Density Functional Approach for Fermion-Boson-Mixtures in Thomas-Fermi Approximation

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Abstract

Density functional theory has been used extensively for the description of boson and fermion gases, but only few studies are available for mixtures of bosons and fermions where two fermions can form bosons as a diatomic molecule. In this thesis, we propose an explicit form of the energy functional underlying the conversion process and explore the particle densities in various parameter regimes.

Contents

Chapter 1

Introduction

1.1 Quantum Many-Body Problem

With the advance of modern quantum mechanics, simple atomic and molecular systems became fairly well understood with the help of the Schrödinger equation. However, when the number of particles in the system starts to increase, wavefunction methods soon encounter the so-called "exponential wall" in computational complexity. Soon as $N \approx O(10)$ the wavefunction can become impractical to solve even using the most powerful computers(5). The problem becomes even more severe when dealing with physical processes that involve millions or even billions of particles (i.e. chemical reaction). Hence, more efficient methods are in demand.

In 1964, a new method was suggested by Hohenberg and Kohn to tackle this many-body problem(3). Instead of calculating the N-particle wavefunction Ψ of the system,

$$\Psi = \Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N).$$ (1.1)

They used the one-particle density function $n(\vec{r})$ of the particles to represent the system. The density function can be formally regarded as a contracted version of N-particle wavefunction,

$$n(\vec{r}) = N \int \Psi^*(\vec{r}, \vec{r}_2, ..., \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, ..., \vec{r}_N) \mathrm{d}\vec{r}_2 \mathrm{d}\vec{r}_3 ... \mathrm{d}\vec{r}_N,$$ (1.2)

where N is the number of particles. Hence we have the normalization condition

$$N = \int \mathrm{d}\vec{r}\, n(\vec{r}).$$ (1.3)

This approach was motivated by the pioneer works from Thomas and Fermi in the 1920s(8), which, however, it is a relatively rough estimation for many physical systems. Hohenberg and Kohn overcame this deficiency by introducing the so-called Hohenberg-Kohn theorem which links the density function and the external potential bijectively(5).

1.2 Hohenberg-Kohn Theorem

The Hohenberg-Kohn theorem states that for any physical system, the ground state density function $n(\vec{r})$ uniquely determines the underlying external potential, up to an irrelevant constant(3). A simple proof for a non-degenerate ground state is illustrated here. It first makes use of the variational principle which states that any trial wavefunction ψ for the system will lead to an energy no less than the ground state energy E_g of the system,

$$\langle \psi | \hat{H} | \psi \rangle \geq E_{\mathrm{g}} . \tag{1.4}$$

When an external potential V_{ext} is applied, the total energy E can be calculated by

$$E = \langle \psi | (\hat{T} + \hat{U}) | \psi \rangle + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}), \tag{1.5}$$

where $\hat{T}$ is the kinetic energy operator and $\hat{U}$ is the interactive energy operator. Next we consider two systems applied with different external potential energies $V_1(\vec{r})$ and $V_2(\vec{r})$. Let E_1 and E_2 be the ground state energies, and let ψ_1 and ψ_2 be the ground state wavefunctions of the two Hamiltonians. Suppose both potentials lead to the same density n, we have

$$E_1 = \langle \psi_1 | (\hat{T} + \hat{U}) | \psi_1 \rangle + \int \mathrm{d}\vec{r})\, V_{\mathrm{ext}} n(\vec{r}), \tag{1.6}$$

$$E_2 = \langle \psi_2 | (\hat{T} + \hat{U}) | \psi_2 \rangle + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}). \tag{1.7}$$

By virtue of the variational principle,

$$E_1 < \langle \psi_2 | (\hat{T} + \hat{U}) | \psi_2 \rangle + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}), \tag{1.8}$$

$$E_2 < \langle \psi_1 | (\hat{T} + \hat{U}) | \psi_1 \rangle + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}), \tag{1.9}$$

If we add up (1.8) and (1.9),

$$E_1 + E_2 < \langle \psi_1 | (\hat{T} + \hat{U}) | \psi_1 \rangle + \langle \psi_2 | (\hat{T} + \hat{U}) | \psi_2 \rangle + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}) + \int \mathrm{d}\vec{r}\, V_{\mathrm{ext}} n(\vec{r}), \tag{1.10}$$

rearranging the terms we get a contradiction,

$$E_1 + E_2 < E_1 + E_2. \tag{1.11}$$

Hence, we have shown by contradiction that two systems with the same density function must have the same external potential applied. Since the external potential determines the wavefunction and thus the density function, with the introduction of Hohenberg-Kohn Theorem, we can now draw a unique link between a Hamiltonian and its density function and use the density function in place of wavefunction as a representation of a system. In

other words, the total energy E is a functional of the density $n(\vec{r})$.

1.3 Ultracold Gas

In nature there are two types of particles - fermions and bosons. We can identify them by their intrinsic spins. Fermions have half-integer spins, and bosons all have integer spins. Besides spin, their most prominent difference is that fermions obey Pauli's exclusion principle, but bosons do not. This implies that no two identical fermions occupy the same state at the same time, while bosons have no restriction on number of particles per state. This difference becomes more evident when temperature T of the system drops close to 0K, and at $T = 0$ the system reaches its ground state. We call particles at this temperature degenerate gas.

An ultracold fermionic gas follows the so-called "Fermi-Dirac statistics". The total energy of the system, as Hohenberg-Kohn Theorem states, is a functional of the density of fermions. The explicit form of this functional at zero-temperature limit has been worked out by Thomas and Fermi in 1927(8),

$$E = C_F \frac{\hbar}{M} \int \mathrm{d}\vec{r}\, n^{\frac{5}{3}}(\vec{r}) + \int \mathrm{d}\vec{r}\, V(\vec{r})n(\vec{r}), \tag{1.12}$$

where C_F is a dimensionless constant and M is the mass of the fermion. This equation is often referred to Thomas-Fermi approximation, and we will briefly demonstrate the reasoning behind it in the next section.

1.4 Thomas-Fermi Approximation

In a free fermion gas, if a system contains a large number of fermions, uniformly distributed in phase space, and as long as we are interested in the particle number, its density operator at temperature $T = 0$ can be represented as

$$\hat{\rho} = 2\eta(\mu - \hat{H}), \tag{1.13}$$

where μ is the chemical potential and the factor 2 is from the spin multiplicity. For a free fermion gas the Hamiltonian is given by

$$\hat{H} = \frac{\hat{P}^2}{2m}. \tag{1.14}$$

We find the Wigner function of the density function to be ($D = 3$)

$$\nu(\vec{r}, \vec{p}) = \frac{2}{h^3}\eta(\mu - H(\vec{r}, \vec{p})) = \frac{2}{h^3}\eta(\mu - \frac{\vec{p}^2}{2m}), \tag{1.15}$$

which is simply a sphere in the momentum space. The spatial density function can then be easily obtained,

$$\begin{aligned}
n(\vec{r}) &= \frac{2}{h^3}\int d^3\vec{p}\ \eta(\mu - \frac{\vec{p}^2}{2m}) \\
&= \frac{2}{h^3}\int d^3\vec{p}\ \eta(p_f^2 - \vec{p}^2) \\
&= \frac{2}{h^3}\int_0^{p_f} dp\ 4\pi p^2 \\
&= \frac{8\pi p_f^3}{3h^3}.
\end{aligned} \tag{1.16}$$

The Fermi momentum p_f is related to be spatial density of fermions by

$$p_f = \left[\frac{3h^3 n(\vec{r})}{8\pi}\right]^{\frac{1}{3}}. \tag{1.17}$$

We can then evaluate the kinetic energy of the ensemble to be

$$\begin{aligned}
E_K &= \int\int d^3\vec{r}d^3\vec{p}\ \nu(\vec{r}, \vec{p})\frac{\vec{p}^2}{2m} \\
&= \int d^3\vec{r}\int dp\ 4\pi p^2\frac{2}{h^3}\eta(p_f^2 - p^2)\frac{p^2}{2m} \\
&= \frac{4\pi}{mh^3}\int d^3\vec{r}\int_0^{p_f} dp\ p^4 \\
&= \frac{4\pi}{mh^3}\int d^3\vec{r}\ \frac{p_f^5}{5}.
\end{aligned} \tag{1.18}$$

Substituting the expression of p_f (1.17), we get

$$E_{\text{kin}} = \frac{3h^2}{10m}(\frac{3}{8\pi})^{\frac{2}{3}}\int d^3\vec{r}\ n^{\frac{5}{3}}. \tag{1.19}$$

This is the Thomas-Fermi approximation of the kinetic energy. Although our calculation is done for $D = 3$, similar arguments can be carried out for lower dimensions. In fact, the explicit form of the functional can be obtained by a simple dimensional analysis. Suppose the energy functional of a D-dimensional system has the form

$$E_{\text{kin}} = C_D\frac{\hbar^2}{m}\int d^D\vec{r}\ n^k. \tag{1.20}$$

The dimension of $\frac{\hbar^2}{m}$ is

$$[\frac{\hbar^2}{m}] = [E][L]^{-2}, \tag{1.21}$$

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the dimension of n is

$$[n] = [L]^{-D}, \tag{1.22}$$

and the dimension of integral is

$$[n^k \mathrm{d}^D \vec{r}] = [L]^{-kD+D}. \tag{1.23}$$

Thus, comparing with (1.21), we get

$$-kD + D = -2,$$
$$k = \frac{D+2}{D}, \tag{1.24}$$

and then we have

$$E_{\mathrm{kin}} = C_D \frac{\hbar^2}{m} \int \mathrm{d}^D \vec{r} \, n^{\frac{D+2}{D}}. \tag{1.25}$$

Here C_D is a dimensionless constant that can be derived using the same method illustrated earlier. For example, for a one-dimensional system

$$C_1 = \frac{\pi^2}{24}. \tag{1.26}$$

and the energy is given by

$$E_{\mathrm{kin}} = \frac{\hbar^2 \pi^2}{24m} \int \mathrm{d}x \, n^3. \tag{1.27}$$

1.5 Bose-Einstein Condensate

In a boson gas, unlike for fermions, there is no restriction on the number of bosons per state. When $T = 0K$, all the bosons occupy the ground state of the system to minimize the total energy. This behaviour of boson gases is called Bose-Einstein condensate.

