma^{(1)}$ we compute the expectation values of the observables. In solving the NLSE, we shall assume that $\phi(\mathbf{R})$ varies slowly enough that we can also neglect the kinetic-energy operator. The expressions for the local quantities obtained in this manner are identical to the perturbation results for the dilute homogeneous Bose gas with the (zeroth-order) chemical potential equal to $\mu_{\mathrm{eff}}(\mathbf{R})$.

To make the dependence on the scattering length explicit, we replace the potential by a pseudopotential

$$V_{\mathrm{pseudo}}(\mathbf{r})=\lambda\,\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{46}$$

where $\lambda=4\pi\hbar^2a/m$ and the derivative operator is necessary to remove the divergency in the ground-state free energy [21]. Furthermore, we shall assume that $\phi(\mathbf{R})$ varies slowly enough that we can also neglect the kinetic-energy operator in solving the NLSE (42):

$$\lambda[\phi^{(1)}(\mathbf{R})]^2=\mu_{\mathrm{eff}}(\mathbf{R}), \tag{47}$$

where μ_{eff} is the effective chemical potential (44). The functional derivatives (41) are

$$\frac{\delta F^{(1)}}{\delta\Delta}=-\lambda[\phi^{(1)}(\mathbf{R})]^2,$$

$$\frac{\delta F^{(1)}}{\delta\rho}=\frac{p^2}{2m}-\mu_{\mathrm{eff}}(\mathbf{R})+2\lambda[\phi^{(1)}(\mathbf{R})]^2. \tag{48}$$

Consequently, the single iteration value for the Bogoliubov transformation parameter σ is equal to

$$\tanh[2\sigma_0^{(1)}(\mathbf{R},\mathbf{p})]=\frac{\lambda\phi^2(\mathbf{R})}{(p^2/2m)-\mu_{\mathrm{eff}}(\mathbf{R})+2\lambda\phi^2(\mathbf{R})}=\frac{\mu_{\mathrm{eff}}(\mathbf{R})}{(p^2/2m)+\mu_{\mathrm{eff}}(\mathbf{R})}, \tag{49}$$

which can be recognized as the dilute uniform gas result if we set $\mu_{\rm eff}=\mu$.

The expression for the Bogoliubov parameter $\sigma_0^{(1)}$ from Eq. (49) is what we would have obtained with an effective energy density neglecting the interaction energies of the particles out of the condensate, $V_{\rm dir}$, $V_{\rm exch}$, and $V_{\rm pair}$. In other words, the effective ground-state energy is $F_{\rm eff}=\int d^3R\ \ f_{\rm eff}(\mathbf{R})$, where

$$f_{\rm eff}(\mathbf{R})=-\mu_{\rm eff}(\mathbf{R})\phi^2(\mathbf{R})+\frac{\lambda}{2}\phi^4(\mathbf{R})+\int_{\mathbf{p}}\left[\left(\frac{p^2}{2m}-\mu_{\rm eff}(\mathbf{R})\right.\right.$$
$$\left.\left.+2\lambda\phi^2(\mathbf{R})\right)\rho_W(\mathbf{R},\mathbf{p})-\lambda\phi^2(\mathbf{R})\Delta_W(\mathbf{R},\mathbf{p})\right]. \quad (50)$$

We obtain the results for the observable quantities by calculating their expectation values from the single iteration $\sigma_0^{(1)}$ of Eq. (49). For example, the condensate wave function is determined from the NLSE

$$\lambda\phi^2(\mathbf{R})\approx\mu_{\rm eff}(\mathbf{R})-U^{(1)}(\mathbf{R}), \quad (51)$$

where the potential $U(\mathbf{R})$ is the sum of the generalized potentials at zero momentum (43),

$$U^{(1)}(\mathbf{R})=U^{(1)}_{\rm exch}(\mathbf{R},0)+U^{(1)}_{\rm dir}(\mathbf{R})-U^{(1)}_{\rm pair}(\mathbf{R},0), \quad (52)$$

evaluated with the single-iteration value for σ. The single-iteration values for the generalized potentials are computed to be

$$U^{(1)}_{\rm exch}(\mathbf{R},0)=U^{(1)}_{\rm dir}(\mathbf{R})=\frac{\lambda}{3\pi^2}[\mu_{\rm eff}(\mathbf{R})]^{3/2}m^{3/2},$$

$$U^{(1)}_{\rm pair}(\mathbf{R},0)=-\frac{\lambda}{\pi^2}\ [\mu_{\rm eff}(\mathbf{R})]^{3/2}m^{3/2}. \quad (53)$$

