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M.Sc. THESIS IN ENGINEERING OF PHYSICS

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INVESTIGATION OF BOSE-EINSTEIN CONDENSATION FOR DIFFERENT POTENTIALS

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Investigation of Bose-Einstein Condensation for Different Potentials

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Supervisor

Prof. Dr. Hayriye TÜTÜNCÜLER

by

Mustafa KILIN

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ABSTRACT

INVESTIGATION OF BOSE-EINSTEIN CONDENSATION FOR DIFFERENT POTENTIALS

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In this study, we analyze the ground state properties of the condensate for different potentials. These are harmonic oscillator potential which is solved in literature anharmonic and morse potentials which have not been investigated before.

This thesis has two main parts. In the first part, ground state solutions for different potentials are obtained. We have used the Runge-Kutta method to solve time-independent Gross-Pitaevskii equation for determination of the ground state wave function of system.

The second part involves the solution of time-independent Gross-Pitaevskii equation for the same potentials by using Thomas-Fermi Approximation. This approximation method is valid in systems that have very large number of atoms in the condensate.

Key words: Bose-Einstein condensation, Gross-Pitaevskii equation, Thomas-Fermi Approximation.

ÖZET

FARKLI POTANSİYELLER İÇİN BOSE-EINSTEIN YOĞUŞMASININ İNCELENMESİ

KILIN, Mustafa
Yüksek Lisans Tezi, Fizik Mühendisliği Bölümü,
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Bu çalışmada, farklı potansiyeller için yoğuşmanın taban durum özelliklerini analiz ettik. Bu potansiyeller literatür de çözümü olan harmonik potansiyel ve daha önce incelenmemiş olan anharmonik ve morse potansiyelleridir.

Bu tez iki ana kısımdan oluşmaktadır. İlk bölümde taban durum çözümleri farklı potansiyeller içinde elde edildi. Sistemin taban durumu dalga fonksiyonun belirlenmesinde, zamandan bağımsız Gross-Pitaevskii denkleminin çözümü için Runge-Kutta metodunu kullandık.

Tezin ikinci parçası, Thomas-Fermi yaklaşımını kullanarak aynı potansiyeller için zamandan bağımsız Gross-Pitaevskii denkleminin çözümünü içermektedir. Bu yaklaşım yoğuşmadaki atom sayısının fazla olduğu sistemlerde geçerlidir.

Anahtar Kelimeler: Bose-Einstein yoğunlaşması, Gross-Pitaevskii denklemi, Thomas-Fermi Yaklaşımı

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Å	Angstrom
λ	de Broglie wave length
λ_{TD}	Thermal de Broglie wave length
h	Planck constant
k_B	Boltzmann constant
T_c	Critical temperature
$f^0(\epsilon_v)$	Bose distribution function
ϵ_v	Energy in state v
μ	Chemical potential
ζ	Fugacity
$H(p,q)$	Hamiltonian in phase space
$G(\epsilon)$	Number of micro state
$g(\epsilon)$	Density of state
$\Gamma(\alpha)$	Gama function
$\zeta(\alpha)$	Riemann-Zeta function
$\overline{\omega}$	Geometric mean of angular frequency
N	Number of particles
N_0	Number of particle in condensate state

N_{ex}	Number of particles in excited state
$\widehat{H}$	Hamiltonian operator of the N interacting bosons
$\widehat{\Psi}(r)$	Annihilation boson operator
$\widehat{\Psi}^{\dagger}(r)$	Creation boson operator
$\psi_{\alpha}(r)$	Condensate wave function
$\phi_{\alpha}(r)$	Single particle wave function
a_{α}	Annihilation boson operator in Fock space
$a_{\alpha}{}^{\dagger}$	Creation boson operator in Fock space
$\delta_{\alpha,\beta}$	Kronecher delta function
g	S-wave atom-atom interacting potential
$n(r)$	Condensate density
$V_{ext}(r)$	External potential
a	Scattering length

CHAPTER 1

GENERAL INTRODUCTION

Bose-Einstein condensation is phase transition in atomic systems consist of bosons gas at very low temperatures. Bosons are particles with integer spin. The wave function for a system of identical bosons is symmetric under interchange of any two particles. Unlike fermions which have half-odd integer spin and anti-symmetric wave function, bosons may occupy the same single particle state. That is bosons do not obey Pauli Exclusion Principle but fermions obey this principle.