In a degenerate boson gas, let the N-particle wavefunction be Ψ_g and let a single particle wavefunction be ψ_g, the ground state in Bose-Einstein condensate can then be described as

$$\Psi_g = \psi_g(\vec{r}_1)\psi_g(\vec{r}_2)...\psi_g(\vec{r}_N). \tag{1.28}$$

By (1.2), the ground state density $\rho(\vec{r})$ of the system is

$$\rho(\vec{r}) = N \int \Psi_g^*(\vec{r}, \vec{r}_2, ..., \vec{r}_N)\Psi_g(\vec{r}, \vec{r}_2, ..., \vec{r}_N)\mathrm{d}\vec{r}_2\mathrm{d}\vec{r}_3...\mathrm{d}\vec{r}_N$$
$$= N\psi_g^*\psi_g. \tag{1.29}$$

Hohenberg-Kohn theorem states that the energy of the system is a functional of $\rho(\vec{r})$. According to Schrödinger equation, the total kinetic energy of the system can be calculated

as

$$E_{\text{kin}} = -\frac{\hbar^2}{2m} N \int \mathrm{d}\vec{r}\, \psi_g^* \nabla^2 \psi_g(\vec{r}) = \frac{\hbar^2}{2m} N \int \mathrm{d}\vec{r}\, (\nabla \psi_g)^2. \tag{1.30}$$

Since the ground state wavefunction in a one-dimensional system is always nondegenerate, real, and does not change sign(6), according to (1.29) one can then replace $\sqrt{N}\psi_g$ with $\sqrt{\rho}$ and obtain

$$E_{\text{kin}} = \frac{\hbar^2}{2m} \int \mathrm{d}\vec{r}\, (\nabla \sqrt{\rho})^2. \tag{1.31}$$

1.6 Hohenberg-Kohn Variational Theorem

Much of the use of density functional theory comes from this variational theorem first suggested by Hohenberg and Kohn(3). It makes use of the important property of a ground state, that is, the energy being at its minimum. Since energy is a functional of density function $n(\vec{r})$, any first order variation of density $\delta n(\vec{r})$ must vanish. In a system with a fixed number of particles N, the problem becomes a constrained variational problem with a constraint

$$N = \int \mathrm{d}\vec{r}\, n(\vec{r}). \tag{1.32}$$

The variation of E with respect to $n(\vec{r})$ gives

$$\frac{\delta}{\delta n} \left[E + \mu \left(N - \int \mathrm{d}\vec{r}\, n(\vec{r}) \right) \right] = 0, \tag{1.33}$$

where μ is the Lagrange multiplier, and it is often referred to as chemical potential. Once the explicit form of E in n is known, the ground state density can be immediately obtained by simply solving (3.16). This method will be frequently used in the later chapters.

1.7 Particle Conversion

Density functional theory (DFT) has been frequently applied to ultracold bosonic gas(4; 10), ultracold fermionic gas(2; 1), and sometimes even a mixture of both gases(9). However, none of those investigations has considered the possibility of conversion between two types of particles via chemical reactions. For example, two Lithum-6 atoms can combine through the formation of chemical bond and form a Lithum dimer Li_2, which is a boson. In the present thesis, we aim at the description of such a conversion within DFT.

The paper will be structured as follows. In Chapter 2, we will first look at mixture of bosons and fermions but with no interaction between them (i.e. no conversion will occur), and develop necessary techniques to understand it. In Chapter 3 we will make use of the methods and apply them onto interacting mixtures of bosons and fermions (i.e. conversion occurs). In Chapter 4, we will present the numerical solutions that we obtained.

Chapter 2

Mixtures of Non-Interacting Bosons and Fermions

2.1 Energy Functional

Consider a system containing a mixture of non-interacting fermions and bosons where bosons are formed by two fermions as diatomic molecules. By non-interacting we mean that there is no interaction except the Pauli exclusion principle. Let the number of fermions be N_F and the number of bosons be N_B, respectively. Since there is no interaction between the two types of particles, their numbers are separately conserved,

$$
\begin{aligned}
N_F &= \text{Const.} \\
N_B &= \text{Const.}
\end{aligned}
\tag{2.1}
$$

Let the density function of fermions be $n(\vec{r})$, and let the density function of fermions be $\rho(\vec{r})$, the normalization conditions say,

$$
\begin{aligned}
N_F &= \int \mathrm{d}^D \vec{r}\, n(\vec{r}), \\
N_B &= \int \mathrm{d}^D \vec{r}\, \rho(\vec{r}),
\end{aligned}
\tag{2.2}
$$

where D is the dimension of the system. In the zero-temperature limit, the system reaches its ground state. Hohenberg-Kohn theorem hence implies that the total energy of fermions and bosons are functionals of fermion and boson density functions, respectively. Denoting the total energy of fermions as $E^{(\mathrm{F})}$ and that of bosons as $E^{(\mathrm{B})}$, we have

$$
\begin{aligned}
E^{(\mathrm{F})} &= E^{(\mathrm{F})}[n(\vec{r})], \\
E^{(\mathrm{B})} &= E^{(\mathrm{F})}[\rho(\vec{r})].
\end{aligned}
\tag{2.3}
$$

Generally in a system there are many interaction terms that contribute to the total energy, for instance, the contact energy, the magnetic dipole-dipole interaction, etc. All of these have been studied extensively in the literature(1). Bearing in mind that our objective is to

use density functional theory to understand the effects of the particle conversion process. None of these interactions seems to help us with the understanding, and at the same time, they make the calculation more cumbersome. Hence we will ignore these contributions for the time being.

The total energy of the system comes from four major contributions - the kinetic energy of fermions, the kinetic energy of bosons, the potential energy of fermions and the potential energy of bosons. The kinetic energy of fermions, denoted as $E_{\text{kin}}^{(F)}$, is given by Thomas-Fermi approximation,

$$E_{\text{kin}}^{(F)} = C_D \frac{\hbar^2}{m_F} \int d^D \vec{r}\, n^{\frac{D+2}{D}}, \tag{2.4}$$

where m_F is the mass of the fermion particle and C_D is a dimensionless constant depending on the the number of spatial dimensions of the system. With a trapping potential V_F applied on fermions, the potential energy $E_{\text{pot}}^{(F)}$ becomes

$$E_{\text{pot}}^{(F)} = \int d^D \vec{r}\, V_F(\vec{r}) n(\vec{r}). \tag{2.5}$$

Bosons, in the zero-temperature limit, form the Bose-Einstein condensate. We denote the kinetic energy of bosons as $E_{\text{kin}}^{(B)}$, and it is given by (1.31),

$$E_{\text{kin}}^{(B)} = \frac{\hbar^2}{2m_B} \int d^D \vec{r} \left(\nabla \sqrt{\rho(\vec{r})} \right)^2. \tag{2.6}$$

With an external trapping potential V_B, its potential energy is given by

$$E_{\text{pot}}^{(B)} = \int d^D \vec{r}\, V_B(\vec{r}) \rho(\vec{r}). \tag{2.7}$$

Apart from the energy related to the boson-formation (discussed in the next chapter), the total energy of the system E_{TOT} is known.

$$
\begin{aligned}
E_{\text{TOT}} =& E_{\text{kin}}^{(F)}[n] + E_{\text{pot}}^{(F)}[n] + E_{\text{kin}}^{(B)}[\rho] + E_{\text{pot}}^{(B)}[\rho] \\
=& C_D \frac{\hbar^2}{m_F} \int (d^D \vec{r})\, n^{\frac{D+2}{D}} + \int d^D \vec{r}\, V_F(\vec{r}) n(\vec{r}) \\
& + \frac{\hbar^2}{2m_B} \int d^D \vec{r} \left(\nabla \sqrt{\rho(\vec{r})} \right)^2 + \int d^D \vec{r}\, V_B(\vec{r}) \rho(\vec{r}).
\end{aligned} \tag{2.8}
$$

This energy functional is bounded from below as long as trapping potentials are bounded functions since all other terms are positive. Hence, the ground state of this Hamiltonian exists and can be explored through the method of variation.

2.2   Methods of Variation

When the system is in its ground state, the first order variation of energy vanishes with respect to infinitesimal variations in n and ρ. Under the constraints in (2.1) we have a constrained variational problem,

$$\frac{\delta}{\delta n}\left[E_{\text{TOT}} + \mu_F\left(N_F - \int d^D\vec{r}\, n(\vec{r})\right)\right] = 0,$$
$$\frac{\delta}{\delta\rho}\left[E_{\text{TOT}} + \mu_B\left(N_B - \int d^D\vec{r}\, \rho(\vec{r})\right)\right] = 0, \tag{2.9}$$

where μ_F and μ_B are the Lagrange multipliers resulting from the two constraints in (2.1). We call them the chemical potential of fermions, and the chemical potential of bosons, respectively. From (2.9), we can solve for n.

$$\frac{\delta}{\delta n}\left[E_{\text{TOT}} + \mu_F\left(N_F - \int d^D\vec{r}\, n(\vec{r})\right)\right]$$
$$=\frac{\delta}{\delta n}E_{\text{kin}}^{(\text{F})}[n] + \frac{\delta}{\delta n}E_{\text{pot}}^{(\text{F})}[n] - \mu_F\frac{\delta}{\delta n}\int d^D\vec{r}\, n(\vec{r})$$
$$=C_D\frac{\hbar^2}{m_F}\frac{\delta}{\delta n}\int d^D\vec{r}\, n^{\frac{D+2}{D}} + \frac{\delta}{\delta n}\int d^D\vec{r}\, V_F(\vec{r})n(\vec{r}) - \mu_F \tag{2.10}$$
$$=C_D\frac{\hbar^2}{m_F}\frac{D+2}{D}n^{\frac{2}{D}} + V_F - \mu_F = 0,$$

and we get

$$n = \left[(\mu_F - V_F)\frac{Dm_F}{(D+2)\hbar^2 C_D}\right]_+^{\frac{D}{2}}. \tag{2.11}$$

The "+" subscript indicates that we require $n \geq 0$. The boson density ρ can also be obtained from (2.9). However, instead of using the variation of ρ, it is simpler to vary $\sqrt{\rho}$.

$$\frac{\delta}{\delta\sqrt{\rho}}\left[E_{\text{TOT}} + \mu_B\left(N_B - \int d^D\vec{r}\, \rho(\vec{r})\right)\right]$$
$$=\frac{\delta}{\delta\sqrt{\rho}}E_{\text{kin}}^{(\text{B})}[\rho] + \frac{\delta}{\delta\sqrt{\rho}}E_{\text{pot}}^{(\text{B})}[\rho] - \mu_B\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\, \rho$$
$$=\frac{\hbar^2}{2m_B}\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\,(\nabla\sqrt{\rho})^2 + \frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\, V_B(\vec{r})\rho - \mu_B\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\, \rho \tag{2.12}$$
$$=-\frac{\hbar^2}{2m_B}\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\, \sqrt{\rho}\,\nabla^2\sqrt{\rho} + 2V_B\sqrt{\rho} - 2\mu_B\sqrt{\rho}$$
$$=-\frac{\hbar^2}{2m_B}2\nabla^2\sqrt{\rho} + 2V_B\sqrt{\rho} - 2\mu_B\sqrt{\rho} = 0.$$

It simply reduces to the Schrödinger equation of a single boson particle.

$$-\frac{\hbar^2}{2m_B}\nabla^2\sqrt{\rho} + (V_B - \mu_B)\sqrt{\rho} = 0. \tag{2.13}$$

This result is not surprising since we have not yet included any interaction between fermions and bosons. At $T = 0$ all bosons condensate to the ground state and effectively behave like a giant particle.