Thus the condensate density is [Eq. (51)]

$$\phi^2(\mathbf{R})\approx\frac{1}{\lambda}\mu_{\rm eff}(\mathbf{R})-\frac{5}{3\pi^2}[\mu_{\rm eff}(\mathbf{R})]^{3/2}m^{3/2}. \quad (54)$$

The total density n$(\mathbf{R})$, including the correction to $\phi^2(\mathbf{R})$ [Eq. (54)] and the local depletion, is equal to

$$\begin{aligned}n(\mathbf{R})&=\phi^2(\mathbf{R})+\int_{\mathbf{p}}\rho(\mathbf{R},\mathbf{p})\\&\approx\phi^2(\mathbf{R})+\frac{1}{3\pi^2}[\mu_{\rm eff}(\mathbf{R})]^{3/2}m^{3/2}\\&\approx\frac{1}{\lambda}\mu_{\rm eff}(\mathbf{R})-\frac{4}{3\pi^2}[\mu_{\rm eff}(\mathbf{R})]^{3/2}m^{3/2},\end{aligned} \quad (55)$$

resulting in an expression for the density $n(\mathbf{R})$ in terms of the effective chemical potential $\mu_{\rm eff}(\mathbf{R})$. Inverting this relation up to first order in $\sqrt{na^3}$, we obtain

$$\mu_{\rm eff}(\mathbf{R})\approx\lambda n(\mathbf{R})\left[1+\frac{32}{3}\sqrt{\frac{n(\mathbf{R})a^3}{\pi}}\right], \quad (56)$$

which, for the homogeneous case, reduces to the well-known perturbation result.

Finally, in a similar manner, we obtain the local pressure $P(\mathbf{R})$ from the expression for the effective free-energy density [Eq. (50)] $P(\mathbf{R})=-f^{(1)}_{\rm eff}(\mathbf{R})$,

$$P(\mathbf{R})=\frac{\lambda\phi^4(\mathbf{R})}{2}\left[1-\frac{128}{15\pi^2}\sqrt{n(\mathbf{R})a^3}\right]. \quad (57)$$

We can then replace ϕ^2 in Eq. (57) by its single-iteration value [Eq. (54)]. Furthermore, replacing $\mu_{\rm eff}(\mathbf{R})$ in the resulting expression by Eq. (56) results in a local equation of state.

The above results illustrate an important advantage of the Thomas-Fermi description: by neglecting the kinetic-energy operator in the NLSE we recover simple analytical expressions for most quantities. These expressions are the analogs of the perturbation results for the dilute homogeneous Bose gas. It is then of course very important to determine the regime and the conditions under which these results can be trusted.

One source of error in the theory stems from neglecting the Laplacian operator in the NLSE. We can estimate the error by calculating e_L, the ratio of the kinetic energy term $-\nabla^2\phi/2m$, and the nonlinear potential energy in the NLSE $\lambda\phi^3$,

$$e_L(\mathbf{R})=|-\nabla^2\phi/2m\lambda\phi^3|=\left|\frac{-\nabla^2\phi(\mathbf{R})/\phi(\mathbf{R})}{k_c^2(\mathbf{R})}\right|, \quad (58)$$

where $k_c(\mathbf{R})=[8\pi a n(\mathbf{R})]^{1/2}$ is the inverse of the local coherence length $k_c=\lambda_c^{-1}(\mathbf{R})$.