Bose-Einstein condensation which is a long-lasting problem in physics in 1901 [1] began with the idea that it should be discrete radiation emitted from the heated object by Planck but the first foundations of Bose-Einstein condensation was put forward by S. N. Bose and A. Einstein. In 1924 [2] Bose was the definition of the photon statistics. Upon this in 1925 [3] Einstein showed that gas of boson consist of particles that do not interact with each other occupy single particle quantum state. These two theories by combining, have submitted at absolute zero temperature Bose systems transformed into a new state of matter. It is called Bose-Einstein Condensation.

One of the most important features of Bose systems, they are non-homogeneous and are finite dimensional systems. Two body interactions play an important role in non-homogeneous systems. Many body correlation effects between bosons increases the amount of exited atoms located outside of condensation in an interactive Bose system.

Following the work of Bose (1924) [2] and Einstein (1925) [3], Fritz London suggested the connection between the super-fluidity of liquid ^{4}He and Bose-Einstein condensation in 1938 [4]. Liquid ^{4}He is good candidate for Bose-Einstein

Condensation and it has played a good role in the development of physical concepts. However, the interaction between helium atoms is strong, and this reduces the number of atoms in the zero-momentum state at low temperatures. Therefore it is difficult to evaluate directly the occupancy of the zero momentum state.

Pioneering theoretical studies on the behavior of interacting bosons gas was initiated by Bogoliubov in 1947 [5]. Bogoliubov has developed a perturbation expansion for the case where number of atoms excited state and weak interactive atoms became low density, can be neglected.

In 1957 J. Barden, L. N. Cooper and J. R. Schrieffer are published an article associated with super-conductivity. In their theory molecules system has properties similar to that of a charged Bose-Einstein gas, including a Meissner effect and a critical temperature of condensation [6,7].

In 1959 [8] Hecht argued that spin-polarized hydrogen would be a good applicant for a weakly interacting Bose gas. The attractive interaction between electronic spins aligned two hydrogen atoms was guessed to be so weak. Hecht’s paper get little attention, but his conclusions was approved Stwalley and Nosanow [9] in 1976, when improved information about interaction between two hydrogen atoms with their electronic spins fixed was usable.

In 1976 regarding spin-polarized hydrogen made some experiments was followed by several experiments. In 1980 J. T. M. Walraven-Isaac F. Silvera [10], in 1982 Hardy W. N. and his friends [11], 1984 Greytak T. J. and his friends [12] first cooled the hydrogen atoms in a refrigerator, then trapped by magnetic field and farther cooled by evaporating. They came very close to Bose-Einstein condensation.

In1986 [13] laser cooling and in 1987 [14] magneto-optical trapping were advanced to cool and traps atoms. Laser based methods are convenient for alkali atoms and can excite their optical transitions. Laser methods can cool them to very low temperatures due to their good internal energy level structure.

Since Bose-Einstein condensation has been predicted in 1924-1925, it has become a major topic of interest. After this prediction 70 years and after many experimental attempts, in 1995 Bose-Einstein condensation was observed as a result of a series of experiments with weak interaction alkali atoms. This condensate was initially observed in Joint Institute for Laboratory Astrophysics (JILA) by Anderson and his friends in 1995 with rubidium [15], later this experiment was obtained in Massachusetts Institute of Technology (MIT) by Davis and his friends in 1995 with sodium [16], in the same year Bose-Einstein condensation was observed again with lithium by Bradley and his friends [17]. In this experiment atoms have been confined with magnetic traps and cooled to low temperatures which become order of micro-Kelvin. After than magnetic traps have been shut down, atoms began to spread and optical operations have been applied to atoms. Under the certain temperature in the velocity distribution around zero speed a peak has observed and it has been become a proof of Bose-Einstein condensation. Success of these experimental provides unique facility for exploring quantum phenomena on macroscopic scale. Bose-Einstein condensation is a very important event, it is considered that Bose-Einstein condensation will be provide basis important development both in the area of technology and scientific.