2.3 System in a One-Dimensional Harmonic Trap

As an example, we consider a one-dimensional system under harmonic trapping potentials centred at origin with the same frequency ω for bosons and fermions,

$$
\begin{aligned}
V_F &= \frac{1}{2}m_F\omega^2 x^2, \\
V_B &= \frac{1}{2}m_B\omega^2 x^2.
\end{aligned}
\tag{2.14}
$$

Substitute it back to (2.11) and substitute the value for C_1 from (1.26), we find

$$n(\vec{r}) = \left[(\mu_F - \frac{1}{2}m_F\omega^2 x^2)\frac{8m_F}{\hbar^2\pi^2}\right]_+^{\frac{1}{2}}. \tag{2.15}$$

The "+" subscript denotes that when the expression in the bracket is not positive, it is evaluated as zero. In fact, one can see from (2.15), fermions form a centralized packet around origin (see Fig. 2.1) with sharp edges located at

$$x_C = \pm\sqrt{\frac{2\mu_F}{\omega^2}}. \tag{2.16}$$

Next we solve for the density of bosons. Substituting (2.14) back to (2.13) we get

$$-\frac{\hbar^2}{2m_B}\frac{\mathrm{d}^2}{dx^2}\sqrt{\rho} + \frac{1}{2}m_B\omega^2 x^2\sqrt{\rho} = \mu_B\sqrt{\rho}. \tag{2.17}$$

This reduces to the familiar problem of a quantum harmonic oscillator. The system reaches its ground state when

$$\mu_B = \frac{1}{2}\hbar\omega, \tag{2.18}$$

corresponding to a solution of $\sqrt{\rho}$ being

$$\sqrt{\rho} = \sqrt{N_B}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-m_B\omega x^2/2\hbar}. \tag{2.19}$$

Hence the density of bosons is

$$\rho = N_B \left(\frac{m_B \omega}{\pi \hbar}\right)^{\frac{1}{2}} e^{-m_B \omega x^2 / \hbar}. \qquad (2.20)$$

It implies that, at $T = 0$, bosons form a Gaussian distribution centred at origin under a harmonic trap (see Fig. 2.1).
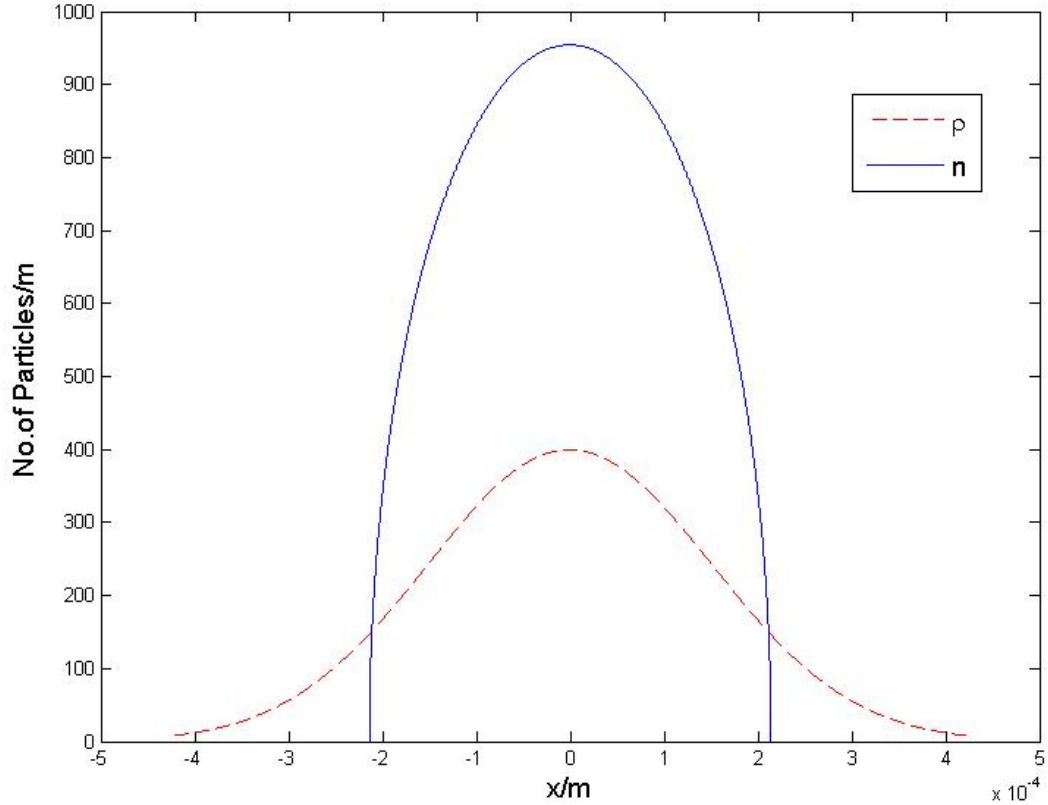

Figure 2.1: Densities of bosons and fermions. The horizontal axis represents the spatial dimension and the vertical axis represents the number of particles per unit length.

2.4 Energy Profile

Having derived the density of fermions $n(\vec{r})$ and the density of bosons $\rho(\vec{r})$, we will next investigate how the energy of the system scales with the increasing particle number. This is particularly important for the theory to be used by experimentalists.

There are two types of particles in the system existing independently of each other, thus

we can investigate them separately. First we look at the total energy of bosons,

$$E_{\text{TOT}}^{(B)} = -\frac{\hbar^2}{2m_B} \int dx \sqrt{\rho} \frac{d^2}{dx^2} \sqrt{\rho} + \int dx \frac{1}{2} m_B \omega^2 x^2 \rho$$
$$= \int dx \sqrt{\rho} \left(-\frac{\hbar^2}{2m_B} \frac{d^2}{dx^2} \sqrt{\rho} + \frac{1}{2} m_B \omega^2 x^2 \sqrt{\rho} \right). \tag{2.21}$$

According to (2.17) and (2.18), we have

$$E_{\text{TOT}}^{(B)} = \int dx \sqrt{\rho} \mu_B \sqrt{\rho}$$
$$= \mu_B N_B = \frac{1}{2} N_B \hbar \omega. \tag{2.22}$$

The energy of bosons scales linearly with the number of bosons. Next we look at how the energy of fermions scales with the number of fermions. From (2.15) we have

$$N_F = \int dx\, n(x)$$
$$= \int dx \left[(\mu_F - \frac{1}{2} m_F \omega^2 x^2) \frac{8m_F}{\hbar^2 \pi^2} \right]_+^{\frac{1}{2}}. \tag{2.23}$$

Define x_c and γ such that

$$\mu_F \equiv \frac{1}{2} m_F \omega^2 x_c^2, \tag{2.24}$$
$$\gamma \equiv \frac{x}{x_c}. \tag{2.25}$$

The integral becomes

$$N_F = \int_0^{x_c} dx \left[\frac{1}{2} m_F \omega^2 (x_c^2 - x^2) \frac{8m_F}{\hbar^2 \pi^2} \right]^{\frac{1}{2}}$$
$$= \int_0^1 d\gamma\, x_c^2 \left[\frac{1}{2} m_F \omega^2 (1 - \gamma^2) \frac{8m_F}{\hbar^2 \pi^2} \right]^{\frac{1}{2}}$$
$$= \frac{2m_F \omega}{\hbar \pi} x_c^2 \int_0^1 d\gamma\, (1 - \gamma^2)^{\frac{1}{2}} \tag{2.26}$$
$$= \frac{2m_F \omega}{\hbar \pi} x_c^2 \frac{\pi}{4}$$
$$= \frac{m_F \omega}{2\hbar} x_c^2.$$

The kinetic energy of fermions is given by

$$
\begin{aligned}
E_{\text{kin}}^{(F)} &= \frac{\hbar^2 \pi^2}{24 m_F} \int \mathrm{d}x \, n^3 \\
&= \frac{\hbar^2 \pi^2}{24 m_F} \int_0^{x_c} \mathrm{d}x \, \left[\frac{1}{2} m_F \omega^2 (x_c^2 - x^2) \frac{8 m_F}{\hbar^2 \pi^2} \right]^{\frac{3}{2}} \\
&= \frac{\hbar^2 \pi^2}{24 m_F} \int_0^1 \mathrm{d}\gamma \, x_c \left[\frac{1}{2} m_F \omega^2 x_c^2 (1 - \gamma^2) \frac{8 m_F}{\hbar^2 \pi^2} \right]^{\frac{3}{2}} \\
&= \frac{\hbar^2 \pi^2}{24 m_F} x_c^4 \left(\frac{2 m_F \omega}{\hbar \pi} \right)^3 \int_0^1 \mathrm{d}\gamma \, (1 - \gamma^2)^{\frac{3}{2}} \\
&= \frac{m_F^2 \omega^3 x_c^4}{16 \hbar},
\end{aligned}
\tag{2.27}
$$

and the potential energy of fermions is

$$
\begin{aligned}
E_{\text{pot}}^{(F)} &= \int \mathrm{d}x \, V_F n(x) \\
&= \frac{1}{2} m_F \omega^2 \int_0^{x_c} \mathrm{d}x \, x^2 \left[\frac{1}{2} m_F \omega^2 (x_c^2 - x^2) \frac{8 m_F}{\hbar^2 \pi^2} \right]^{\frac{1}{2}} \\
&= \frac{1}{2} m_F \omega^2 x_c^3 \frac{2 m_F \omega x_c}{\hbar \pi} \int_0^1 \mathrm{d}\gamma \, \gamma^2 (1 - \gamma^2)^{\frac{1}{2}} \\
&= \frac{m_F^2 \omega^3 x_c^4}{\hbar \pi} \frac{\pi}{16} \\
&= \frac{m_F^2 \omega^3 x_c^4}{16 \hbar} = E_{\text{kin}}^{(F)}.
\end{aligned}
\tag{2.28}
$$

The potential energy of fermions turns out to be exactly the same as its kinetic energy, as expected from the virial theorem. Therefore, the total energy of fermions is given by two times of its kinetic energy

$$
E_{\text{TOT}}^{(F)} = 2 E_{\text{kin}}^{(F)} = \frac{m_F^2 \omega^3 x_c^4}{8 \hbar}
\tag{2.29}
$$

Comparing with (2.26) we find that

$$
E_{\text{TOT}}^{(F)} = \frac{1}{4} N_F^2 \hbar \omega
\tag{2.30}
$$

The total energy of fermions grow quadratically with the number of fermions in the system. Therefore the total energy of the system scales like

$$
E_{\text{TOT}} = N_B \hbar \omega + \frac{1}{4} N_F^2 \hbar \omega
\tag{2.31}
$$

We identify that two scaling laws exist in the system - one is linear with the number of bosons; one is quadratic with the number of fermions. We will call them the "principle scales" of the system. The method presented here relies on direct integrations. However, as we will soon see, in a more complicated system, direct integrations are no longer

practical. We will need to develop an alternative method to identify the principle scales of the system.