Another source of error, which cannot be remedied but is truly inherent to the Thomas-Fermi approximation, stems from the inhomogeneity of the system. This error is also more difficult to estimate, and one benefit of our approach is that the lowest-order nonvanishing term in the gradient expansion can be used to estimate the magnitude of the error. This term is of second order because the first-order term vanishes. We estimate its magnitude (14) by replacing the partial derivatives with respect to the momentum variables by k_c^{-1}, since k_c is a measure of the range in $\mathbf{p}$ of the observable at zero temperature. The relative error for the general product of two arbitrary operators A and B, $e_{\rm i}[AB]$, is then given by

$$e_{\rm i}[AB]\approx\frac{1}{8k_c^2(\mathbf{R})}\left[\frac{\nabla^2A_W}{A_W}+\frac{\nabla^2B_W}{B_W}-2\frac{\boldsymbol{\nabla}A_W\cdot\boldsymbol{\nabla}B_W}{A_WB_W}\right], \quad (59)$$

The validity of the Thomas-Fermi description depends on $X_W^2-Y_W^2=1$ [Eq. (15)], so that we use the accuracy of this equality to test the validity of the local homogeneity description. The expression (15) can also be written as $\exp[\sigma(\mathbf{R},\mathbf{p})]\exp[-\sigma(\mathbf{R},\mathbf{p})]=1$, so that we choose A_W as $\exp[\sigma(\mathbf{R},\mathbf{p})]$ and B_W as $\exp[-\sigma(\mathbf{R},\mathbf{p})]$ to estimate the relative error e_i. In fact, it is more convenient to work with $\exp(4\sigma)$ than $\exp(\sigma)$, so we compute the inhomogeneity error $e_i[\exp(4\sigma)\exp(-4\sigma)]$ of $\exp(4\sigma)$ and divide by 4 [since the relative error of f^n is simply $n\times$ (the relative error of f)]. In this manner, we find that

$$e_i[\exp(\sigma)\exp(-\sigma)]=\frac{1}{4}e_i[\exp(4\sigma)\exp(-4\sigma)] \approx \frac{1}{8k_c^2(\mathbf{R})}\left|\frac{\boldsymbol{\nabla}\exp(4\sigma)}{\exp(4\sigma)}\right|^2. \quad (60)$$

With the single-iteration value for the low-density condensate

$$\exp[4\sigma(\mathbf{R},\mathbf{p})]=1+\frac{2\mu_{\text{eff}}(\mathbf{R})}{p^2/2m}, \quad (61)$$

we find that the inhomogeneity error $e_i(\mathbf{R})$ [Eq. (60)] is equal to

$$e_i(\mathbf{R})=\frac{1}{2}\left|\frac{\mathbf{F}_{\text{ext}}(\mathbf{R})\lambda_c(\mathbf{R})}{(p^2/2m)+2\mu_{\text{eff}}(\mathbf{R})}\right|^2, \quad (62)$$

where $\mathbf{F}_{\text{ext}}$ is the force of the external potential $\mathbf{F}_{\text{ext}}=-\boldsymbol{\nabla}V_{\text{ext}}$. As expected, the error is largest for $\mathbf{p}=\mathbf{0}$, and using the $\mathbf{p}=\mathbf{0}$ value, we obtain a simple position-dependent estimate for the inhomogeneity error $e_i(\mathbf{R})$,

$$e_i(\mathbf{R})=\frac{1}{8}|\mathbf{F}_{\text{ext}}(\mathbf{R})\lambda_c(\mathbf{R})/\lambda\phi^2(\mathbf{R})|^2, \quad (63)$$

where we replaced μ_{eff} by $\lambda\phi^2$. By equating this error (63) to a chosen value $e_{\text{cut}}\ll 1$, reflecting the accuracy we demand from the theory, we can determine the spatial boundary beyond which the Thomas-Fermi theory is less accurate than e_{cut}.

VII. SPHERICALLY SYMMETRIC HARMONIC-OSCILLATOR TRAP

We now specialize $V_{\text{ext}}(\mathbf{R})$ to a harmonic-oscillator potential

$$V_{\text{ext}}(\mathbf{R})=\frac{1}{2}\hbar\omega(R/L)^2, \quad (64)$$

where L is the size of the harmonic-oscillator ground state

$$L=\sqrt{\frac{\hbar}{m\omega}}, \quad (65)$$

and compute the expectation value of important quantities in the low-density limit of the preceding section. In zeroth order in the iteration, we recover the results of Baym and Pethick [20]. From Eq. (47) we see that

$$[\phi^{(0)}(\mathbf{R})]^2=[\mu-V_{\text{ext}}(\mathbf{R})]/\lambda=\frac{R_0^2}{8\pi aL^4}[1-(R/R_0)^2], \quad (66)$$

