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, MA 02138

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

ABSTRACT

We derive a description of the spatially inhomogeneous Bose-Einstein condensate which treats the system locally as a homogeneous system. 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-Bogolubov description, are very attractive: 1. It is simpler than the Hartree-Fock-Bogolubov 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. 2. 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-Bogolubov theory always breaks down. 3. The Thomas-Fermi-Bogolubov description can be generalized to treat the statistical mechanics of the bose gas at finite temperatures.
1 Introduction

The recently reported Bose-Einstein condensates of trapped neutral atoms [1]–[3] represent the first 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 inter-atomic potential. In the atomic-trap experiments, typically $n \sim 10^{12} - 10^{14} \text{cm}^{-3}$, and $a \sim 1 - 5 \text{ nm}$, so that $\sqrt{na^3} \sim 10^{-2} - 3 \times 10^{-5}$. 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 Bogolubov 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]. As pointed out by Kagan, Shlyapnikov, and Walraven [12], the local-density description is valid when

$$\frac{\mu}{\hbar \omega} \gg 1,$$

where $\mu$ is the mean-field energy per particle, or chemical potential, and $\hbar \omega$ is the zero-point energy in the trap.

In this paper, we derive such a description 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-Pitaevski 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 shall discuss in future work. In this paper we focus on the bose gas at zero temperature.

The paper is organized as follows. In section 2, we generalize the usual Bogolubov transformation to describe spatially inhomogeneous condensates. In section 3, 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 sections 4 and 5, 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 section 6 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 section 7. Finally, in section 8, we derive a density of states of the trapped weakly interacting condensate within the spirit of the Thomas-Fermi approximation.

2 Generalized Bogolubov Transformation

The Bogolubov quasi-particle concept \[13\] provides a very elegant description of the interacting Bose-Einstein condensate. The quasi-particles are represented by creation (\(\eta^\dagger\)) and annihilation (\(\eta\)) 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 \(\mathbf{k}\), the Bogolubov transformation which relates the quasi-particle and regular particular operators, takes on a particularly simple form,

\[
\begin{align*}
\eta^\dagger_k &= x_k a^\dagger_k + y_k a_{-k}, \\
\eta_k &= x_k a_k + y_k a^\dagger_{-k},
\end{align*}
\]

(2)

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

\[
x_k^2 - y_k^2 = 1,
\]

(3)

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

\[
\begin{align*}
a^\dagger_k &= x_k \eta^\dagger_k - y_k \eta_{-k}, \\
a_k &= x_k \eta_k - y_k \eta^\dagger_{-k},
\end{align*}
\]

(4)

which is the inverse transformation of (2).

It is useful to define the following quantities, the “distribution function” \(\rho\) and the “pairing function” \(\Delta\):

\[
\begin{align*}
\rho_k &= \langle a^\dagger_k a_k \rangle = \frac{1}{2} \left[ \cosh 2\sigma_k - 1 \right], \\
\Delta_k &= -\langle a_k a_{-k} \rangle = \frac{1}{2} \sinh 2\sigma_k,
\end{align*}
\]

(5)

where the brackets \(\langle \rangle\) 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) only applies to homogeneous systems, whereas the treatment of a general (inhomogeneous) condensate, as we shall show below, involves a Bogolubov 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, \( \hat{\Psi}(x) \) and \( \hat{\Psi}^\dagger(x) \), 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 \( \hat{\psi}(x) \) and \( \hat{\psi}^\dagger(x) \), which are displaced from the original fields \( \hat{\Psi}(x) \) and \( \hat{\Psi}^\dagger(x) \) by the expectation value \( \phi(x) \) of \( \hat{\Psi}(x) \),

\[
\begin{align*}
\hat{\Psi}(x) & = \hat{\psi}(x) + \phi(x), \\
\hat{\Psi}^\dagger(x) & = \hat{\psi}^\dagger(x) + \phi^*(x),
\end{align*}
\]

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

\[
\langle \hat{\psi}(x) \rangle = \langle \hat{\psi}^\dagger(x) \rangle = 0.
\]