2.5   Scale Transformation

We consider a scale transformation on the densities of fermions and bosons.

$$
\begin{aligned}
n(x) &\to \lambda^{\alpha+1} n(\lambda x), \\
\rho(x) &\to \lambda^{\alpha+1} \rho(\lambda x).
\end{aligned}
\tag{2.32}
$$

This transformation is specially designed such that the number of particles scales with λ^α (for $\lambda \neq 0$). For example, after the scale transformation the number of fermions becomes

$$
N_F \to \int \mathrm{d}x \, \lambda^{\alpha+1} n(\lambda x) = \lambda^\alpha \int \mathrm{d}(\lambda x) \, n(\lambda x) = \lambda^\alpha N_F.
\tag{2.33}
$$

Similarly,

$$
N_B \to \lambda^\alpha N_B.
\tag{2.34}
$$

Various energy terms also scale accordingly under the transformation. Since fermions and bosons are non-interacting at this stage, we will talk about them separately. The kinetic energy of fermions scales according to

$$
\begin{aligned}
E_{\mathrm{kin}}^{(\mathrm{F})} &\to C_1 \frac{\hbar^2}{m_F} \int \mathrm{d}x \, \lambda^{3\alpha+3} [n(\lambda x)]^3 \\
&= C_1 \frac{\hbar^2}{m_F} \lambda^{3\alpha+2} \int \mathrm{d}(\lambda x) \, [n(\lambda x)]^3 \\
&= \lambda^{3\alpha+2} E_{\mathrm{kin}}^{(\mathrm{F})}.
\end{aligned}
\tag{2.35}
$$

Its potential energy scales like

$$
\begin{aligned}
E_{\mathrm{pot}}^{(\mathrm{F})} &\to \int \mathrm{d}x \, \frac{1}{2} m_F \omega^2 x^2 \lambda^{\alpha+1} n(\lambda x) \\
&= \lambda^{\alpha-2} \int \mathrm{d}(\lambda x) \, \frac{1}{2} m_F \omega^2 (\lambda x)^2 n(\lambda x) \\
&= \lambda^{\alpha-2} E_{\mathrm{pot}}^{(\mathrm{F})}.
\end{aligned}
\tag{2.36}
$$

Hence, the total energy of fermions becomes

$$
E_{\mathrm{TOT}}^{(\mathrm{F})} = \lambda^{3\alpha+2} E_{\mathrm{kin}}^{(\mathrm{F})} + \lambda^{\alpha-2} E_{\mathrm{pot}}^{(\mathrm{F})},
\tag{2.37}
$$

and the system reaches its ground state when $\lambda = 1$. If the number of fermions is fixed, any first order change of the total energy resulting from a variation of λ will vanish at $\lambda = 1$. For a given potential N_F entirely determines the total energy of the ground state.

It follows that

$$\delta N_F \frac{\partial E_{\text{TOT}}^{(\text{F})}}{\partial N_F} = \delta \left(\lambda^{3\alpha+2} E_{\text{kin}}^{(\text{F})} + \lambda^{\alpha-2} E_{\text{pot}}^{(\text{F})} \right). \tag{2.38}$$

Taking derivative of λ on both sides, we get

$$\frac{dN_F}{d\lambda}\Big|_{\lambda=1} \frac{\partial E_{\text{TOT}}^{(\text{F})}}{\partial N_F} = \frac{d\lambda^{3\alpha+2}}{d\lambda}\Big|_{\lambda=1} E_{\text{kin}}^{(\text{F})} + \frac{d\lambda^{\alpha-2}}{d\lambda}\Big|_{\lambda=1} E_{\text{pot}}^{(\text{F})}. \tag{2.39}$$

Evaluating the derivatives, and setting $\lambda = 1$ we get

$$\alpha N_F \frac{\partial E_{\text{TOT}}^{(\text{F})}}{\partial N_F} = (3\alpha + 2) E_{\text{kin}}^{(\text{F})} + (\alpha - 2) E_{\text{pot}}^{(\text{F})}. \tag{2.40}$$

We have the freedom to choose α. Let $\alpha = 0$,

$$0 = 2E_{\text{kin}}^{(\text{F})} - 2E_{\text{pot}}^{(\text{F})}. \tag{2.41}$$

One immediately finds that the kinetic energy of fermions is the same as the potential energy of fermions, a result that we have observed earlier. Next let $\alpha = 2$, we get

$$N_F \frac{\partial E_{\text{TOT}}^{(\text{F})}}{\partial N_F} = 4E_{\text{kin}}^{(\text{F})}. \tag{2.42}$$

Define a "power operator" P_x of the form

$$P_x \equiv x \frac{\partial}{\partial x}, \tag{2.43}$$

it effectively picks up the power of x in its operand as an eigenvalue. For example,

$$(x \frac{\partial}{\partial x}) x^\alpha = \alpha \, x^\alpha. \tag{2.44}$$

From equations (2.4-2.7), we know

$$\begin{aligned} P_\hbar E_{\text{TOT}}^{(\text{F})} &= 2E_{\text{kin}}^{(\text{F})} \\ P_\omega E_{\text{TOT}}^{(\text{F})} &= 2E_{\text{pot}}^{(\text{F})} \\ P_{m_F} E_{\text{TOT}}^{(\text{F})} &= -E_{\text{kin}}^{(\text{F})} + E_{\text{pot}}^{(\text{F})}. \end{aligned} \tag{2.45}$$

Comparing with (2.41), we have

$$\begin{aligned} P_{m_F} E_{\text{TOT}}^{(\text{F})} &= 0, \\ P_\hbar E_{\text{TOT}}^{(\text{F})} &= P_\omega E_{\text{TOT}}^{(\text{F})}. \end{aligned} \tag{2.46}$$

We find that $E_{\text{TOT}}^{(\text{F})}$ is independent of m_F and its powers in $\hbar$ are always the same as its powers in ω, implying the energy to be a function of $\hbar\omega$. Comparing with (2.42),

$$2P_\hbar E_{\text{TOT}}^{(\text{F})} = P_{N_F} E_{\text{TOT}}^{(\text{F})} = 2P_\omega E_{\text{TOT}}^{(\text{F})}. \tag{2.47}$$

Its powers in N_F are twice of its powers in $\hbar$, yielding the total energy of fermions to be a function of $N_F^2 \hbar \omega$, a result that we have observed before through direct integration. One can carry out the same argument for boson and easily get $E_{\mathrm{TOT}}^{(\mathrm{B})}$ being a function of $N_B \hbar \omega$. This method does not require integrations and is capable of deriving the principle scales of the system, hence we will use it to study the principle scales of interacting system in the next chapter.

Chapter 3

Mixture of Interacting Bosons and Fermions

3.1 Energy Functional

The system becomes more interesting when we allow fermions to form diatomic bosons. Then, one immediately finds that the number of fermions and the number of bosons are no longer conserved separately. Instead, a unique combination of the two particle numbers is kept as a constant,

$$\frac{1}{2}N_F + N_B \equiv N = \text{Const.}. \tag{3.1}$$

We now introduce an interaction term to the total energy of the system to represent the interaction between two particles. (2.8) then has an additional term E_I,

$$E_{\text{TOT}} = E_{\text{kin}}^{(\text{F})}[n] + E_{\text{pot}}^{(\text{F})}[n] + E_{\text{kin}}^{(\text{B})}[\rho] + E_{\text{pot}}^{(\text{B})}[\rho] + E_I[n, \rho]. \tag{3.2}$$

However, to our knowledge there is no literature on the explicit form of this additional interaction energy functional. We propose that it is of the following form,

$$E_I[n, \rho] = -\int \mathrm{d}^D \vec{r} \, B\rho + A \int \mathrm{d}^D \vec{r} \sqrt{\rho} n. \tag{3.3}$$

The first term in (3.3) is well justifiable. We know that each boson is a composition of two fermions via chemical bond, and the energy associated with each bond is given by the binding energy B. The binding energy density is therefore product of binding energy and the density of bosons. The second term in (3.3), instead, has no classical analogue. Its justification lies in the formalism of second quantization of quantum mechanics which motivates the coupling of $\sqrt{\rho}$ and n.

In second quantization approach, instead of dealing directly with wavefunctions one deals with creation and annihilation operators. We can create a boson using boson creation operator $\hat{b}^\dagger$

$$\hat{b}^\dagger |N_B\rangle = \text{const.}|N_B + 1\rangle. \tag{3.4}$$

The number in the ket indicates the number of particles in the system. Similarly one can remove a fermion from the system using the fermion annihilation operator $\hat{f}$.

$$\hat{f}|N_F\rangle = \text{const.}|N_F - 1\rangle. \tag{3.5}$$

Consider a process where two fermions are destroyed and one boson is created, it can be represented as

$$\hat{b}^\dagger \hat{f}\hat{f}|N_B, N_F\rangle = \text{const.}|N_B + 1, N_F - 2\rangle. \tag{3.6}$$

Since such an interpretation corresponds, in Schrödingers picture, to an overlap of two fermions and one boson wavefunctions, it is suggestive that the interaction process can be approximated by

$$\hat{b}^\dagger \hat{f}\hat{f} \longrightarrow \psi_b \psi_f \psi_f, \tag{3.7}$$

where ψ_b is the wavefunction of boson and ψ_f is the wavefunction of a fermion. Hence, the energy term is proportional to the product of the three wavefunctions with coupling constant A. This is, of course, not meant to be a rigorous justification, but it is suggestive enough that one should make an attempt to compute its consequence. This term will be referred to as the overlapping term or overlapping effect in the later sections.

With the energy functional known, one may want to directly apply variational theorem to get the densities of fermions and bosons. However, this is not advisable at this stage because the system may not even have a ground state energy (i.e. not bounded from below). As a first step, one has to check the boundedness of the Hamiltonian.