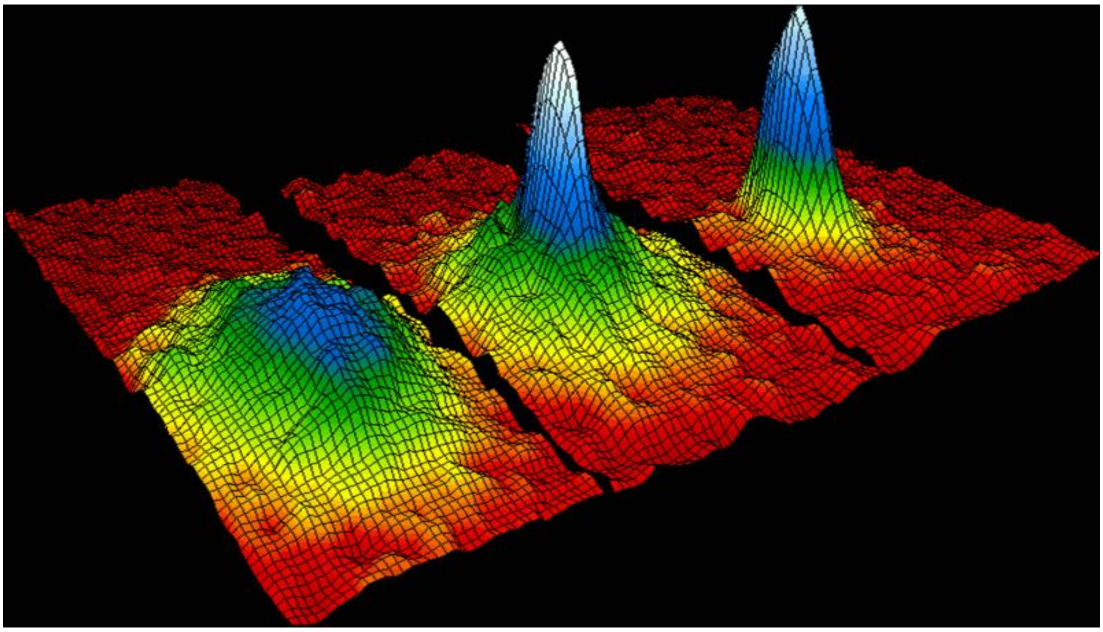

Figure 1.1 Rubidium atoms velocity distribution [15].

This figure is rubidium atoms velocity distribution image in the experiment made by Anderson and his friends in 1995. The left figure is image of the gas at above the condensation temperatures, the center figure is image of the gas just after the appearance of the condensate, and the right figure is image of pure condensate after evaporation is made. Colors denote numbers of atoms in the velocity distribution. Red one is minimum and white one is maximum.

In 1995 in the experiment made with weak interactive alkali atoms become low density (^{87}Rb, ^{23}Na and ^{7}Li [15] [16] [17]), occurrence of the atomic cloud to single quantum state is observed. In later years Bose-Einstein condensation has been observed with ^{1}H (Fried and his friends) [18] in 1998, ^{14}K (Monduga and his friends) [19] in 2001, semi-stable ^{4}He (Santos and his friends) [20] in 2001, ^{133}Cs (Weber and his friends) [21] in 2003 and in the Li_2 molecules (Jochim and his friends) [22] in 2002.

Before we start the theoretical literature survey of the Bose-Einstein condensation, briefly we can give some information about experimental survey of the studies at low temperature.

When all physical particles lose kinetic energies in accordance with traditional theory, as a result of this, they slow down by losing their speed. Similarly atoms or atomic mixtures slow down when they lose their kinetic energy. One of the simplest ways to slow down particles reduces momentum of the particles. If it is provided that the momentum of a moving particle release, it will slow down by losing energy. Cooling is a process realized by lowering the temperature. There is no physical response of the temperature for a single particle. The temperature which is a form of energy has a physical mean for a particle system and kinetic energy of this system is a parametric measurement of temperature. Therefore, to reduce the kinetic energy of particle in the system corresponds to lower the temperature of the system that is cooling the system. On the other hand trapping is known that their motion restrict towards the all freedom degrees of atoms. The aim of the studies in this area is to cool the order of the micro-Kelvin or below the temperature of particles by preventing conversion of atomic gases to a solid or liquid [9].

