1 Thomas-Fermi Theory

The Thomas-Fermi method \cite{1,2} was designed for the calculation of the electron density in a heavy atom, by treating the electrons as locally free. Lieb and Simon \cite{3} 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 \cite{4}, and by Oliva \cite{5}, and recently reconsidered by Chou, Yang, and Yu \cite{6}. I shall describe some work on this subject, done in collaboration with E. Timmermans and P. Tommasini \cite{7}.

First, let us review the original method of Thomas and Fermi. Suppose $V(r) = -e\Phi(r)$ denotes the effective potential energy of an electron in an atom, at a distance $r$ from the nucleus. (See Fig.1).

The condition that the electron is in a bound orbit is that

$$\frac{\hbar^2 k^2}{2m} + V(r) \leq 0 \quad (1)$$

---

1 Contribution to Workshop on Bose-Einstein Condensation, Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, (August 19-30, 1996).
where $k$ is the local wave vector. Assume that all available states are occupied. Then the local Fermi momentum $\hbar k_F(r)$ is given by

$$\frac{\hbar^2 k_F^2(r)}{2m} + V(r) = 0$$

which gives

$$\hbar k_F = \sqrt{2m\epsilon\Phi(r)}$$

We know that $k_F(r)$ is related to the local density $n(r)$ by

$$2(4\pi/3)k_F^3 = n(r)$$

where the factor 2 comes from spin. This relates the density to the potential $\Phi(r)$. We now use the Poisson equation

$$\nabla^2 \Phi(r) = -4\pi[Z\epsilon\delta(r) - en(r)]$$

For $r \neq 0$ this equation is of the form

$$\nabla^2 \Phi(r) + C\Phi^{3/2}(r) = 0$$

where $C$ is a constant. One can solve this equation, and then obtain $n(r)$. A comparison between Thomas-Fermi and Hartree results for Rb is sketched in Fig.2.

![Figure 2: Electron density in Rb: Comparison between Thomas-Fermi and Hartree approximations.](image)

The essence of the method is that one assumes there is a local chemical potential $\mu_{\text{eff}}(r)$, related to the true chemical potential $\mu$ by

$$\mu_{\text{eff}}(r) = \mu - V(r)$$

In the earlier discussion, the chemical potential (Fermi energy) was taken to be zero.
2 Ideal Bose Gas in External Potential

Can we apply this idea to a Bose gas? Let us first consider an ideal Bose gas in an external potential, at a temperature $T$ above the transition point. Take the potential to be harmonic:

$$V(r) = \frac{1}{2}m\omega^2r^2$$  \hspace{1cm} (8)

For the Thomas-Fermi idea to be applicable, we require

$$\frac{\hbar\omega}{kT} \ll 1$$  \hspace{1cm} (9)

Above the transition temperature, the density is related to the fugacity $z = \exp(-\mu/kT)$ through

$$n = \frac{1}{\lambda^3}g_{3/2}(z)$$  \hspace{1cm} (10)

where $\lambda = \sqrt{2\pi\hbar^2/mkT}$ is the thermal wavelength, and

$$g_{3/2}(z) = \sum_{\ell=1}^\infty \frac{z^\ell}{\ell^{3/2}}$$  \hspace{1cm} (11)

This suggests that in the presence of an external potential we take the local density to be

$$n(r) = \frac{1}{\lambda^3}g_{3/2}\left(z e^{-\beta V(r)}\right)$$  \hspace{1cm} (12)

where $\beta = 1/kT$. Integrating both sides over all space, we obtain an expression for the total number of particles:

$$N = \frac{1}{\lambda^3} \int d^3r g_{3/2} \left(z e^{-\beta V(r)}\right)$$  \hspace{1cm} (13)

We know that $g_{3/2}(z)$ is bounded for $0 \leq z \leq 1$. So the right side is bounded. This forces Bose-Einstein condensation when $N$ exceeds the bound. The number of atoms in the condensate $N_0$ is given through

$$N = N_0 + \frac{1}{\lambda^3} \int d^3r g_{3/2} \left(z e^{-\beta V(r)}\right)$$  \hspace{1cm} (14)

In this intuitive approach, however, the Bose condensate was not described accurately.