We introduce the Bogolubov transformation as a general linear transformation relating the displaced fields to the quasi-particle fields, \( \hat{\xi}(x) \) and \( \hat{\xi}^\dagger(x) \),

\[
\begin{align*}
\hat{\psi}(x) & = \int d^3z \left[ X(x, z)\hat{\xi}(z) - Y(x, z)\hat{\xi}^\dagger(z) \right], \\
\hat{\psi}^\dagger(x) & = \int d^3z \left[ X^*(x, z)\hat{\xi}^\dagger(z) - Y^*(x, z)\hat{\xi}(z) \right],
\end{align*}
\]

which is the generalization of Eq.(3). The non-local nature of the generalized Bogolubov transformation (8) should not be surprising – the ‘homogeneous’ Bogolubov transformation (2) can be written in the same form with the special feature, due to the homogeneity of the system, that \( X(x, y) \) and \( Y(x, y) \) only depend on \( x - y \).

Requiring the quasi-particle fields to be canonical, leads to

\[
\int d^3z \left[ X(x, z)X(z, y) - Y(x, z)Y(z, y) \right] = \delta(x - y),
\]

which is the generalization of (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 Bogolubov 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 new 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.
3 Wigner Representation and Gradient Expansion

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

$$\rho_W(R, p) = \int d^3r \, \Psi^*(R + r/2)\Psi(R - r/2) \exp(ip \cdot r),$$

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 [14] 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, $\rho_W$ 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 $(2\pi)^{-3}\rho_W$,

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

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

etc. More recently, the many-particle generalization of the Wigner distribution has found many important applications in diverse areas such as nuclear [15] and solid state physics [16].

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

$$A_W(R, p) = \int d^3r \, A(R + r/2, R - r/2) \exp(ip \cdot r),$$

and its inverse

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

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 [15] – [16]. The gradient expansion shows that, to first order, a ‘product’ operator $C(x, x') = \int d^3z \, A(x, z)B(z, x')$, in the Wigner representation simply gives the algebraic product of $A$ and $B$, $C_W(R, p) \approx A_W(R, p)B_W(R, p)$. The higher-order corrections to this approximation can be written as a series of terms containing successively higher-order derivatives in the $(R, p)$-coordinates,

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

$$- \frac{1}{8} \sum_{j=1}^{3} \left[ \frac{\partial^2 A_W}{\partial R_j^2} \frac{\partial^2 B_W}{\partial p_j^2} + \frac{\partial^2 A_W}{\partial p_j^2} \frac{\partial^2 B_W}{\partial R_j^2} - 2 \frac{\partial^2 A_W}{\partial R_j \partial p_j} \frac{\partial^2 B_W}{\partial R_j \partial p_j} \right] + \cdots.$$
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 Bogolubov transformation, $X(x, y), Y(x, y)$, of the previous section. 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 Bogolubov transformation,

$$X^2_W(R, p) - Y^2_W(R, p) \approx 1.$$  

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

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

The local $\sigma$ parametrization of the Bogolubov transformation is crucial to the Thomas-Fermi description and it is upon the validity of (15) that the Thomas-Fermi theory rests. The error introduced to (15) due to the inhomogeneity of the system can be estimated by the lowest order non-vanishing term in the gradient expansion (14). Notice that the first order term in the gradient expansion of (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.

### 4 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, $F = \int d^3R f(R)$, where $f(R)$ 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 inter-atomic 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 $\mu$, the chemical potential:

$$\hat{H} - \mu \hat{N} = \int d^3x \hat{\Psi}^\dagger(x) \hat{h}(x) \hat{\Psi}(x) + \frac{1}{2} \int d^3x d^3y \hat{\Psi}(y) \hat{\Psi}(x) \hat{V}(|x - y|) \hat{\Psi}(x) \hat{\Psi}(y),$$

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

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

where $V_{ext}(x)$ is the external potential.
The presence of a condensate displaces the field operators $\hat{\Psi}(x)$ by their expectation value $\phi(x)$. To generate the variational free energy, we shall use the mean field approximation, in which terms of first and third order in $\psi$ and $\psi^\dagger$ vanish and the fourth order term factorizes as follows:

$$\langle \hat{\psi}(y)^\dagger \hat{\psi}(x)^\dagger \hat{\psi}(x)\hat{\psi}(y) \rangle \approx \Delta^*(y, x)\Delta(y, x) + \rho(y, x)\rho(x, y) + \rho(x, x)\rho(y, y).$$

The variational nature of this procedure is insured 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.