In 1908, the Dutch physicist Heike Kammerligh Onnes achieved helium liquefaction at -269°C (4.2 K) temperature. Until this time, by using liquid nitrogen was reached to 77 K temperature. As known from the kinetic theory, motion, rotation and translation of atoms and molecules stop at 0 K (-273.15°C). In this very low temperature matters begin to show different feature. The first of these features, “below the specific temperature, resistance of certain substance decreases to zero” discovered in 1911 by Kammerligh Onnes that is, it is superconductivity. Generally, some good non-conductive materials have been observed to be super conductive at liquid helium temperature. In the nucleus of isotope He formed fluid which has two protons and neutrons show a property like frictionless flow (super-fluidity) at 2.18 K temperature. But, in the atomic boson gases phase transition predicted by Bose and Einstein require much lower temperature.

In order to descend to low temperatures in the range of micro-Kelvin, laser light has been used (light amplification by stimulated emission of radiation). On this subject, the aim of first studies would rather the idea of cooling than slow down atoms to increase the accuracy of spectroscopic studies [10].

Laser shows several differences compared with normal light. Normal light includes different frequency ranges as an electro-magnetic wave and just as it shows the spherical expansion so laser is coherent and monochromatic. Laser can be controlled and have high density to examine some features of physical systems since 1960.

First time in 1968 Letokhow suggested that atomic trapping with electromagnetic waves can be accomplished. After than 1970 Ashkin calculated what would happen light pressure in an atom where a light beam became in resonance. On this subject, in years maintained different studies firstly Hansch and Schawlow (1975) showed that laser light can be used for cooling of atoms. Physical reason of the slowdown of atoms can be explained that atoms absorb photon from the outside. Because photon absorption is to change the momentum of the atoms when conditions are satisfied, it is possible to slow down motion of atom by using this method. If three dimension laser systems are used, atom can be cooled in the direction of all degrees of freedom. Alkali atoms are quite convenient to laser-based methods because optical transition of they can be excited with available laser and they have appropriate internal energy level in order to cool low temperature.

The low temperature which is obtained by using laser cooling technique is limited with energy of a single photon. As a result, the number of atom in the volume λ_{DB}^3 is very smaller than number of atom required for BEC. In the 1980 the first successful experiment achieved with laser cooling method was carried out by Balykin and Letokhow in Moscow and in same year by Phillips and his friends in the Gaithersburg. Immediately after, at below limits prescribed by earlier theories of

Phillips, Chı and Cohen-Tnnoudji, the cooling method was developed. After cooling with the laser has been achieved, Chu and his study friends in the Bell laboratory was trapped atoms cooled by optical traps. Because optical traps are too small and weak, physically in order to collect a sufficient number of atoms good traps had been required. After that, magnetic-traps were used but in 1986 more original magneto-optical tapping method suggested by Dalibard. Beside at that time this technique was developed by Chu and Pritchard's groups. Until that day, magneto-optic traps which were developed, has been best method and so both cooling and trapping of atoms has been achieved as quite safe [11].

In the non-homogeneous systems, Gross-Pitaevskii equation which gives the experimental results correspond to the data is derived by Gross in 1961 [23] [24] and Pitaevskii in 1961 [25] independently of each other and by using different techniques. GP equation gives a very good mean-field description of condensation at low density. In 1995 following the experimental observation of Bose-Einstein condensation, interested in Bose-Einstein condensation has increased both experimental and theoretical. In later years, while the solution of GP equation have been made, take into account the different potentials, numerical methods, dimensions and geometries theoretical studies have been carried, in 1995 Mark Edwards and K. Burnett [26] solved numerical solution of non-linear Schrödinger equation for small samples of trapped neutral atoms, in 1999 A. Gammal and his friends [27] improved numerical approach, in 2000 Sadhan K. Adhikari [28] solved 2-D GP equation and in 2009 Cheng Luo [29] brought a new model Bose-Einstein condensation with GP equation.