where R_0 is the size of the condensate $R_0=\sqrt{2\mu/\hbar\omega}L$. In zeroth order, all particles are in the condensate, so that $N=\int_{\mathbf{R}}\phi^2(\mathbf{R})$,

$$\mu^{(0)}=\frac{\hbar\omega}{2}\left(\frac{15aN}{L}\right)^{2/5}, \quad (67)$$

and, consequently,

$$R_0=L\left(\frac{15aN}{L}\right)^{1/5}. \quad (68)$$

The local coherence length $\lambda_c(\mathbf{R})$ is given by

$$\lambda_c(\mathbf{R})=\frac{L^2}{\sqrt{R_0^2-R^2}}. \quad (69)$$

Before we proceed to calculate the perturbation corrections to the observables, we test the validity of the low-density Thomas-Fermi formalism by calculating the errors. The error due to neglecting the Laplacian in the NLSE, $e_L(\mathbf{R})$ [Eq. (58)], is easily computed with Eq. (69):

$$e_L(\mathbf{R})=\left(\frac{L}{R_0}\right)^4\frac{[3-2(R/R_0)^2]}{(1-(R/R_0)^2)^3}, \quad (70)$$

from which we see that the Laplacian can be omitted in the NLSE on condition that the size of the condensate is much larger than the size of the ground state $R_0\gg L$ or $(15aN/L)^{1/5}\gg 1$. The error due to the departure of the BEC from homogeneity, $e_i(\mathbf{R})$ [Eq. (60)], is

$$e_i(\mathbf{R})=\frac{1}{2}\left(\frac{L}{R_0}\right)^4\frac{(R/R_0)^2}{[1-(R/R_0)^2]^3}. \quad (71)$$

Again, notice that e_i is small over most of the condensate region ($R<R_0$) if $R_0\gg L$.

In Fig. 1 we show the density $[\phi^{(0)}(R)]^2/[\phi^{(0)}(R=0)]^2$ [Eq. (66)] and both errors e_L and e_i as a function of the distance to the middle of the trap. The curves are calculated for a harmonic-oscillator trap of $L=1$ μm and an interatomic interaction with scattering length $a=5$ nm. The dotted lines correspond to $N=10^3$ atoms in the trap and the full line gives the results for $N=10^6$ atoms. Notice that for 10^3 particles, the Laplacian error is already substantial ($\sim 10\%$) in the middle of the trap. Consequently, in this example of 1000 atoms, neglecting the Laplacian operator in the NLSE is not a valid approximation. The Thomas-Fermi-Bogoliubov approximation is of the local-density type and cannot account for finite-size effects. If the e_L or e_i errors are too large, the effect of finite-size features, such as the curvature of the condensate wave function, is expected to be larger than the effects of the fluctuations calculated in the Thomas-Fermi approximation.

On the other hand, for 10^6 atoms, e_i and e_L become only of the order of 10% at $R=9.0L$, whereas $R_0=9.4L$, which shows that the Thomas-Fermi description and neglecting the Laplacian operator are valid approximations in almost all of the condensate region. Under this condition, it is meaningful to calculate the perturbation corrections to the expectation