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 $\phi$ and their functional dependence on $\rho$ and $\Delta$:

1. $h_1$ is the one-body contribution of zeroth order in $\phi$ to the ground state energy,

$$h_1 = \frac{1}{2} \int d^3x \int d^3y \hat{h}(x)\rho(y, x)\delta(x - y).$$

2. In analogy with the Hartree-Fock theory, we call $V_{\text{dir}}$ given below, the direct energy contribution to the energy,

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

3. Using the same analogy to the Hartree-Fock treatment, the exchange energy, $V_{\text{exch}}$, is equal to

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

4. Standard Hartree-Fock theory does not describe pairing and the pairing energy, $V_{\text{pair}}$,

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

is consequently absent from the Hartree-Fock expressions.

In second order in $\phi$, we find contributions that can be obtained from the above terms by replacing either $\Delta(x, y)$ or $\rho(x, y)$ by $\phi(x)\phi(y)$.

5. For example, the one-body contribution, due to the kinetic and potential energy of the condensate is $h^\phi_1$, where

$$h^\phi_1 = \int d^3x \phi(x)\hat{h}(x)\phi(x).$$

6. $V^\phi_{\text{dir}}$ 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),

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

7. Similarly, $V^\phi_{\text{exch}}$ is the exchange contribution of second order in $\phi$,

$$V^\phi_{\text{exch}} = \frac{1}{2} \int d^3x \int d^3y \phi(y)\phi(y)\rho(y, x)V(|x - y|).$$
8. We represent the pairing energy of the condensate with the particles out of the condensate by $V_{\text{pair}}^\phi$:

$$V_{\text{pair}}^\phi = \frac{1}{2} \int d^3x \ d^3y \ \phi(y)\phi(x)\Delta(y, x)V(|x - y|). \quad (27)$$

9. Finally, we denote the contribution of fourth order in $\phi$, representing the interaction energy of the condensate with itself, by $V^{\phi\phi}$:

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

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

$$F = \left\langle \hat{H} - \mu \hat{N} \right\rangle = h_1 + V_{\text{dir}} + V_{\text{exch}} + V_{\text{pair}} + h_1^\phi + 2V_{\text{dir}}^\phi + 2V_{\text{exch}}^\phi - 2V_{\text{pair}}^\phi + V^{\phi\phi}, \quad (29)$$

where the minus sign of the $V_{\text{pair}}^\phi$ 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 $R$ over which is integrated. For the sake of notational convenience we introduce the following integration symbol

$$\int_p \equiv (2\pi)^{-3} \int d^3p, \quad \int_R \equiv \int d^3R. \quad (30)$$

The terms of zero order in $\phi$ then give

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

$$V_{\text{exch}} = \int_R \int_p \int_{p'} \rho_W(R, p)v(p - p')\rho_W(R, p') \rho_W(R, p'),$$

$$V_{\text{pair}} = \int_R \int_p \int_{p'} \Delta_W(R, p)v(p - p')\Delta_W(R, p'),$$

$$V_{\text{dir}} = \int_R \int_r \int_{p} \int_{p'} \int_{q} \rho_W(R - r/2, p)\rho_W(R + r/2, p') \exp(iq \cdot r)v(q), \quad (31)$$

where $v$ is the Fourier transform of the interaction potential, $v(q) = \int d^3rV(r)\exp(-iq \cdot r)$.

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

$$Q_W(R, p) = \int r \phi(R + r/2)\phi(R - r/2) \exp(ip \cdot r). \quad (32)$$
Notice that the contributions of second order in $\phi$, are non-local 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 non-local integrals can be approximated by local expressions. We illustrate this point by considering the exchange ($V_{\text{exch}}^\phi$) and pairing ($V_{\text{pair}}^\phi$) energies. The key to obtain local expressions is to notice that $Q_W(R, p)$ varies with respect to $p$ on the scale of $R_0^{-1}$, where $R_0$ is the size of the condensate. On the other hand, $v(p - p')$ varies on the scale of $l_r^{-1}$ where $l_r$ is the range of the atom-atom interaction. Typically $R_0 \gg l_r$ so that $Q_W(R, p)$ varies much more rapidly with respect to $p$ than $v(p - p')$. In fact, when $p$ is large enough to make $v(p - p')$ significantly different from $v(p')$, $Q_W(R, p) \approx 0$. Thus, we can replace $v(p - p')$ by $v(p')$ in the integrands:

\[
\begin{align*}
V_{\text{exch}}^\phi & \approx \frac{1}{2} \int_{R} \int_{p} \int_{p'} \phi(R + r/2)\phi(R - r/2) \exp(i p \cdot r) v(p') \rho_W(R, p') \\
& = \frac{1}{2} \phi^2(R) \int_{R} \int_{p'} v(p') \rho_W(R, p'), \\
V_{\text{pair}}^\phi & \approx \frac{1}{2} \phi^2(R) \int_{R} \int_{p'} v(p') \rho_W(R, p').
\end{align*}
\]

The same considerations regarding the relative magnitude of the relevant length scales show that we can similarly simplify the expression of the $\phi^4$ interaction energy, $V_{\phi}^\phi$, and the direct interaction energies, $V_{\text{dir}}^\phi$ and $V_{\phi}^\phi$. 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 $\rho(x, x) \approx \rho(y, y)$ if $|x - y| \leq l_r$. Thus, we can replace $\rho(x, x)$ by $\rho(y, y)$ in an integrand if it is accompanied by $V(|x - y|)$:

\[
\begin{align*}
V_{\text{dir}}^\phi & \approx \frac{1}{2} \int d^3 x \int d^3 y \rho^2(x, x) V(|x - y|) \\
& = \frac{1}{2} v(0) \int_{R} \int_{p} \int_{p'} \rho_W(R, p) \rho_W(R, p'), \\
V_{\text{dir}}^\phi & \approx \frac{1}{2} v(0) \int_{R} \int_{p} \phi^2(R) \rho_W(R, p), \\
V_{\phi}^\phi & \approx \frac{1}{2} v(0) \int_{R} \phi^4(R).
\end{align*}
\]

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 non-local operator, in the $\hbar^\phi$ -contribution to the energy. In fact, it is the non-locality of this term that gives rise to a generalized Gross-Pitaevski or non-linear Schrodinger equation (NLSE). The resulting (almost-local) ground state free energy is $F = \int d^3 R f(R)$, where

\[
\begin{align*}
f(R) &= \int_{p} \left[ \frac{p^2}{2m} + V_{\text{ext}}(R) - \mu \right] \rho(R, p) + v_{\text{exch}}(R) + v_{\text{dir}}(R) + v_{\text{pair}}(R) \\
& \quad + \phi(R) \left[ \frac{-\nabla^2}{2m} + V_{\text{ext}}(R) - \mu \right] \phi(R) + 2v_{\text{exch}}^\phi(R) + 2v_{\text{dir}}^\phi(R) - 2v_{\text{pair}}^\phi(R) \\
& \quad + \frac{1}{2} v(0) \phi^4(R),
\end{align*}
\]
where the exchange, direct and pairing energy densities are the integrands of the corresponding interaction energy contributions to the free energy:

\[ v_{\text{exch}}(\mathbf{R}) = \frac{1}{2} \int_p \int_{p'} \rho(\mathbf{R}, \mathbf{p}) v(\mathbf{p} - \mathbf{p}') \rho_W(\mathbf{R}, \mathbf{p}') , \]

\[ v_{\text{pair}}(\mathbf{R}) = \frac{1}{2} \int_p \int_{p'} \Delta_W(\mathbf{R}, \mathbf{p}) v(\mathbf{p} - \mathbf{p}') \Delta_W(\mathbf{R}, \mathbf{p}') , \]

\[ v_{\text{dir}}(\mathbf{R}) = \frac{1}{2} v(0) \int_p \int_{p'} \rho_W(\mathbf{R}, \mathbf{p}) \rho_W(\mathbf{R}, \mathbf{p}') , \]

\[ v_{\phi}^\text{exch}(\mathbf{R}) = \frac{1}{2} \phi^2(\mathbf{R}) \int_p \rho_W(\mathbf{R}, \mathbf{p}) v(\mathbf{p}) , \]

\[ v_{\phi}^\text{pair}(\mathbf{R}) = \frac{1}{2} \phi^2(\mathbf{R}) \int_p \Delta_W(\mathbf{R}, \mathbf{p}) v(\mathbf{p}) , \]

\[ v_{\phi}^\text{dir}(\mathbf{R}) = \frac{1}{2} \phi^2(\mathbf{R}) v(0) \int_p \rho_W(\mathbf{R}, \mathbf{p}) . \]  

(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 \( F[\rho, \Delta, \phi; \mu] \).