In this thesis, up to now experimental and theoretical studies gave inspiration us, following these studies, Bose -Einstein condensation system have been examined under different potentials and with different solution methods. Before the calculations, in chapter 2, definition of Bose-Einstein condensation have been described, also the behavior of an ideal Bose gas and thermodynamic properties at low temperatures is surveyed in the non-interacting systems. This chapter also forms the theoretical foundations of Bose-Einstein condensation. Furthermore it is examined behavior of the critical temperatures of atoms which began condensation.

In chapter 3 a system formed gas of bosons is considered in presence of interactions at low temperatures. These systems are rare and there are weak interactions in there which is defined by Gross-Pitaevskii equation which describes the structure and distribution of condensation. This equation was derived independently by Gross 1961 [23] [24] and Pitaevskii 1961 [25]. For bosons which are trapped by external potential, ground state solutions have been determined by different methods and approaches.

In chapter 4, the numerically solution of the time-independet Gross-Pitaevskii equation are defined, for harmonic, anharmonic and morse potentials and after that condensate probability density of these solutions are drowned versus the boundary of potentials. Secondly, these graphs are propagated for different value of chemical potentials. After these calculations are done, for solution of Gross-Pitaevskii equation a approximation is applied it is called Thomas-Fermi approximation, for this approximation the graph of condensate probability density are drowned. Finally in this chapter, for same potentials, chemical potential versus the graph of number of particles are drowned.

Finally in chapter 5 we define the conclusion for our all calculations which are made in chapter 4.

CHAPTER 2

THEORETICAL FOUNDATIONS
OF BOSE-EINSTEIN CONDENSATION

2.1 WHAT IS THE BOSE-EINSTEIN CONDENSATION

In order to understand the Bose-Einstein Condensation, primarily the physical properties of classical and quantum gases should be research closely. It is known that, gas forms of molecules and atomic particles that move freely in space. Gases can be examined in to two class like that classical and quantum gases. At high enough temperatures the behavior of all the gases is defined as classical.

The average distance between gas molecules is relatively large and they just interact weakly. At any time only a very smart part of the collection of molecules interact with each other through collisions. Under normal conditions, average distances between molecules are about the order of 30 A^0 (10^{-10} m) and it is 10 times the diameter of a molecules.

When potential energy of interaction between molecules of a gas system was compared with the kinetic energy of motion between molecules of it, if potential energy is smaller than kinetic energy, the system is called ideal gas. At the high enough temperatures such gas represented distribution function and owned free energy obtained by using Maxwell-Boltzman statistics and this statistical mechanic is called classical approximation [30].

When it goes to the low temperatures, quantum effects be based on particles cannot be distinguished from each other begin to appears.

In quantum mechanics there is a de Broglie wavelength accompanied a particle with p momentum and it is defined as [31]

$$\lambda = \frac{h}{p} \tag{2.1}$$

In a system occurring from *N* particles, let’s take average momentum *p* according to equipartition theorem, at temperature *T* in the gas system the average energy of each particle is;

$$\in = \frac{p^2}{2m} = \frac{3}{2} k_B T \tag{2.2}$$

$$\frac{(h/\lambda)^2}{2m} = \frac{3}{2} k_B T \tag{2.3}$$

$$\lambda = \left(\frac{h^2}{3mk_B T} \right)^{1/2} \tag{2.4}$$

In Eq. (2.4) λ denotes de Broglie wavelength. In here, because an approximation calculation is made, de Broglie wavelength can be taken to equal to the λ_{TD} thermal de Broglie wavelength [32].

$$\lambda_{TD} = \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{1/2} \tag{2.5}$$

In Eq. (2.5) λ_{TD} thermal de Broglie wavelength is a boundary condition which describes the classical limit and quantum limit. When temperature *T* decreases in there, λ_{TD} thermal de Broglie wavelength increases. In the quantum mechanics the minimum amplitude of the wave packets which represents particles close to λ_{TD} thermal de Broglie wavelength. When distance between two particles with decreasing the temperature is going to come λ_{TD} thermal de Broglie wavelength which represents the particles, quantum effects has began to appear.