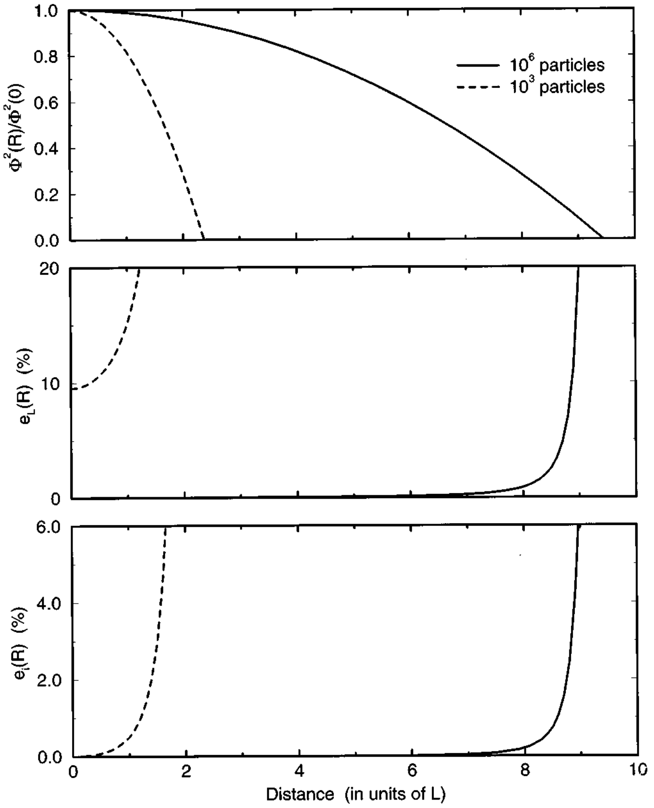

FIG. 1. (a) Condensate density for $N = 10^3$ and 10^6. (b) Error incurred in neglecting the kinetic term in the NLSE. (c) Error incurred in the Thomas-Fermi approximation. The length scale on the horizontal axis is in units of L, the extent of the ground-state wave function. Calculations are done for $L = 10^{-4}$ cm and scattering length $a = 5 \times 10^{-7}$ cm.

values of the observable quantities. Including the perturbation correction, the local density (55) is equal to

$$n(R) = \frac{R_0^2}{8\pi a L^4}[1-(R/R_0)^2]\left[1 - \frac{2\sqrt{2}}{3\pi}\frac{aR_0}{L^2}\sqrt{1-(R/R_0)^2}\right]. \tag{72}$$

The number of trapped particles N is obtained by integrating over the density $n(\mathbf{R})$,

$$N = \int_{\mathbf{R}} n(R) = 4\pi \int_0^{R_0} dR\, R^2 n(R), \tag{73}$$

which leads to

$$N = \frac{1}{15}\frac{L}{a}\left(\frac{2\mu}{\hbar\omega}\right)^{5/2} - \frac{\sqrt{2}}{24}\left(\frac{2\mu}{\hbar\omega}\right)^{3}. \tag{74}$$

The inverse relation μ as a function of N can be obtained by solving for μ iteratively in Eq. (74), which gives, up to second iteration, the result

$$\mu = \frac{\hbar\omega}{2}\left(\frac{15a}{L}\right)^{2/5} N^{2/5}\left[1 + \frac{\sqrt{2}}{60}\left(\frac{15a}{L}\right)^{6/5} N^{1/5}\right]. \tag{75}$$

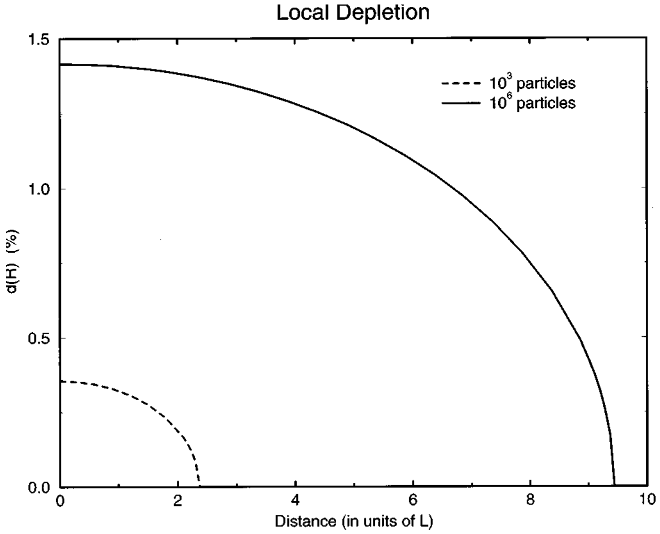

FIG. 2. Depletion, defined as $d(R) = [n(\mathbf{R}) - \phi^2(\mathbf{R})]/\phi^2(\mathbf{R})$, for the same systems as Fig. 1.

Similarly, we obtain the condensate density from Eq. (54) or the local depletion $d(\mathbf{R}) = \{n^{(1)}(\mathbf{R}) - [\phi^{(1)}(\mathbf{R})]^2\}/[\phi^{(1)}(\mathbf{R})]^2$:

$$d(R) = \frac{2\sqrt{2}}{3\pi}\frac{aR_0}{L^2}\sqrt{1-(R/R_0)^2}. \tag{76}$$

In Fig. 2, we show the local depletion as a function of position for the same parameters as those of Fig. 1. The local pressure is shown in Fig. 3.