As it turns out, the problem can be solved exactly [5]:

$$n(r) = \frac{z_1}{1 - z_1} |\psi_0(r)|^2 + \frac{1}{\lambda^3}G(z, r)$$  \hspace{1cm} (15)

where $\psi_0(r)$ is the ground-state wave function in the potential, and

$$G(z_1, r) = \frac{1}{(2\ell)^{3/2}} \sum_{\ell=1}^\infty z_1^\ell \left\{ \frac{\exp[-(r/r_0)^2\tanh(\ell\ell/2)]}{[1 - \exp(-2\ell\ell)]^{3/2}} - \exp[-(r/r_0)^2] \right\}$$  \hspace{1cm} (16)
with

\[
\begin{align*}
    z_1 &= z e^{-3\hbar\omega/2kT} \\
    \epsilon &= \hbar\omega/kT \\
    r_0 &= \sqrt{kT/2\pi m\omega^2}
\end{align*}
\]

The explicit occurrence of \(\psi_0(r)\) shows that Bose condensation occurs in the ground state \(\psi_0\) of the potential. The zero-momentum state is irrelevant here. The total number of particles is

\[
N = \frac{z_1}{1 - z_1} + \frac{1}{\Lambda^3} \int \! d^3r G(z, r)
\]

which shows that the condensation is a continuous process, though it may appear to be abrupt, when \(N\) is so large that the first term can be neglected except near \(z_1 = 1\).

The Thomas-Fermi approximation is good when \(\epsilon \ll 1\). In that case we have

\[
G(z_1, r) \approx g_{3/2} \left( z_1 e^{-\beta V(r)} \right)
\]

and therefore

\[
n(r) \approx \frac{z_1}{1 - z_1} \left| \psi_0(r) \right|^2 + \frac{1}{\Lambda^3} g_{3/2} \left( z_1 e^{-\beta V(r)} \right)
\]

which is similar to the naive formula, except for a better representation of the condensate. (The replacement of \(z\) by \(z_1\) is inconsequential.) The lesson is that a purely intuitive approach is not satisfactory, and we need a systematic method.

3 Uniform Dilute Interacting Bose Gas

The underlying idea of the Thomas-Fermi approach is to treat a nonuniform condensate as locally uniform, with a slowly varying density. I will first review the properties of a uniform Bose gas in the dilute limit, with interparticle interactions taken into account through a scattering length \(a \geq 0\).

The annihilation operator \(a_k\) of a particle of momentum \(\hbar k\) satisfies the commutation relation

\[
[a_k, a_{k'}^\dagger] = \delta_{kk'}
\]

We make a Bogolubov transformation to quasiparticle operators \(\eta_k\):

\[
a_k = x_k \eta_k - y_k \eta_k^\dagger \quad (k \neq 0)
\]

and require that the transformation be canonical, i.e.

\[
\left[ \eta_k, \eta_{k'}^\dagger \right] = \delta_{kk'}
\]

This leads to the condition

\[
x_k^2 - y_k^2 = 1
\]
which can be satisfied by putting

\[
\begin{align*}
    x_k &= \cosh \sigma_k \\
    y_k &= \sinh \sigma_k
\end{align*}
\]

This a convenient parametrization, because interesting quantities find simple expressions:

\[
\begin{align*}
    \rho_k &\equiv \langle a_k^\dagger a_k \rangle = \frac{1}{2} [ \cosh (2\sigma_k) - 1 ] \\
    \Delta_k &\equiv -\langle a_k a_{-k} \rangle = \frac{1}{2} \sinh (2\sigma_k)
\end{align*}
\]

where \( \rho_k \) measures the depletion of the unperturbed condensate:

\[
N_0 = N - \sum_{k \neq 0} \rho_k
\]

and \( \Delta_k \), is a measure of off-diagonal long range order.