There is a critical temperature T_c which began appearing these effects. The particle density of a gas that is the number of particles per unit volume is represented by number n, the volume of surrounding a particle is $1/n$ and average distance between particles is $1/n^{1/3}$ (that is volume between particles). So the criterion which is searched and compared with the thermal de Broglie wavelength and average distance between particles is given by;

Classical case $$\lambda \ll \frac{1}{n^{1/3}} \rightarrow n\lambda^3 \ll 1 \tag{2.6}$$

Quantum case $$\lambda \gg \frac{1}{n^{1/3}} \rightarrow n\lambda^3 \gg 1 \tag{2.7}$$

In the volume of $n\lambda^3 = 1$ which separates the two limit (classical and quantum case) temperature T_c is called critical temperature or degeneracy temperature.

In order to understand the physical behaviors of a gas where quantum effects dominates, according to quantum statistics, properties and numbers of the situations that can be described should be known. In the quantum mechanics the case of a system is defined by wave function of system. The absolute square of the amplitude of the wave function is proportional to the probability of finding of the system in a particular situation. Since the particles that have the same structural properties (mass, electric charge, etc…) cannot be distinguished from each other, interchange of two particles should not change the physical observables of the system. Because of this fundamental principle, in the quantum mechanics the wave functions which define a system that occur identical particles have to indicate the symmetric or anti-symmetric behavior under interchange of two particles.

If spin of particles is half integer, they are called fermions (electron, proton, neutron, etc…). The wave functions of such particles are anti-symmetric and obey Fermi-Dirac statistics [33] [34].

If spin of particle is odd integer, they are called bosons (phonon, photon, K and π meson, etc...). The wave functions of such particles are symmetric and obey Bose-Einstein statistics (1924-1925 by Albert Einstein, by Satyendra Nath Bose).

At high temperature between bosons and fermions don't have certain difference at the observable behaviors of them. But when the system's temperature reaches to sufficient low temperature, it shows quite different statistical behavior. As a result of the anti-symmetric wave function, fermions obey Pauli Exclusion Principle (1925 by Wolf Gang Pauli), so at the same time maximum one fermion particle can exists in the same quantum state, whereas bosons which have symmetric wave function occupy in the same quantum state without limitation.

We consider that a boson gas that is equal to total integer spin and non-zero mass. But before dealing with boson gas, we should describe what is the boson gas? The total spin of a Bose particle must be an integer, and therefore a boson made up fermions must contain an even number of them. Neutral atoms contain equal numbers of electrons and protons, and therefore the statistics that an atom obeys is determined solely by the number of neutrons N: if N is even, the atom is a boson and if it is odd, the atom is a fermion. The alkalis have odd atomic number Z, boson alkali atoms have odd mass numbers A [35].

In the boson gas consist of boson alkali atoms, molecules can move freely, in the sufficiently high temperatures, at the classical limit, according to quantum mechanics a particle with momentum p that accompanied de Broglie wavelength λ_{DB} must be small compare with average distance between molecules. If average distance between molecules is much bigger than λ_{DB} , de Broglie wavelength cannot interference each other sufficiently. This particle obeys Newton mechanics. If bosons gas begins to approach the limit temperature T_c, as described with equation (2.5), particles accompanied wave length λ_{DB} begin to grow.

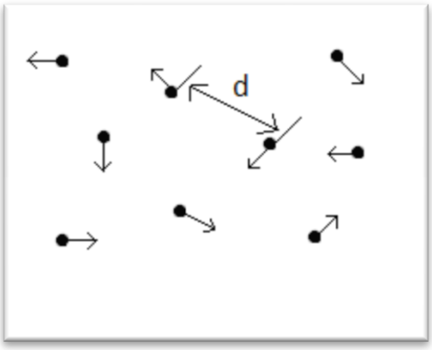

Figure 2.1 At high temperature T, thermal speed V and density $1/n^{1/3}$ "look like billiard balls".

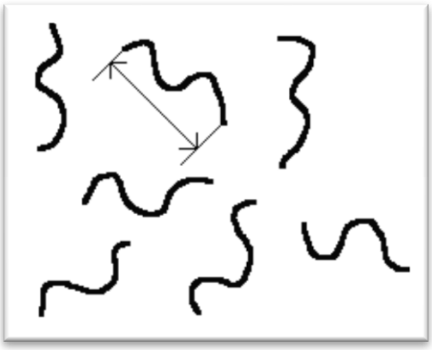

Figure 2.2 At low temperature T, de Broglie wavelength $\lambda_{DB} = h/mV \propto T^{-1/2}$ “wava packets”.