Notice that the depletion (76) vanishes at the edge of the condensate. This behavior is different from the result of the hydrodynamic Thomas-Fermi description [12], which yields a depletion that diverges at the edge of the condensate. This divergence can be related to the surface modes [22], which cannot be described by a local-density approximation such as the Thomas-Fermi-Bogoliubov technique. Regarding the difference between the hydrodynamic and Thomas-Fermi-Bogoliubov results, we remind the reader that both approximations break down before the edge is reached, and the significance of the behavior of any quantity in this region is questionable.

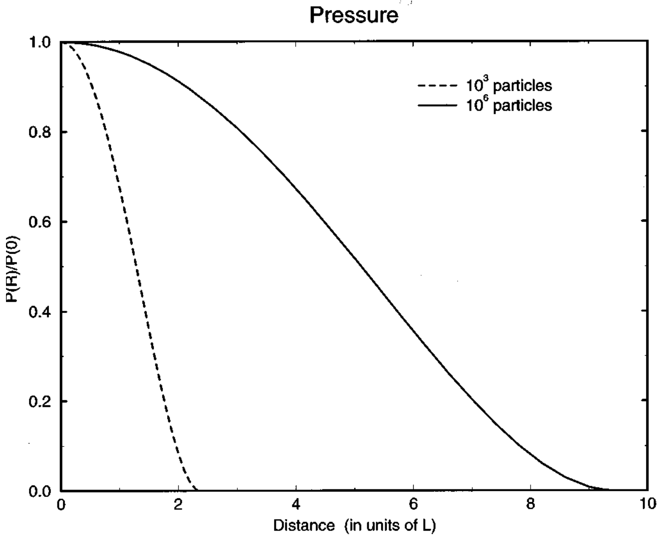

FIG. 3. Pressure for the same systems as in Fig. 1.

TABLE I. Results for the spherically symmetric harmonic-oscillator trap.

Size of the condensate	$R_0 = L\left(\frac{15aN}{L}\right)^{1/5}$
Chemical potential	$\mu = \frac{\hbar\omega}{2}\left(\frac{15aN}{L}\right)^{2/5}$
Condensate density	$\phi^2(R) = \frac{R_0^2}{8\pi a L^4}[1-(R/R_0)^2]$
Local coherence length	$\lambda_c(R) = \frac{L^2}{\sqrt{R_0^2 - R^2}}$
Local depletion	$d(R) = \frac{2\sqrt{2}}{3\pi}\frac{aR_0}{L^2}\sqrt{1-(R/R_0)^2}$
Error due to neglecting the Laplacian	$e_L(R) = \left(\frac{L}{R_0}\right)^4 \frac{[3-2(R/R_0)^2]}{[1-(R/R_0)^2]^3}$
Error due to the inhomogeneity	$e_i(R) = \frac{1}{2}\left(\frac{L}{R_0}\right)^4 \frac{(R/R_0)^2}{[1-(R/R_0)^2]^3}$

To conclude this section, we repeat that the condition for the validity of the Thomas-Fermi description is that the size of the condensate exceeds the size of the ground state of the trap $R_0 \gg L$. An equivalent condition is that the coherence length in the middle of the condensate is smaller than the size of the ground state $\lambda_c(R=0) \ll L$ or that the chemical potential exceeds the ground-state energy $\mu \gg \hbar\omega/2$. These statements do not depend on the details of the trapping potential. Of course, the shape of the condensate, the boundary where the Thomas-Fermi description breaks down, and the expectation values of the local observables do depend on the shape of the potential. In this section we gave the results for a spherically symmetric harmonic-oscillator potential. For the convenience of the reader we tabulate several of the results up to first nonvanishing order in Table I.

VIII. DENSITY OF STATES

In the Thomas-Fermi picture, the system is locally equivalent to a uniform system. Therefore, there are local excitations, which in the low-density regime are described by the energy spectrum

$$\epsilon_p(\mathbf{R}) = \sqrt{[p^2/2m + \mu_{\text{eff}}(\mathbf{R})]^2 - \mu_{\text{eff}}^2(\mathbf{R})} + \mu, \tag{77}$$

which is well known from the Bogoliubov treatment of the uniform case. The local dispersion relation (77) describes a phonon with position-dependent sound velocity.