5 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 previous 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 Bogolubov 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 \( \rho_W \) and \( \Delta_W \) are parametrized by \( \sigma \) [17], \( F[\sigma, \phi; \mu] = F[\rho_W(\sigma), \Delta_W(\sigma), \phi; \mu] \). We obtain the condensate wave function \( \phi_0(\mathbf{R}) \) and Bogolubov parameter \( \sigma_0(\mathbf{R}, \mathbf{p}) \) that describe the condensate by varying \( \sigma \) and \( \phi \) independently to get a minimum in \( F \):

\[ \frac{\delta F}{\delta \phi(\mathbf{R})}_{\sigma = \sigma_0, \phi = \phi_0} = 0 , \quad \text{(NLSE)} \]

\[ \frac{\delta F}{\delta \sigma(\mathbf{R}, \mathbf{p})}_{\sigma = \sigma_0, \phi = \phi_0} = 0. \]  

(37)

The \( \phi \) variation, \( \delta F/\delta \phi = 0 \), gives the non-linear Schrödinger Equation (NLSE). The \( \sigma \) 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 \( \Delta = \frac{1}{2} \sinh(2\sigma) \) [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

\[ \tanh(2\sigma_0) = -\frac{\delta F/\delta \Delta_W}{\delta F/\delta \rho_W} . \]  

(38)

Now, several terms of the NLSE, as well as the functional derivatives \( \delta F/\delta \Delta \) and \( \delta F/\delta \rho \) [38], depend on \( \sigma_0 \) and \( \phi_0 \) 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 $\sigma$-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,

$$U_{\text{exch}}(R, p) = \frac{\delta V_{\text{exch}}}{\delta \rho W(R, p)} = \int_{p'} v(p-p')\rho W(R, p'),$$

$$U_{\text{dir}}(R) = \frac{\delta V_{\text{dir}}}{\delta \rho W(R, p)} = v(0) \int_{p'} \rho W(R, p'),$$

$$U_{\text{pair}}(R, p) = \frac{\delta V_{\text{pair}}}{\delta \Delta W(R, p)} = \int_{p'} v(p-p')\Delta W(R, p'),$$

(39)

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

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

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

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

(40)

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

$$\frac{\delta F}{\delta \Delta W(R, p)} = U_{\text{pair}}(R, p) - \phi^2(R)v(p),$$

$$\frac{\delta F}{\delta \rho W(R, p)} = \frac{p^2}{2m} + V_{\text{ext}}(R) - \mu$$

$$+ U_{\text{exch}}(R, p) + U_{\text{dir}}(R, p) + \phi^2(R) [v(p) + v(0)] \ .$$

(41)

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

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

(42)

where the potential $U(R)$, is equal to:

$$U(R) = U_{\text{dir}}(R) + U_{\text{exch}}(R, 0) - U_{\text{pair}}(R, 0) \ .$$

(43)

This potential term, which stems from the interaction of the condensate with the particles out of the condensate, is absent in the simplest (low density limit) form of the NLSE, usually encountered in the literature.
The equations, (40) (41) (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 [17], are recovered by putting $V_{\text{ext}} = 0$ and by assuming that $\phi$ 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 $\mu$ and $V_{\text{ext}}$ in the self-consistent mean field equations always appear as $\mu - V_{\text{ext}}(\mathbf{R})$, so that it is natural to define a local effective chemical potential:

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

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 $\mu$. One observable we can obtain in this manner is $N$, the number of trapped particles,

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

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 $N$.

6 Low Density Limit

The self-consistent equations, (40) (41) (42) and (43) can be solved iteratively. In the low density regime, where $\sqrt{n a^3} \ll 1$, we approximate the result by the expressions obtained after a single iteration, starting from $\sigma_0^{(0)} = 0 (U_{\text{exch}}^{(0)} = U_{\text{dir}}^{(0)} = U_{\text{pair}}^{(0)} = 0$, where the superscript indicates the order of the iteration). With this first guess we solve the NLSE and obtain the functional derivatives (41), $\delta F/\delta \rho$, $\delta F/\delta \Delta$, yielding the first-order $\sigma-$parameter (38), $\sigma^{(1)}$, and the generalized potentials (39), $U^{(1)}_{\text{dir}}$, $U^{(1)}_{\text{exch}}$, $U^{(1)}_{\text{pair}}$. With these single iteration expressions we compute the expectation values of the observable quantities.