3.2   Boundedness of Hamiltonian

First let us take a closer look at the Hamiltonian of the system as in (3.2),

$$\begin{aligned}
E_{\text{TOT}} &= E_{\text{kin}}^{(\text{F})}[n] + E_{\text{pot}}^{(\text{F})}[n] + E_{\text{kin}}^{(\text{B})}[\rho] + E_{\text{pot}}^{(\text{B})}[\rho] + E_I[n, \rho] \\
&= C_D \frac{\hbar^2}{m_F} \int \mathrm{d}^D \vec{r}\, n^{\frac{D+2}{D}} + \int \mathrm{d}^D \vec{r}\, V(\vec{r}) n(\vec{r}) \\
&\quad + \frac{\hbar^2}{2m_B} \int \mathrm{d}^D \vec{r} \left(\nabla \sqrt{\rho(\vec{r})}\right)^2 + \int \mathrm{d}^D \vec{r}\, V_B(\vec{r}) \rho(\vec{r}) \\
&\quad - \int \mathrm{d}^D \vec{r}\, B\rho + A \int \mathrm{d}^D \vec{r}\, \sqrt{\rho}\, n.
\end{aligned} \tag{3.8}$$

Evidently only terms that are negative contribute to possible unboundedness, and one can easily see that term $-\int \mathrm{d}^D \vec{r}\, B\rho$ is bounded from below.

$$-\int \mathrm{d}^D \vec{r}\, B\rho = -BN_B \geq -BN. \tag{3.9}$$

Hence, for bounded potential energies (then, without loss of generality, $V_F, V_B \geq 0$) the only term that matters is the conversion energy when $A < 0$.

$$A \int \mathrm{d}^D \vec{r} \sqrt{\rho} n. \tag{3.10}$$

In fact one can also show that this term is bounded from below for $D = 1$. Let $A' = -A > 0$ and consider the combination of two terms as follows and we can claim that

$$E_{\mathrm{TOT}} > C_1 \frac{\hbar^2}{m_F} \int \mathrm{d}x \, n^3 - A' \int \mathrm{d}x \, \sqrt{\rho} n - BN. \tag{3.11}$$

Using Cauchy-Schwarz inequality on the second term,

$$-A' \int \mathrm{d}x \, \sqrt{\rho} n \geq -A' \left(\int \mathrm{d}x \, \rho \right)^{\frac{1}{2}} \left(\int \mathrm{d}x \, n^2 \right)^{\frac{1}{2}}$$
$$\geq -A' \sqrt{N} \left(\int \mathrm{d}x \, n^2 \right)^{\frac{1}{2}}. \tag{3.12}$$

We can apply Cauchy-Schwarz inequality on it again and get

$$-A' \sqrt{N} \left(\int \mathrm{d}x \, n^2 \right)^{\frac{1}{2}} \geq -A' \sqrt{N} \left[\left(\int \mathrm{d}x \, n \right)^{\frac{1}{2}} \left(\int \mathrm{d}x \, n^3 \right)^{\frac{1}{2}} \right]^{\frac{1}{2}}$$
$$\geq -A' N^{\frac{3}{4}} \left(\int \mathrm{d}x \, n^3 \right)^{\frac{1}{4}}. \tag{3.13}$$

Substitute (3.13) back to (3.11) and let

$$\kappa \equiv \left(\int \mathrm{d}x \, n^3 \right)^{\frac{1}{4}}, \tag{3.14}$$

we get

$$E_{\mathrm{TOT}} \geq C_1 \frac{\hbar^2}{m_F} \kappa^4 - A' N^{\frac{3}{4}} \kappa - BN, \tag{3.15}$$

and the right hand side is clearly a polynomial of κ and bounded from below. Hence we have shown that the ground state energy of such Hamiltonian exists and one can now apply Hohenberg-Kohn variational theorem.

3.3 Methods of Variation

We know that when the system resides in the ground state, the total energy is stationary with respect to variations of fermion and boson densities. With the new constraint given

by (3.1), instead of having two different Lagrange multipliers, we have only one.

$$\frac{\delta}{\delta n}\left\{E_{\text{TOT}} + \mu\left[N - \int d^D\vec{r}\left(\frac{1}{2}n+\rho\right)\right]\right\} = 0,$$
$$\frac{\delta}{\delta\rho}\left\{E_{\text{TOT}} + \mu\left[N - \int d^D\vec{r}\left(\frac{1}{2}n+\rho\right)\right]\right\} = 0. \tag{3.16}$$

Here μ is the new Lagrange multiplier. Solving it using the same method as non-interacting case, we get the density of fermions.

$$\frac{\delta}{\delta n}\left[E_{\text{TOT}} + \mu\left(N - \int d^D\vec{r}(\frac{1}{2}n+\rho)\right)\right]$$
$$= C_D\frac{\hbar^2}{m_F}\frac{\delta}{\delta n}\int d^D\vec{r}\, n^{\frac{D+2}{D}} + \frac{\delta}{\delta n}\int d^D\vec{r}\, V_F(\vec{r})n(\vec{r})$$
$$+ A\frac{\delta}{\delta n}\int d^D\vec{r}\,\sqrt{\rho}\, n - \frac{1}{2}\mu$$
$$= C_D\frac{\hbar^2}{m_F}\frac{D+2}{D}n^{\frac{2}{D}} + V_F + A\sqrt{\rho} - \frac{1}{2}\mu = 0, \tag{3.17}$$

yielding

$$n = \left[(\frac{1}{2}\mu - V_F - A\sqrt{\rho})\frac{Dm_F}{(D+2)\hbar^2 C_D}\right]^{\frac{D}{2}}_+. \tag{3.18}$$

Similarly we get the density of bosons by variation w.r.t. $\sqrt{\rho}$.

$$\frac{\delta}{\delta\sqrt{\rho}}\left[E_{\text{TOT}} + \mu\left(N - \int d^D\vec{r}(\frac{1}{2}n+\rho)\right)\right]$$
$$= \frac{\hbar^2}{2m_B}\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\,(\nabla\sqrt{\rho})^2 + \frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\, V_B(\vec{r})\rho$$
$$- B\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\,\rho + A\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\,\sqrt{\rho}\, n - \mu\frac{\delta}{\delta\sqrt{\rho}}\int d^D\vec{r}\,\rho$$
$$= -\frac{\hbar^2}{2m_B}2\nabla^2\sqrt{\rho} + 2V_B\sqrt{\rho} - 2B\sqrt{\rho} + A\, n - 2\mu\sqrt{\rho} = 0, \tag{3.19}$$

yielding

$$-\frac{\hbar^2}{2m_B}\nabla^2\sqrt{\rho} + (V_B - B - \mu)\sqrt{\rho} = -\frac{1}{2}An. \tag{3.20}$$

The introduction of boson-fermion interaction effectively adds an inhomogeneity to (3.20) and at the same time, it modifies the trapping potential that fermions see into an effective potential,

$$V_{\text{eff}} = V_F + A\sqrt{\rho}. \tag{3.21}$$

The effective chemical potentials of fermions and bosons, in comparison with (2.11)-(2.13), are related to the combined Lagrange multiplier via

$$
\begin{aligned}
\mu_{\text{eff}}^{\text{(F)}} &= \frac{1}{2}\mu, \\
\mu_{\text{eff}}^{\text{(B)}} &= \mu + B, \\
2\mu_{\text{eff}}^{\text{(F)}} &= \mu_{\text{eff}}^{\text{(B)}} - B.
\end{aligned}
\tag{3.22}
$$

If we adjust $A \to 0$, we will effectively reduce to the non-interacting problem with chemical potentials of bosons and fermions connected in a specific way as governed by (3.22).

3.4   System in a One-Dimensional Harmonic Trap

As what we did for non-interacting system, we will again focus on a one-dimensional system (i.e. $D = 1$) to simplify the problem. External harmonic trapping potentials are applied to both bosons and fermions

$$
\begin{aligned}
V_F &= \frac{1}{2}m_F\omega^2 x^2, \\
V_B &= \frac{1}{2}m_B\omega^2 x^2.
\end{aligned}
\tag{3.23}
$$

Substituting it back to (3.18-3.20) we get

$$
n = \left[(\frac{1}{2}\mu - \frac{1}{2}m_F\omega^2 x^2 - A\sqrt{\rho})\frac{32m_F}{h^2}\right]^{\frac{1}{2}},
\tag{3.24}
$$

$$
-\frac{\hbar^2}{2m_B}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sqrt{\rho} + (\frac{1}{2}m_B\omega^2 x^2 - B - \mu)\sqrt{\rho} = -\frac{1}{2}An.
\tag{3.25}
$$

Clearly (3.25) is a nonlinear differential equation with no obvious analytic solutions. To extract some useful information from this set of equations, we consider two cases according to the value of A that we choose.

3.4.1   No Overlapping Effect

We first investigate what will happen when $A = 0$. We call it "no overlapping" because when $A = 0$, the overlapping term in the total energy functional no longer contributes. (3.24-3.25) reduce to

$$
n = \left[(\frac{1}{2}\mu - \frac{1}{2}m_F\omega^2 x^2)\frac{32m_F}{h^2}\right]^{\frac{1}{2}}_+
\tag{3.26}
$$

$$
-\frac{\hbar^2}{2m_B}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sqrt{\rho} + (\frac{1}{2}m_B\omega^2 x^2 - B - \mu)\sqrt{\rho} = 0
\tag{3.27}
$$

It seems that it reproduces the non-interacting problem discussed earlier, but in fact this is not the case. Instead of having two independent chemical potentials μ_F and μ_B, now there is only one chemical potential μ connecting the two types of particles. In other words, the particles can still inter-convert but just that the conversion is "free of charge" in a way that it does not cost any extra energy other than the binding energy B. To solve for the densities, one identifies that (3.27) is simply the familiar one dimensional harmonic oscillator equation with a ground state yielding

$$\mu = \frac{1}{2}\hbar\omega - B. \tag{3.28}$$

When $B \geq \frac{1}{2}\hbar\omega$, the chemical potential becomes non-positive, which makes fermions distribution vanish because the density function $n(x)$ has to be strictly positive. Hence all fermions will form bosons and condensate to the ground state of bosons. When $B \leq \frac{1}{2}\hbar\omega$, the fermion distribution becomes non-vanishing.

$$n(x) = \left[(\frac{1}{4}\hbar\omega - \frac{1}{2}B - \frac{1}{2}m_F\omega^2 x^2)\frac{32m_F}{h^2} \right]^{\frac{1}{2}}. \tag{3.29}$$

x_c, defined to be the boundary of fermion distribution, is then related to B via

$$\frac{1}{2}m_F\omega^2 x_c^2 = \frac{1}{4}\hbar\omega - \frac{1}{2}B \implies x_c = \sqrt{\frac{\hbar\omega - 2B}{2m_F\omega^2}}. \tag{3.30}$$