To obtain the excitation of the whole system we compute the density of states using the formula

$$g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i), \tag{78}$$

where Σ_i represents the sum over all excited states. In the spirit of the Thomas-Fermi approximation we take

$$g(\epsilon) = \int_{\mathbf{R}} \int_{\mathbf{p}} \delta(\epsilon - \epsilon_{\mathbf{p}}(\mathbf{R})). \tag{79}$$

After integration over the momentum variable, we obtain

$$g(\epsilon) = \frac{1}{2\pi^2} \int_{\mathbf{R}} p_\epsilon^2(\mathbf{R}) \left| \frac{\partial \epsilon}{\partial p} \right|^{-1}, \tag{80}$$

where $p_\epsilon(\mathbf{R})$ is the momentum of a particle at position $\mathbf{R}$ with energy ϵ. When calculating the remaining integral over space, we need to distinguish between spatial region I with condensate and a second region II without condensate, shown schematically in Fig. 4. It is necessary to break up the integral (80) over the different integration regions, because the dispersion relations for the excitations are different. In region I we use the Bogoliubov spectrum (77), whereas in region II the atoms are essentially free particles moving in the trap:

$$\epsilon_p(\mathbf{R}) = \frac{p^2}{2m} + V_{\text{ext}}(\mathbf{R}). \tag{81}$$

The density of states is then the sum of the integrals over regions I and II:

$$\begin{aligned} g(\epsilon) = \frac{\sqrt{2}}{2} \frac{m^{3/2}}{\pi^2} \Bigg[& (\epsilon - \mu) \int_{\text{I}} d^3R \\ & \times \frac{\sqrt{\sqrt{[\epsilon-\mu]^2 + \mu_{\text{eff}}^2(\mathbf{R})} - \mu_{\text{eff}}(\mathbf{R})}}{\sqrt{[\epsilon-\mu]^2 + \mu_{\text{eff}}^2(\mathbf{R})}} \\ & + \int_{\text{II}} d^3R \sqrt{\epsilon - V_{\text{ext}}(\mathbf{R})} \Bigg]. \end{aligned} \tag{82}$$

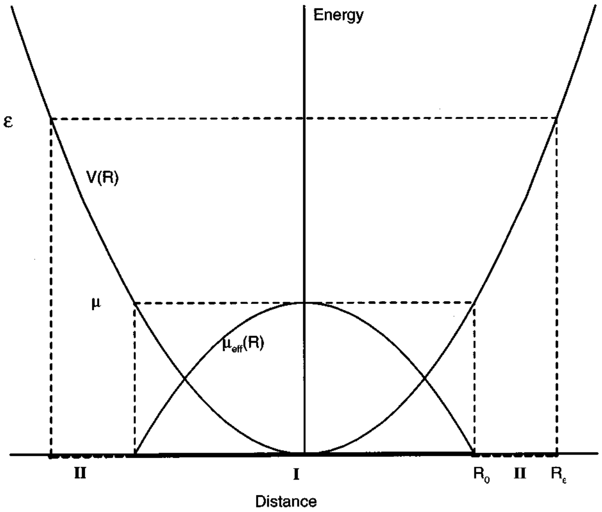

FIG. 4. Schematic representation of the region with (region I) and without condensate (region II) for a BEC in a harmonic trap. The condensate density is proportional to $\mu_{\text{eff}}(\mathbf{R})$, which is a "mirror image" of the trapping potential. Particles in the condensate have energy μ and a particle excited up to energy ϵ can move into region II as far as the classical turning point R_ϵ.