In solving the NLSE, we shall assume that $\phi(\mathbf{R})$ varies slowly enough that we can also neglect the kinetic energy operator. To make the dependence on the scattering length explicit, we replace the potential by a pseudopotential,

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

where $\lambda = 4\pi \hbar^2 a / m$ and the derivative operator is necessary to remove the divergence in the ground state free energy [19].

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):

$$
\lambda \left[ \phi^{(1)}(\mathbf{R}) \right]^2 = \mu_{\text{eff}}(\mathbf{R}),
$$

where $\mu_{\text{eff}}$ is the effective chemical potential (44). The functional derivatives (41) are

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

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

(48)
Consequently, the single iteration value for the Bogolubov transformation parameter $\sigma$ is equal to

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

$$= \frac{\mu_{\text{eff}}(\mathbf{R})}{(p^2/2m) + \mu_{\text{eff}}(\mathbf{R})},$$

(49)

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

The expression for the Bogolubov 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, $V_{\text{dir}}, V_{\text{exch}}$ and $V_{\text{pair}}$. In other words, the effective ground state energy is $F_{\text{eff}} = \int d^3 R f_{\text{eff}}(\mathbf{R})$, where

$$f_{\text{eff}}(\mathbf{R}) = \int_{\mathbf{p}} \left[ \left( \frac{p^2}{2m} - \mu_{\text{eff}}(\mathbf{R}) + 2\lambda \phi^2(\mathbf{R}) \right) \rho_{\mathbf{W}}(\mathbf{R}, \mathbf{p}) - \lambda \phi^2(\mathbf{R}) \Delta_{\mathbf{W}}(\mathbf{R}, \mathbf{p}) \right]$$

$$- \mu_{\text{eff}}(\mathbf{R}) \phi^2(\mathbf{R}) + \frac{\lambda}{2} \phi^4(\mathbf{R}).$$

(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:

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

(51)

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

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

(52)

evaluated with the single-iteration value for $\sigma$. The single-iteration values for the generalized potentials are computed to be:

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

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

(53)

Thus, the condensate density is (51)

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

(54)

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

$$n(\mathbf{R}) = \phi^2(\mathbf{R}) + \int_{\mathbf{p}} \rho(\mathbf{R}, \mathbf{p})$$

$$\approx \phi^2(\mathbf{R}) + \frac{1}{3\pi^2} \left[ \mu_{\text{eff}}(\mathbf{R}) \right]^{3/2} m^{3/2}$$

$$\approx \frac{1}{\lambda} \mu_{\text{eff}}(\mathbf{R}) - \frac{4}{3\pi^2} \left[ \mu_{\text{eff}}(\mathbf{R}) \right]^{3/2} m^{3/2},$$

(55)
resulting in an expression for the density, $n(R)$, in terms of the effective chemical potential $\mu_{\text{eff}}(R)$. Inverting this relation up to first order in $\sqrt{n a^3}$, we obtain

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

(56)

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

Finally, in a similar manner, we obtain the local pressure $P(R)$ from the expression for the effective free energy density (50),

$$
P(R) = -f_{\text{eff}}^{(1)}(R),
$$

(57)

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

We can then replace $\phi^2$ in (57) by its single-iteration value (54). Furthermore, replacing $\mu_{\text{eff}}(R)$ in the resulting expression by (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 analogues 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. This approximation, although convenient, is not part of the Thomas-Fermi description. It is always possible to calculate the condensate wave function numerically from the NLSE and proceed from there with the iteration of the self-consistent Thomas-Fermi equations (57)!. Nevertheless, if we omit the Laplacian term, we can estimate the error by calculating $e_L$, the ratio of the kinetic energy term, $-\nabla^2 \phi/2m$, and the non-linear potential energy in the NLSE, $\lambda \phi^3$,

$$
e_L(R) = \frac{1}{2} \left| -\nabla^2 \phi / 2m \lambda \phi^3 \right| = \left| \frac{-\nabla^2 \phi(R)}{k_c^2(R)} \phi(R) \right|.
$$

(58)

where $k_c(R) = \left[ 8\pi a^3(R) \right]^{1/2}$ is the inverse of the local coherence length, $k_c = \lambda^{-1}_c(R)$.