In the Bogolubov method, the annihilation operator for the zero-momentum state \( a_0 \) is equated to the c-number \( \sqrt{N} \). Explicit solution of the problem gives

\[
\tanh (2\sigma_k) = \frac{\mu}{(\hbar^2 k^2 / 2m) + \mu}
\]

where \( \mu \) is the chemical potential:

\[
\mu = \frac{4\pi a \hbar^2 n}{m} \left( 1 + \frac{32}{3} \sqrt{\frac{n a^3}{\pi}} \right)
\]

with \( n \) the particle density. Note that this cannot be continued to negative \( a \); apparently, new physics arises when the scattering length turns negative. The excitation energy of a quasiparticle of momentum \( p \) is given by

\[
\epsilon_p = \sqrt{\left( \frac{p^2}{2m} + \mu \right)^2 - \mu^2}
\]

### 4 Quasiparticle Field Operator

In the uniform case, the field operator \( \Psi(\mathbf{r}) \) can be put in the form

\[
\Psi(\mathbf{r}) = a_0 + \psi(\mathbf{r})
\]

with

\[
\psi(\mathbf{r}) = \Omega^{-1/2} \sum_{k \neq 0} a_k e^{i\mathbf{k} \cdot \mathbf{r}}
\]

where \( \Omega \) is the spatial volume. We have

\[
[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')
\]
since $a_0$ is treated as a c-number. We can introduce a quasiparticle field operator:

$$\xi(r) \equiv \Omega^{-1/2} \sum_{k \neq 0} \eta_k e^{ikr}$$

(34)

Note that the relation between $\psi$ and $\xi$ is non-local:

$$\psi(r) = \int d^3y [X(x, y)\xi(y) - Y^*(x, y)\xi^+(y)]$$

(35)

where

$$X(x - y) = \Omega^{-1/2} \sum_{k \neq 0} x_k e^{ik(x-y)}$$

$$Y(x - y) = \Omega^{-1/2} \sum_{k \neq 0} y_k e^{ik(x-y)}$$

(36)

For a non-uniform Bose gas, we write

$$\Psi(r) = \phi(r) + \psi(r)$$

(37)

where $\phi(r)$ is a c-number function, such that

$$\langle \psi(r) \rangle = 0$$

(38)

where $\langle \rangle$ denotes ground state expectation value. We transform to quasiparticle operators by putting

$$\psi(r) = \int d^3y [X(x, y)\xi(y) - Y^*(x, y)\xi^+(y)]$$

(39)

The requirement

$$[\xi(r), \xi^+(r')] = \delta(r - r')$$

(40)

leads to the condition

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

(41)

The fulfillment of this condition in a simple fashion will guide our formulation of the Thomas-Fermi approximation.

## 5 Wigner Representation

In quantum mechanics, the Wigner distribution associated with a wave function $\psi(r)$ is defined by

$$\rho_W(R, p) \equiv \int d^3r \psi^*(R + r/2)\psi(R - r/2)e^{ip\cdot r/\hbar}$$

(42)

That is, we take the off-diagonal density at two different points in space, and Fourier analyze with respect to the relative separation. This is illustrated in Fig.3.
The Wigner distribution is not positive-definite, and hence not a probability; but it acts as a quasi-distribution function in phase space:

\[
(\psi, f\psi) \equiv \int d^3r \psi^*(r) f(r)\psi(r) = \int \frac{d^3R d^3p}{\hbar^3} f(R)\rho_W(R, p)
\]

\[
(\psi, \rho\psi) \equiv \int d^3r \psi^*(r) \frac{\hbar}{i} \nabla \psi(r) = \int \frac{d^3R d^3p}{\hbar^3} \frac{\hbar}{i} \nabla \rho_W(R, p)
\] (43)

For a function \(X(x, y)\) that depends on two spatial points, we define its Wigner transform as

\[
X_W(R, p) \equiv \int d^3r X(R + r/2, R - r/2)e^{ip\cdot r}
\] (44)

with the inverse transform

\[
X(x, y) = \int \frac{d^3p}{(2\pi)^3} e^{-ip\cdot(x-y)}X_W((x + y)/2, p)
\] (45)