Therefore, as the binding energy gets larger, the support of the fermion density gradually decreases and eventually vanishes when $B = \frac{1}{2}\hbar\omega$. For fixed B the total number of fermions remains fixed when the total particle number N, as defined in (3.1), varies. However this does not apply to bosons since (3.27) is a linear differential equation whose solution is only determined up to an multiplicative constant. The latter is only determined by invoking normalization condition. Therefore given a fixed N, we can then uniquely determine the boson density to be

$$\begin{aligned} \sqrt{\rho} &= \sqrt{N_B}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m_B\omega x^2/2\hbar} \\ &= \sqrt{N - \frac{1}{2}N_F}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m_B\omega x^2/2\hbar}. \end{aligned} \tag{3.31}$$

This indicates when we add in new particles to the system, all of them become bosons although there is a non-vanishing fermion density. This is plausible as fermions cannot occupy the same state. As the fermion number increases it gradually requires more energy and becomes energetically unfavorable to be fermions. This trend is illustrated in Fig. 3.1. It shows that the number of fermions remains at a constant while the number of bosons increases linearly as the total number of particle increases.
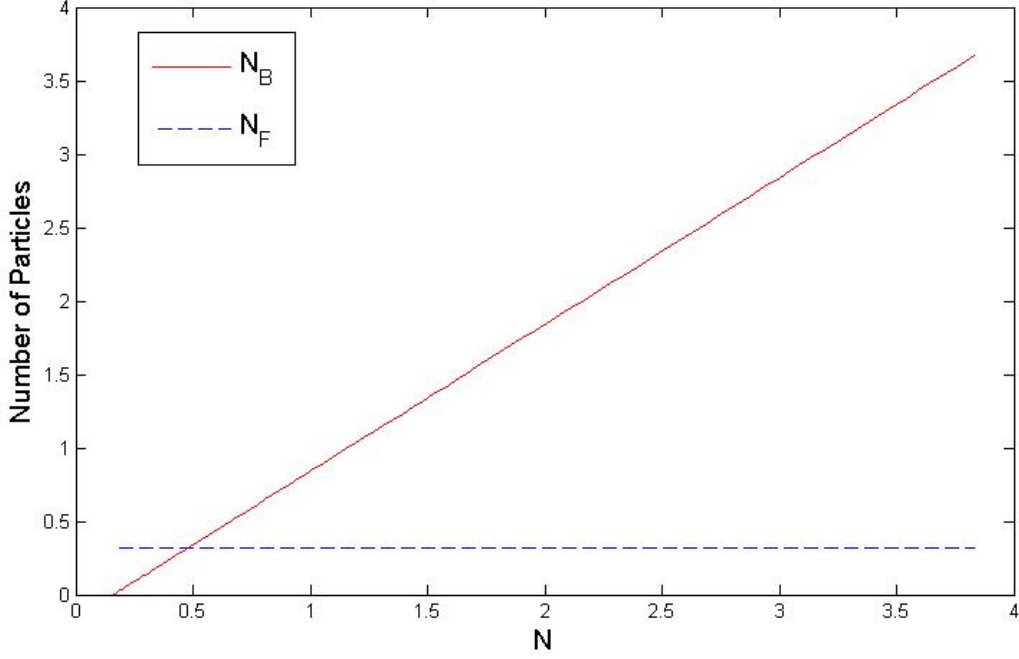
Figure 3.1: N_F and N_B against N. The solid line represents the number of bosons in the system, and the dashed line represents the number of fermions.

3.4.2 Weak Overlapping Effect

Next we investigate the case when A is not zero but a very small number (i.e. $|A| << 1$) such that the density of bosons remains approximately unaffected. We call the non-interacting solutions obtained in (3.29) and (3.31) as n_0 and ψ_0, and we will calculate the first order corrections to the fermion density. Let the first order corrected fermion density be n_1, we have

$$n_1 = \left[(\frac{1}{2}\mu - \frac{1}{2}m_F\omega^2 x^2 - A\psi_0)\frac{32m_F}{h^2} \right]^{\frac{1}{2}}. \tag{3.32}$$

Using (3.31) one gets

$$n_1 = \left[(\frac{1}{2}\mu - \frac{1}{2}m_F\omega^2 x^2 - A\sqrt{N_B}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m_B\omega x^2/2\hbar})\frac{32m_F}{h^2} \right]^{\frac{1}{2}}. \tag{3.33}$$

The fermions are effectively exposed to a potential

$$V_{\text{eff}}(x) = \frac{1}{2}m_F\omega^2 x^2 + A\sqrt{N_B}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m_B\omega x^2/2\hbar}. \tag{3.34}$$

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After a superposing with a Gaussian function, the effective potential, instead of having zero potential at origin, now has a slightly positive potential with magnitude

$$E_0 = A\sqrt{N_B}\left(\frac{m_B\omega}{\pi\hbar}\right)^{\frac{1}{4}}.$$

(3.35)

As a consequence, fermions no longer peak at the origin, but instead, they form two peaks at some distance from the origin. We find the location of peaks by requiring

$$\frac{\mathrm{d}}{\mathrm{d}x}V_{\mathrm{eff}} = 0,$$

(3.36)

yielding

$$x = \pm\sqrt{\frac{2\hbar}{m_B\omega}\ln\left(\frac{m_B E_0}{m_F\hbar\omega}\right)}.$$

(3.37)

In the case when the overlapping effect is not weak, we can only rely on numerical tools to get approximate solutions of the densities (discussed in the next chapter). However, if we are only concerned about how the total energy of system scales with the particle number, we can apply the scale transformation to find the principle scales of the system.

3.5 Scale Transformation

We apply the same scale transformation to the densities of fermions and bosons

$$\begin{aligned}
n(x) &\to \lambda^{\alpha+1}n(\lambda x),\\
\rho(x) &\to \lambda^{\alpha+1}\rho(\lambda x).
\end{aligned}$$

(3.38)

The conserved quantity N scales according to

$$N = N_B + \frac{1}{2}N_F \to \lambda^\alpha N.$$

(3.39)

We have discussed in Chapter 2 that the kinetic energy and potential energy of fermions scale by

$$\begin{aligned}
E_{\mathrm{kin}}^{(\mathrm{F})} &\to \lambda^{3\alpha+2}E_{\mathrm{kin}}^{(\mathrm{F})},\\
E_{\mathrm{pot}}^{(\mathrm{F})} &\to \lambda^{\alpha-2}E_{\mathrm{pot}}^{(\mathrm{F})}.
\end{aligned}$$

(3.40)

By the same method we can find how other terms in the total energy scale,

$$\begin{aligned}
E_{\mathrm{kin}}^{(\mathrm{B})} &\to \lambda^{\alpha+2}E_{\mathrm{kin}}^{(\mathrm{B})},\\
E_{\mathrm{pot}}^{(\mathrm{B})} &\to \lambda^{\alpha-2}E_{\mathrm{pot}}^{(\mathrm{B})}.
\end{aligned}$$

(3.41)

Define E_B and E_A to be

$$E_B = -\int \mathrm{d}x\, B\rho,$$

$$E_A = \int \mathrm{d}x\, A\sqrt{\rho}n, \tag{3.42}$$

and they scale according to

$$E_B \to \lambda^\alpha E_B,$$

$$E_A \to \lambda^{\frac{3}{2}\alpha+\frac{1}{2}} E_A. \tag{3.43}$$

When $\lambda = 1$, variational principle requires that the first order changes of E_{TOT} must be entirely resulted from the first order changes in the particle number. We call E_{TOT} as E for now. We have

$$\alpha N \frac{\partial E}{\partial N} = (3\alpha + 2)E_K^F + (\alpha + 2)E_K^B + (\alpha - 2)E_P^F$$

$$+ (\alpha - 2)E_P^B + \alpha E_B + (\frac{3}{2}\alpha + \frac{1}{2})E_A. \tag{3.44}$$

Let $\alpha = 0$ we get

$$0 = 2E_K^F + 2E_K^B - 2E_P^F - 2E_P^B + \frac{1}{2}E_A. \tag{3.45}$$

Let $\alpha = 2$ we get

$$N\frac{\partial E}{\partial N} = 4E_K^F + 2E_K^B + E_B + \frac{7}{4}E_A. \tag{3.46}$$

making use of the power operators defined in (2.43), we have

$$P_N E = 4E_K^F + 2E_K^B + E_B + \frac{7}{4}E_A;$$

$$P_\hbar E = 2E_K^F + 2E_K^B;$$

$$P_{\omega_F} E = 2E_P^F;$$

$$P_{\omega_B} E = 2E_P^B;$$

$$P_{m_F} E = -E_K^F + E_P^F;$$

$$P_{m_B} E = -E_K^B + E_P^B;$$

$$P_B E = E_B;$$

$$P_A E = E_A. \tag{3.47}$$

Note that we have distinguished the two frequencies in the trapping potentials and the masses of the two types of particles in order to attain wider generality. The number of variables to keep track doubles and hence we need a systematic treatment. System of linear equations is often efficiently solved via linear algebra techniques, so we propose the following linear algebra procedures to solve this problem. First we collect the linear

dependence of power operators on energy terms in a matrix form,

$$\begin{pmatrix} 4 & 2 & 0 & 0 & 1 & \frac{7}{4} \\ 2 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 2 & 2 & -2 & -2 & 0 & \frac{1}{2} \end{pmatrix}. \tag{3.48}$$

The rows represent P_N, $P_\hbar$, P_{ω_F}, P_{ω_B}, P_{m_F}, P_{m_B}, P_B, P_A as in (4.3) and the last row represents the "null vector" given in (4.2). The columns represent E_K^F, E_K^B, E_P^F, E_P^B, E_B and E_A, respectively. In order to find the inter-dependence of different power operators, we need to find the nullspace of the transpose of the matrix. It turns out that the nullspace is spanned by three vectors v_1, v_2 and v_3, writing them in their row forms

$$\begin{aligned} v_1 &= \left(0, -1, 1, 1, 0, 0, -\frac{1}{2}, 1, 1\right), \\ v_2 &= \left(1, -1, -1, 0, 2, 0, -1, -\frac{7}{4}, 0\right), \\ v_3 &= \left(0, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 1, 1, 0, 0, 0\right). \end{aligned} \tag{3.49}$$

Each of these vectors represents an inter-dependence among the power operators. Note that the last element of each vector does not matter since it represents a "null vector", we simply ignore them. To eliminate the redundancies in the equations we form a new matrix from these three row vectors and compute the reduced row-echelon form of the matrix,

$$\begin{pmatrix} 1 & 0 & -2 & -1 & 0 & -2 & -1 & -\frac{3}{4} \\ 0 & 1 & -1 & -1 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & -\frac{1}{4} \end{pmatrix}. \tag{3.50}$$

Each row of this matrix can be translated into an equation. For example, the first row represents

$$P_N E = -2P_{\omega_F}E - P_{\omega_B}E - 2P_{m_B}E - P_B E - \frac{3}{4}P_A E. \tag{3.51}$$

An easy way to solve it is, instead of writing out the equations in their full-forms, we multiply -1 to all the elements and replace the first non-zero element of each row by a "$*$". We get

$$\begin{pmatrix} * & 0 & 2 & 1 & 0 & 2 & 1 & \frac{3}{4} \\ & * & 1 & 1 & 0 & 0 & 0 & -\frac{1}{2} \\ & & & * & -1 & 0 & \frac{1}{4} \end{pmatrix} \tag{3.52}$$

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Now we read the matrix column-by-column. Each number in a column represents the power of the "∗" variable that goes with current variable. For example, column 3 represents ω_F, the column is read as ω_F goes with N^2 and $\hbar^1$. By this methods, we get that the total energy of the system depends on five specific combinations of the parameters in the system,

$$N\hbar\omega_B, \ \ N^2\hbar\omega_F, \ \ N^2\frac{m_B}{m_F}, \ \ NB, \ \ N^{\frac{3}{4}}A\hbar^{-\frac{1}{2}}m_F^{\frac{1}{4}}. \tag{3.53}$$

Hence, the full expression of the energy must be a function of these five parameters.