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 gradient expansion offers a ‘handle’ on this quantity. Indeed, we use the lowest order non-vanishing term in the gradient expansion to estimate the error. This term is of second order because the first order term vanishes. We estimate its magnitude (59) 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 $p$ of the observable at zero temperature. The relative error for the general product of two arbitrary operators $A$ and $B$, $e_i [AB]$, is then given by

$$
e_i [AB] \approx \frac{1}{8k_c^2(R)} \left[ \nabla^2 A_W A_W + \nabla^2 B_W B_W - 2 \nabla A_W \cdot \nabla B_W \right].
$$

(59)

The validity of the Thomas-Fermi description depends on $X_W^2 - Y_W^2 = 1$ (53), so that we use the accuracy of this equality to test the validity of the local homogeneity description. The expression (53) can also be written as $\exp(4\sigma) = 1$, so that we choose $A_W$ as $\exp[\sigma(R, p)]$ and $B_W$ as $\exp[-\sigma(R, p)]$ to estimate the relative error $e_i$. In fact, it is more convenient to work with $\exp(4\sigma)$ then $\exp(\sigma)$, so that 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

$$e_i [\exp(\sigma) \exp(-\sigma)] = \frac{1}{4} e_i [\exp(4\sigma) \exp(-4\sigma)]$$

$$\approx \frac{1}{8k_c^2(R)} \left| \frac{\nabla \exp(4\sigma)}{\exp(4\sigma)} \right|^2.$$  (60)

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

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

we find that the inhomogeneity error, $e_i(R)$ (60), is equal to

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

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

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

where we replaced $\mu_{\text{eff}}$ 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 $e_{\text{cut}}$.

7 Spherically Symmetric Harmonic Oscillator Trap

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

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

where $L$ is the size of the harmonic oscillator ground state,

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

and compute the expectation value of important quantities in the low density limit of the previous section.

In zeroth order in the iteration, we recover the results of Baym and Pethick. From (47) we see that

$$\left[\phi^{(0)}(R)\right]^2 = [\mu - V_{\text{ext}}(R)]/\lambda$$

$$= \frac{R_0^2}{8\pi aL^4} [1 - (R/R_0)^2]$$  (66)
where $R_0$ is the size of the condensate, $R_0 = \sqrt{\frac{\bar{\mu}}{\bar{h} \omega} L}$. In zeroth order, all particles are in the condensate, so that $N = \int_R \phi^2(R)$, and

$$\mu^{(0)} = \frac{\hbar \omega}{2} \left( \frac{15aN}{L} \right)^{2/5},$$  \hspace{1cm} (67)$$

and consequently,

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

The local coherence length, $\lambda_c(R)$ is given by

$$\lambda_c(R) = \frac{L^2}{\sqrt{R_0^2 - R^2}}. \hspace{1cm} (69)$$

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, $e_L(R)$, is easily computed with (69):

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

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, $e_i(R)$, is

$$e_i(R) = \frac{1}{2} \left( \frac{L}{R_0} \right)^4 \frac{(R/R_0)^2}{(1 - (R/R_0)^2)^3}. \hspace{1cm} (71)$$

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, $|\phi^{(0)}(R)|^2/|\phi^{(0)}(R = 0)|^2$, 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 $L = 1 \mu m$ and an inter-atomic 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. In contrast, only at $R = 1.8L$ (to be compared to $R_0 = 2.4L$) does the inhomogeneity error become of comparable magnitude. This indicates that even for as few as 1000 particles in the trap, the Thomas-Fermi description could be reasonably accurate for these parameters, provided one keeps the kinetic energy term in solving the NLSE. For $10^6$ atoms, $e_i$ and $e_L$ only become 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 values of the observable quantities. Including the perturbation correction, the local density (53) is equal to

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

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

$$N = \int_R n(R) = 4\pi \int_0^{R_0} dR \ R^2 \ n(R), \hspace{1cm} (73)$$
Figure 1: (a) Condensate density for \( N = 10^3 \) and \( 10^6 \); (b) Error incurred in neglecting kinetic term in NLSE; (c) Error incurred in Thomas-Fermi approximation. Length scale on horizontal axis is in units of \( L \), the extend of the ground state wave function. Calculations are done for \( L = 10^{-4} \) cm, scattering length \( a = 5 \times 10^{-7} \) cm.
which leads to

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

The inverse relation, $\mu$ as a function of $N$, can be obtained by solving for $\mu$ iteratively in the previous equation, which gives up to second iteration, the following result:

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

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

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

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).