If \(C(x, y)\) has the form

\[
C(x, y) = \int d^3z A(x, z)B(z, y)
\] (46)

then its Wigner transform takes the form

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

\[
-\frac{1}{8} \sum_{j=1}^3 \left( \frac{\partial^2 A_W}{\partial R_j^2} \frac{\partial^2 B_W}{\partial p_j^2} + \frac{\partial^2 B_W}{\partial R_j^2} \frac{\partial^2 A_W}{\partial p_j^2} - 2 \frac{\partial^2 A_W}{\partial R_j \partial p_j} \frac{\partial^2 B_W}{\partial R_j \partial p_j} \right) + \cdots
\] (47)

The second term is the classical Poisson bracket \(\{A_W, B_W\}_{PB}\). It and the subsequent terms all depend on spatial derivatives, and would be small if the system is nearly uniform. Thus our version of Thomas-Fermi approximation consists of keeping only the first term. Errors incurred can be estimated by calculating the next non-vanishing term.

In terms of the Wigner transform, we can write

\[
\int d^3z X(x, z)X(z, y) = X_W(R, p)X_W(R, p) + \frac{1}{2i}\{X_W, X_W\}_{PB} + \cdots
\] (48)
where the second terms vanishes identically. Thus, for such an integral, errors incurred in
using the Thomas-Fermi approximation starts with subsequent terms. The condition on $X$
and $Y$ therefore reads

$$\begin{align*}
X^2_W(R, p) - Y^2_W(R, p) &\approx 1
\end{align*}$$

and is solved by setting

$$\begin{align*}
X_W(R, p) &= \cosh \sigma(R, p) \\
Y_W(R, p) &= \sinh \sigma(R, p)
\end{align*}$$

This make the problem very similar to the uniform case.

At zero temperature, the criterion for the validity of the Thomas-Fermi approximation is

$$\bar{h} \omega / \mu \ll 1$$

where $\bar{h} \omega$ is the characteristic energy of the external potential, and $\mu$ is the chemical potential. For the dilute interacting Bose gas, $\mu$ is of order of the scattering length. Thus, the Thomas-Fermi approximation can be used only when there are interparticle interactions.

## 6 Variational Calculation

We study the system defined by the Hamiltonian $H$, with

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

where $V(x)$ is the interparticle potential, and

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

with $V_{ext}(x)$ the external potential. The ground state free energy is

$$F = \langle H - \mu N \rangle$$

where $\langle \rangle$ means expectation value with respect to the ground state of $H - \mu N$. As mentioned before, we displace the field by writing $\Psi = \phi + \psi$, where $\phi$ is a c-number function, such that $\langle \psi \rangle = 0$. We assume a trial form for the ground state, so that $\langle F \rangle$ has the same form as in mean-field theory, i.e., we can put

$$\langle \psi \dagger(y) \psi \dagger(x) \psi(x) \psi(y) \rangle = \Delta^*(y, x) \Delta(x, y) + \rho(y, x) \rho(x, y) + \rho(y, y) \rho(x, x)$$

where

$$\begin{align*}
\rho(x, y) &= \langle \psi \dagger(x) \psi(y) \rangle \\
\Delta(x, y) &= -\langle \psi(x) \psi(y) \rangle
\end{align*}$$

The ground state free energy $F[\phi, \rho, \Delta; \mu]$ is a functional of $\phi$, $\rho$, and $\Delta$, and also depends on $\mu$ as a parameter. The requirement $\langle \psi \rangle = 0$ means that there are no terms in $F$ linear in $\phi$. 

8
Although we do not need the trial state explicitly, it can be explicitly constructed if desired. One can show that the wave functional of this state is of Gaussian form \[^8\]. Thus, we have a true variational problem.

We rewrite the functions $\rho$ and $\Delta$ in $F[\phi, \rho, \Delta; \mu]$ in terms of their Wigner transforms, and implement our version of the Thomas-Fermi approximation, as explained before. We transform to quasiparticle field operators, and find that, as in the uniform case, $\rho_W$ and $\Delta$ are parametrized by a single function:

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

$$\Delta_W(R, p) = \frac{1}{2} \sinh(2\sigma(R, p))$$

(57)

The Free energy reduces to the form $F = \int d^3R f(R)$. We obtain equations for $\sigma$ and $\phi$ by minimizing $F$. The equation for $\phi$ is a modified Gross-Pitaevskii or non-linear Schrödinger equation (NLSE):

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

(58)

where $U(r)$ is a self-consistent potential that depends on $\sigma$. It is unimportant for low densities.