Chapter 4

Numerical Approach

4.1 Approach

We now consider (3.24 - 3.25) numerically. First, define a critical distance x_c such that

$$\mu = m_F \omega^2 x_c^2. \tag{4.1}$$

Then we know for sure that for $A \geq 0$ and $x > x_c$, the fermion density vanishes, and the density of bosons reduces to a second-order linear differential equation,

$$-\frac{\hbar^2}{2m_B}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sqrt{\rho} + (\frac{1}{2}m_B\omega^2 x^2 - B - \mu)\sqrt{\rho} = 0. \tag{4.2}$$

If we define

$$
\begin{aligned}
k &\equiv \frac{m_B\omega}{\hbar}, \\
z &\equiv \sqrt{2k}\,x, \\
a &\equiv -\frac{\mu + B}{\hbar\omega},
\end{aligned}
$$

(4.2) becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\sqrt{\rho} - (\frac{1}{4}z^2 + a)\sqrt{\rho} = 0. \tag{4.3}$$

Differential equations of this form have well known solutions in terms of the parabolic cylinder functions, and the two independent solutions of (4.3) are given by $U(a, z)$ and $V(a, z)$(7). The explicit forms of the two functions are not relevant in what follows, it is their asymptotic behaviours for large z that are important. If $z \to \infty$,

$$U(a, z) \rightarrow e^{-\frac{z^2}{4}}z^{-a-\frac{1}{2}}, \tag{4.4}$$

$$V(a, z) \rightarrow \sqrt{\frac{2}{\pi}}e^{\frac{z^2}{4}}z^{a-\frac{1}{2}}, \tag{4.5}$$

one finds that $U(a, z)$ decays to zero for large z whereas $V(a, z)$ increases exponentially. Hence, the solution $\sqrt{\rho}$ in the region $x > x_c$ can only be

$$\sqrt{\rho} = fU(a, z), \tag{4.6}$$

where f is an arbitrary multiplicative constant which will be referred to as the "shooting parameter". We can now choose any point x_0 in the region $x > x_c$, substitute it into (4.6) along with an arbitrary choice of shooting parameters f and start numerical integration of (3.25) from $x = x_0$ towards $x = -x_0$. Among the results obtained, we first pick the solutions that are strictly positive, since $\sqrt{\rho}$ cannot be negative, and then we select those that are even, since the system is symmetric about the origin.

4.2   Density Profile

Following the procedures described in Section 4.1, we identify solutions of different kinds as we vary the chemical potential μ. Fig. 4.1 shows a solution with one fermion peak centred at the origin and two boson peaks located at some distance away from the origin.
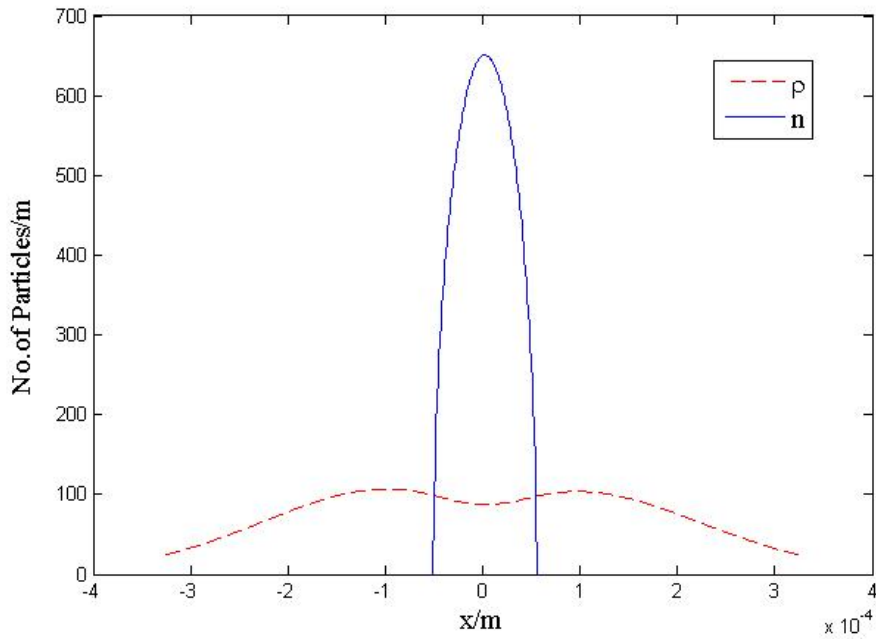

Figure 4.1: A density plot of fermions and bosons. The solid line represents the density of fermions and the dashed line represents the density of bosons.

Fig. 4.2 shows a different kind of solution which has two fermion peaks located at some distance away from origin and a Gaussian-like boson distribution centred at the origin.
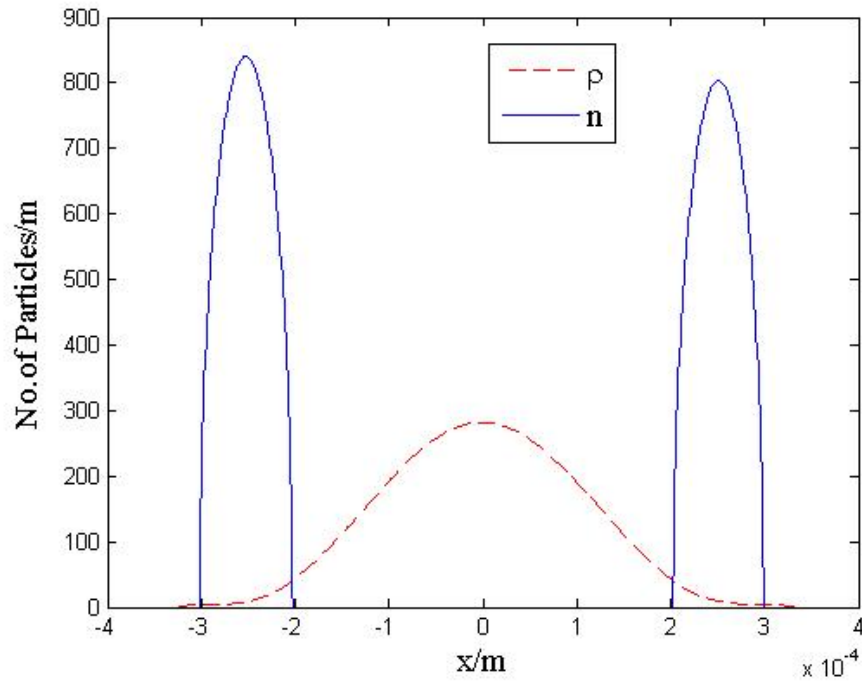
Figure 4.2: A density plot of fermions and bosons. The solid line represents the density of fermions and the dashed line represents the density of bosons.

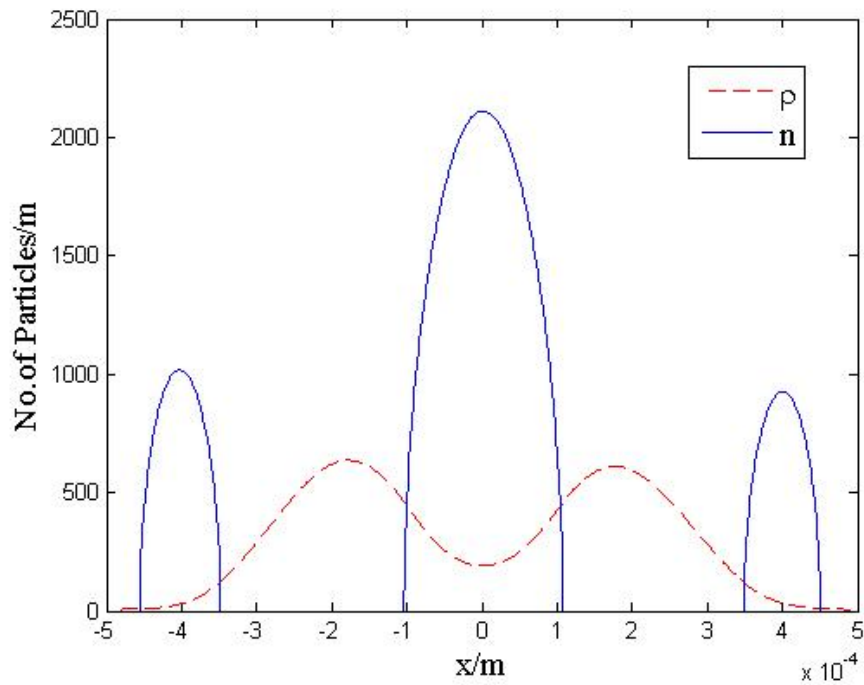There are also solutions with three fermion peaks, as shown in Fig. 4.3

Figure 4.3: A density plot of fermions and bosons. The solid line represents the density of fermions and the dashed line represents the density of bosons.

An alternating pattern of bosons and fermions is observed in all solutions obtained, which shows that the bosons and fermions behave, to some extend, "mutually exclusive". This is in fact not unexpected. When the density of fermions overlaps significantly with the density of bosons, the overlapping term in the total energy increases (since we set $A > 0$) and becomes energetically unfavorable. Hence, it is expected that the densities of bosons and fermions will be spatially "exclusive" in the ground state.

Each solution that we obtained is associated with two parameters - the shooting parameter f and the chemical potential μ. In the next section we will explore how these two parameters are related.