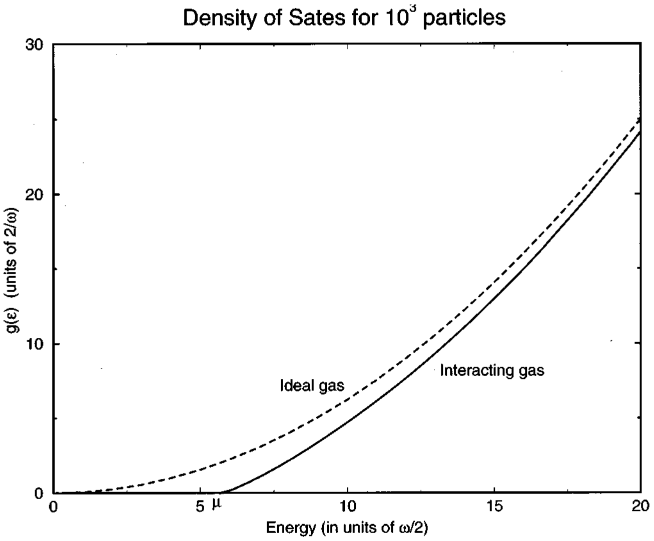

FIG. 5. Density of states calculated in the Thomas-Fermi approach described in the paper. The system is a BEC of $N=10^3$ particles interacting with a scattering length $a=5\times10^{-7}$ cm in a harmonic trap with ground state of extent $L=10^{-4}$ cm.

For the special case of a spherically symmetric harmonic oscillator trap, we find the expression for the density of states

$$g(\epsilon)=\frac{4}{\pi}\,\frac{\mu^2}{(\hbar\omega)^3}\Bigg[(\epsilon/\mu-1)\int_0^1 dr\sqrt{1-r}\times\frac{\sqrt{\sqrt{(\epsilon/\mu-1)^2+r^2}-r}}{\sqrt{(\epsilon/\mu-1)^2+r^2}}+2\int_1^{\epsilon/\mu} dr\; r^2\sqrt{\epsilon/\mu-r^2}\Bigg]. \tag{83}$$

In Figs. 5 and 6 we show the density of states for the system discussed in Sec. VII, $L=1$ μm, $a=5$ nm, $N=10^3$ (Fig. 5), and $N=10^6$ (Fig. 6). The dotted lines show the result for the interacting Bose gas and the full line shows the density of states of the ideal gas in the same trap. The density of states starts from the chemical potential μ, consistent with Eq. (77), which implies that the energies are measured from the bottom of the potential well so that a particle of zero momentum in the condensate has energy μ. If we were to set out the density of states as a function of excitation energy $\epsilon-\mu$, the density of states curves for the interacting BEC systems would be shifted to the left by an amount μ. In contrast to the homogeneous BEC, the density of states for the interacting case, as a function of the excitation energy, grows faster than the density of states of the ideal gas. The reason is purely geometrical: the phonon has a much larger volume in coordinate space available (at least the volume of the condensate) than the noninteracting boson that received the same amount of energy and can only move near the bottom of the potential well. This effect outweighs the fact that the momentum space volume available to the phonon is less than the momentum space volume available to the noninteracting particle with the same energy. Of course, as mentioned previously, the Thomas-Fermi model does not describe finite-size effects such as surface modes. These could alter the density of states somewhat. In analogy with an incompressible spherical fluid, surface modes might be expected to appear in the low-energy region [23]. Related to surface effects, we remark that the sharpness of the boundary between regions I and II is an artifact of neglecting the Laplacian operator in the NLSE. Nevertheless, except for a region near the boundary, we argue that the rest of the space is well described and that the contribution of the near-boundary region is comparatively small so that the error that is introduced in the integral (80) is small provided the Thomas-Fermi description is valid in most of the condensate region.

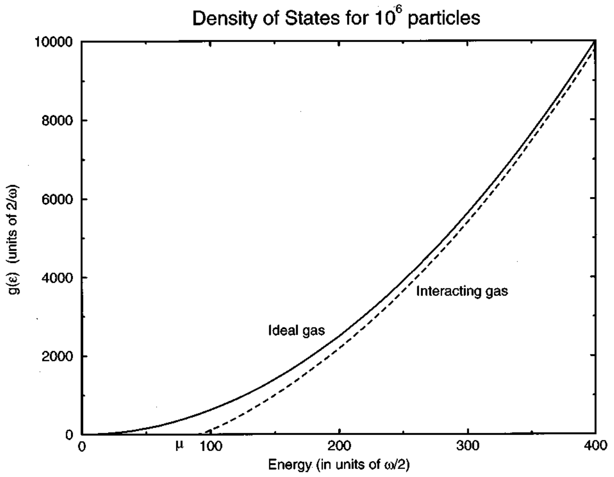

FIG. 6. Density of states for the same system as in Fig. 5, but with $N=10^6$ particles.

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