7 Dilute Interacting Gas in Harmonic Trap

I will just quote some results for a dilute gas in a harmonic trap. The external potential is

$$V_{\text{ext}} = \frac{\hbar \omega}{2} \left( \frac{r}{L} \right)^2$$

(59)

For particles of mass $m$,

$$L = \sqrt{\frac{\hbar}{m \omega}}$$

(60)

which is the extend of the ground state wave function. For the interparticle interaction, we use a pseudopotential

$$\frac{4\pi a \hbar^2}{m} \delta(r) \frac{\partial}{\partial r} r$$

(61)

The sole effect of the differential operator above is the removal of a divergence in the ground state energy. The three important lengths in the problem are

$$L \quad \text{(Extend of ground state wave function)}$$

$$a \quad \text{(Scattering length)}$$

$$R_0 \quad \text{(Extend of condensate)}$$

(62)

They are illustrated in Fig.4.
Figure 4: Length scales in atomic trap. Ground state wave function is $\psi_0(r)$. Condensate wave function is $\phi_0(r)$.

For low densities, the non-linear coupled equations for $\sigma$ and $\phi$ are solved by iteration, and one iteration suffices. The chemical potential is found to be

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

(63)

The requirement $\hbar \omega/\mu \ll 1$ means

$$\frac{L}{aN} \ll 1$$

(64)

The extend of the condensate is given by

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

(65)

For the method to be valid we must have $R_0 >> L$. By neglecting the term $\nabla^2 \phi$ in the NLSE, we find

$$\phi^2(r) = \frac{R_0^2}{8\pi a L^4} \left[ 1 - \left( \frac{r}{R_0} \right)^2 \right]$$

(66)

In Fig.5 we show the shape of the condensate and estimated errors. Fig.5(a) shows $\phi(r)$ as a function of $r$ in units of $L$, for $N=10^3$, and $10^6$.

Fig.5(b) shows the errors arising from the neglect of $\nabla^2 \phi$. This is “trivial,” as it can be corrected through numerical computation.

Fig.5(c) shows the errors incurred due to the Thomas-Fermi approximation, and are intrinsic to the method. They are small except at the edge of the condensate.
Figure 5: (a) Condensate wave functions 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 extent of the groundstate wave function. Calculations are done for $L = 10^{-4}$ cm, scattering length=$5 \times 10^{-7}$ cm.
8 Quasiparticle Excitation

The local excitation energy should be measured from the chemical potential:

$$\epsilon_p(r) = \mu + \sqrt{\left[ \frac{p^2}{2m} + \mu_{\text{eff}}(r) \right]^2 - \mu_{\text{eff}}^2(r)}$$  \hfill (67)

where

$$\mu_{\text{eff}}(r) = \mu - V_{\text{ext}}(r)$$  \hfill (68)

It describes a phonon with a position-dependent sound velocity. The excitation energy density of the system is given by

$$g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i)$$  \hfill (69)

where $\epsilon_i$ is the energy of the $i$th excited state. In the spirit of the Thomas-Fermi approximation, we take

$$g(\epsilon) = \int \frac{d^3r d^3p}{h^3} \delta(\epsilon - \epsilon_p(r))$$  \hfill (70)

The results for $N = 10^3$ and $10^6$ are shown in Fig.6 and Fig.7, with comparison to the ideal gas.

Further details can be found in [7].

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Density of States for $10^3$ particles

$L = 10^4$ cm $\quad a = 5 \times 10^{-7}$ cm

Figure 6: Density of states in harmonic trap, for $N = 10^3$. $g(\varepsilon)$ (units of $2/\omega$) vs. $\mu$ (in units of $\omega/2$).
Density of States for $10^6$ particles

$L = 10^4$ cm $a = 5 \times 10^{-7}$ cm

Figure 7: Same as Fig. 6, but for $N = 10^6$. 

$g(\epsilon)$ (units of $2/\omega$)

Energy (in units of $\omega/2$)

Ideal gas

Interacting gas

$\mu$
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