4.3   Shooting Parameters

If we collect all the "successful" shooting parameters f and plot them against their corresponding x_c - a quantity that is related to μ through (4.1). We get the graph shown in Fig. 4.4.
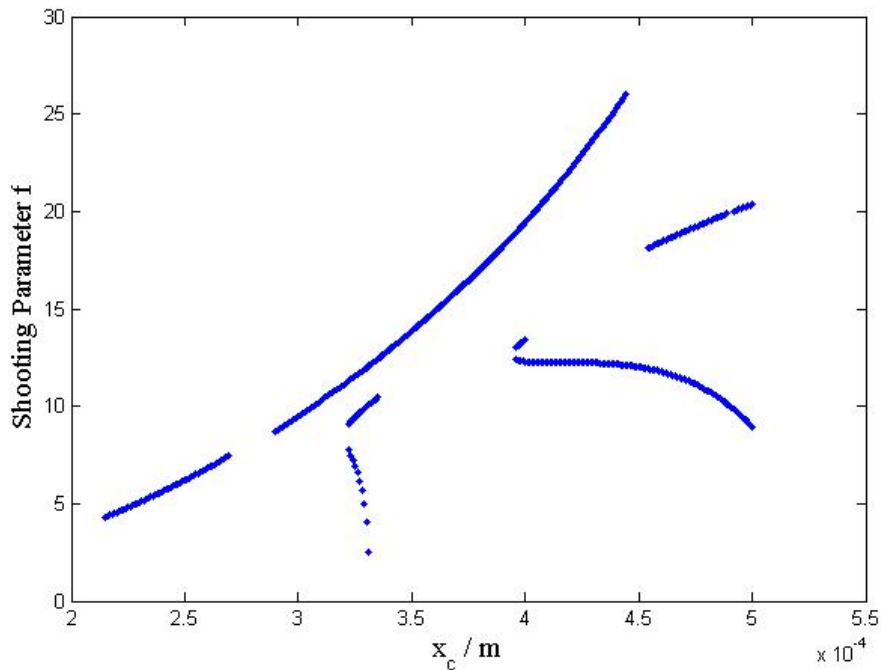

Figure 4.4: Shooting parameter f against x_c

It shows that each chemical potential does not correspond to a unique shooting parameter f since the plot consists of many different branches. The missing points along the branches are likely to be resulted from numerical errors. At $x_c \approx 3.3 \times 10^{-4}$m, the system emerges from one branch to three branches. We will take a closer look at this region and examine how the densities differ along different branches. As shown in Fig. 4.5, the two lower branches seem to originate from a single point, and the lowest branch disappears after
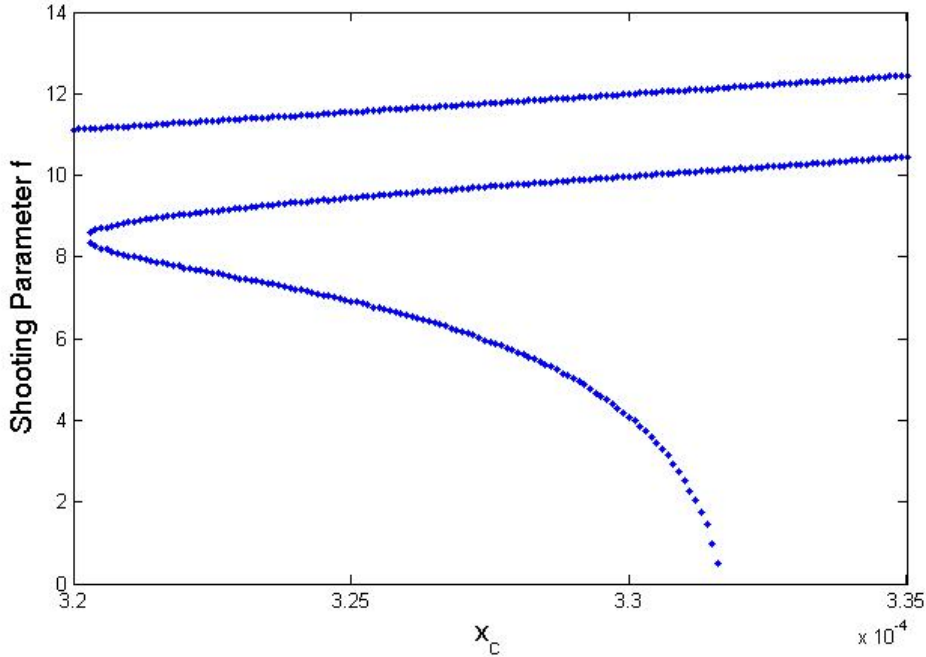
reaching $f = 0$.

Figure 4.5: Shooting parameter f against x_c. A closer plot at $x_c \approx 3.3 \times 10^{-4}$m

If we take shooting parameters from three different branches and plot their densities, we will find that they all correspond to different kinds of densities. For example, the top branch in Fig. 4.5 corresponds to densities of the same kind as in Fig. 4.1 (i.e. one single fermion peak located at the origin), while the lowest branch has densities of the same kind as in Fig. 4.2 (i.e. two fermion peaks located at some distance away from the origin).

However, not all of the branches represent the true ground state of the physical system because different branches are likely to have different total energies, and also from our experience in quantum mechanics, the more nodes there are in the system the higher the total energy is. To verify this we have to study how the total energy of the system changes with the chemical potential.

4.4 Energy Profiles

Knowing the densities of fermions and bosons, one can easily calculate the total energy of the system. The shooting parameters are plotted against x_c in the nearby region of $x_c = 3.3 \times 10^{-4}$m (where branching occurs) and are shown in Fig. 4.6(a). The corresponding total energies E_{TOT} are then plotted against N, the number of particles, and are shown in Fig. 4.6(b).
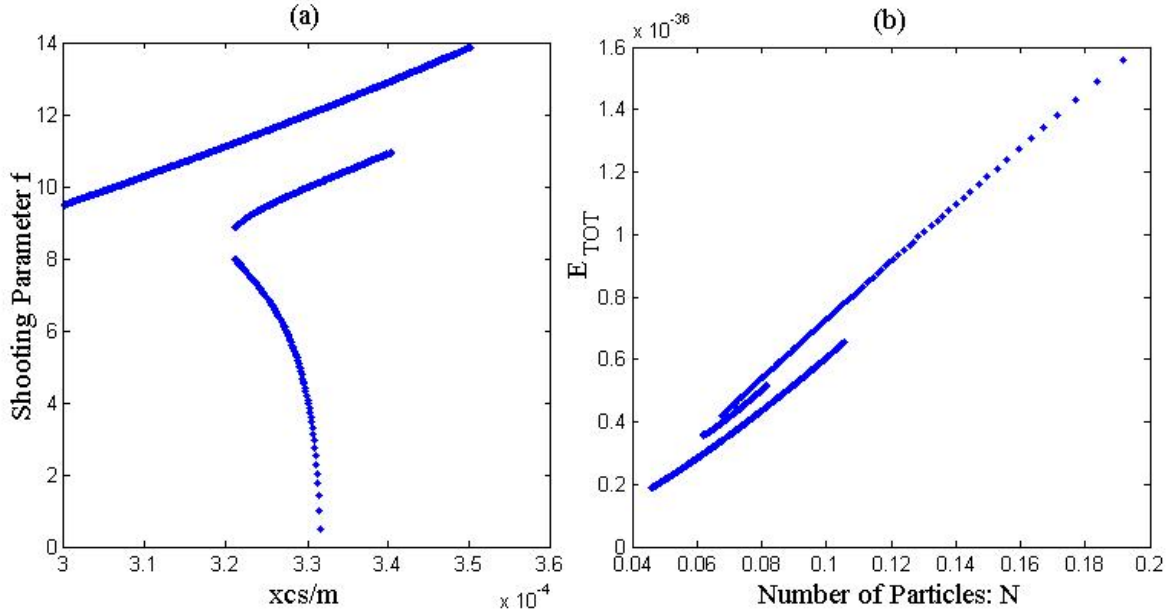
Figure 4.6: f against x_c (left), E_{TOT} against N (right)

The reason that E_{TOT} is plotted against N instead of x_c is that the chemical potential is only an auxiliary parameter that we set to minimize the total energy, and it is not a physical quantity, whereas the total number of particles is a physical quantity that can be measured directly in experiments. It can be easily seen that the three branches of in Fig. 4.6(a) also correspond to three branches in Fig. 4.6(b). Clearly, the lowest branch in Fig. 4.6(b) represents the ground state energies curve , and it turns out that this branch corresponds to densities of the same kind as Fig. 4.1 (with a single fermion peak at the origin). This matches our expectation that the densities with fewer nodes are likely to have a lower total energy. The ground state of the system, based on the numerical results that we have gathered so far, always seem to correspond to a single fermion peak at the origin with two boson peaks at some distance away from the origin (See Fig. 4.1). This formation of a boson shell that encloses fermions in its center can be experimentally verified.

Chapter 5

Future Works

The present work explored a simple physical system - a mixture of inter-converting bosons and fermions. To illustrate how density functional theory sheds light on the problem we made some physically motivated simplifications. First of all, the system is constrained in one-dimensional space, which, although greatly simplified the calculation, also to some extend, may have contributed to the difficulty of the problem. One easily see that when we change the system to two-dimensional, the differential equation for bosons becomes an ordinary linear differential equation w.r.t $\sqrt{\rho}$ (3.18, 3.20). This is certainly worth exploring.

We have, in fact, not justified so far why we restrict the parameter A to be positive. We have proven in a one-dimensional system that the Hamiltonian is bounded from below even if $A < 0$. The dynamics can be even richer when $A < 0$, but its physical implication may need a careful re-examination because physically it implies a decrease in energy, hence a large stability, when bosons and fermions are heavily packed together. There are many other contributions to the total energy of the system, for example, the contact potential and dipole-dipole interaction. We ignored these terms for simplicity and in order to prevent them from interfering our study on conversion process. However, most certainly these terms do matter in practice. Any experiments that attempt to verify the results presented should take into consideration on the side effects from the other energy terms.

As we mentioned before, the ansatz that we proposed to be responsible for the particle conversion process is more of an educated guess than a derived result. Experimental attempts will greatly help to validate this approach, and variation of energy with respect to particles is a good starting point of experimental testing.

Chapter 6

Conclusion

Fermions to bosons conversion, a process that has rarely been previously studied in the context of density functional theory, is explored both analytically and numerically in the paper. The calculation is primarily based on an ansatz that is proposed to account for the interaction energy during particle conversion. It is of form

$$E_I[n, \rho] = -\int \mathrm{d}^D \vec{r} \, B\rho + A \int \mathrm{d}^D \vec{r} \, \sqrt{\rho} n \tag{6.1}$$

With the introduction of this term, the dynamics becomes surprisingly rich including decentralization of particles, formation of shells and possible phase transitions as number of particles changes. Without doubt the density functional approach provides a unique insight into the dynamics of particle exchange process. It not only derives the spatial density distributions of bosons and fermions, but also shed light on how energy scales as the number of particles varies, an important property that experimentalists may find interesting.

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