![Local Depletion Graph](image)

**Figure 2:** Depletion, defined as $d(R) = [n(R) - \phi^2(R)] / \phi^2(R)$, for the same systems as Fig. (1).

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 non-vanishing order in table I.
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 following energy spectrum:

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

(77)

which is well known from the Bogolubov 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

$$g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i),$$

(78)

where \(\sum_i\) represents the sum over all excited states. In the spirit of the Thomas-Fermi approximation we take

$$g(\epsilon) = \int_R \int_p \delta(\epsilon - \epsilon_p(R)).$$

(79)

After integration over the momentum variable, we obtain

$$g(\epsilon) = \frac{1}{2\pi^2} \int_R \rho_p^2(R) \left| \frac{\partial \epsilon_p}{\partial p} \right|^{-1},$$

(80)

where \(\rho_p(R)\) is the momentum of a particle at position \(R\) with energy \(\epsilon\). 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

8 Density of States

![Figure 3: Pressure for the same systems as Fig. (1).](image-url)
Figure 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 $\mu_{\text{eff}}(R)$, which is a 'mirror image' of the trapping potential. Particles in the condensate have energy $\mu$ and a particle excited up to energy $\epsilon$ can move into region (II) as far as the classical turning point $R_\epsilon$.

The density of states is then the sum of the integrals over region (I) and (II):

$$g(\epsilon) = \sqrt{2} \frac{m^{3/2}}{\pi^2} \left[ (\epsilon - \mu) \int_{(I)} d^3R \frac{\sqrt{\epsilon - \mu}^2 + \mu_{\text{eff}}^2(R) - \mu_{\text{eff}}(R)}{\sqrt{\epsilon - \mu}^2 + \mu_{\text{eff}}^2(R)} \right. + \left. \int_{(II)} d^3R \sqrt{\epsilon - V_{\text{ext}}(R)} \right].$$  \hspace{1cm} (82)

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

$$g(\epsilon) = \frac{4}{\pi} \frac{\mu^2}{(\hbar \omega)^3} \left[ (\epsilon/\mu - 1) \int_0^1 dr \sqrt{1 - r} \frac{\sqrt{(\epsilon/\mu - 1)^2 + r^2 - r}}{\sqrt{(\epsilon/\mu - 1)^2 + r^2}} \right. + \left. 2 \int_1^{\epsilon/\mu} dr \ r^2 \sqrt{\epsilon/\mu - r^2} \right].$$  \hspace{1cm} (83)

In Figs. (5) and (6) we show the density of states for the system discussed in the previous section, $L = 1\mu m$, $a = 5\ nm$, $N = 10^3$ (Fig. (5)) and $N = 10^6$ (Fig. (6)). The dotted
Figure 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 $a = 5 \times 10^{-7}$ cm, in a harmonic trap with ground state of extend $L = 10^{-4}$ cm.

Figure 6: Density of states for the same system as in Fig. (6), but with $N = 10^6$ particles.
lines show the result for the interacting bose gas, 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 $\mu$, consistent with (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 $\mu$. 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 $\mu$. 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 non-interacting 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 non-interacting particle with the same energy.

Of course, the sharpness of the boundary between region (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 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.

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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**      | $\phi^2(R) = \frac{R_0^2}{8\pi aL^2} \left[ 1 - (R/R_0)^2 \right]$ |
| **Local Coherence Length**  | $\lambda_c(R) = \frac{L^2}{\sqrt{R_0^2 - R^2}}$       |
| **Local Depletion**         | $d(R) = \frac{3\sqrt{7} aR_0}{L^2} \sqrt{1 - (R/R_0)^2}$ |
| **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 the inhomogeneity** | $e_i(R) = \frac{1}{2} \left( \frac{L}{R_0} \right)^4 \frac{(R/R_0)^2}{(1-(R/R_0)^2)^3}$ |