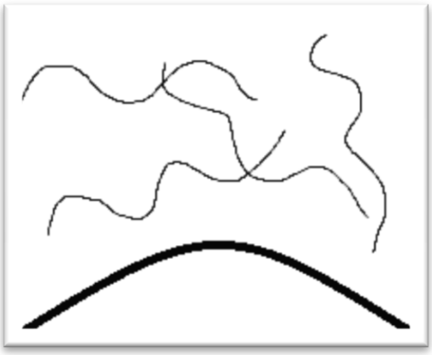

Figure 2.3 T=T$_c$ Bose-Einstein Condensation begin to occur, matter waves overlap

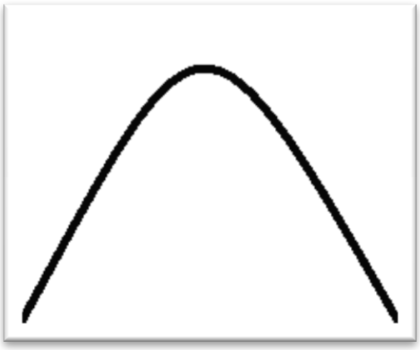

Figure 2.4 T=0 pure boson condensation, giant matte wave

At high temperature, because de Broglie wavelength λ_{DB} is quite small the interaction of the atoms with each other is small enough to be neglected and gas exhibit classical behavior. As shown in Figure 2.1 because the intermolecular distance is too large, de Broglie wavelength accompanied particle is small sufficiently and it cannot be interference with each other, such particles obey Newton's mechanics. Atom can be considered as billiard ball in these conditions which is in the dilute gas limit of weak interactions between atoms. As shown in Figure 2.2 wavelength of the atoms begin to increase at low temperature and the atoms of gas can be considered as wave packets with of the order of the λ_{DB}. In the Figure 2.3 when system approaches to critical temperature T_c, distances between atoms are comparable size with λ_{DB} wavelength and at this temperature atomic wave packets start to overlap. On the bosons a phase transition is observed and Bose-Einstein Condensation begins to form. Finally as shown in Figure 2.4 when the temperature close to zero point, a thermal cloud of atoms excited vanishes and all the atoms occupy in the same quantum state. In this case the system is represented by large wave of a single matter [36].

Energy and momentum of particles reaching the ground state energy are zero, so that the phase transition occurs. By this way the collection of particles in the ground state energy is called Bose-Einstein Condensation (BEC). Because this phase transition which occurs at low temperature to resemble condensation of vapor, it is called BEC. Condensation of the boson gas is quite different from a classical condensation of vapor, but there are same resembles between condensations of boson gas and vapour. For example, at $T < T_c$ like pressure of saturated vapour gas, boson gas pressure does not depend on volume but depend to temperature of gas.

In a phase transition, it is considered that individual characteristics of the particles lost and all particles occupy the single particle quantum state. In this case, in the BEC observed in the rarely alkali gases movement of any particles do not leave other ones therefore in the condensate the movement of all the atoms not take into account separately but take into consideration like movement of a single large atom.

2.2 THE NON-INTERACTING BOSE GAS

Before surveying the behavior of interacting Bose gas, in the present chapter, properties of a non-interacting Bose gas is debated in a trap. In a semi classical approximation, equilibrium properties of systems shall be calculated, in which the energy spectrum is treated as a continuum. For this approach to be valid the temperature must be large compared with $\Delta\in/k$, where $\Delta\in$ denotes the separation between neighboring energy levels and k is the Boltzmann constant [35]. As known, at temperature below the Bose-Einstein condensation temperature the lowest state is not properly accounted for if one simply replaces sums by integral and it must be included explicitly. [30]

In Sec. 2.2.1, the statistical distribution function is discussed, as is single-particle density of states. In the calculations of thermodynamics properties, density of states is a very important ingredient and in Sec. 2.2.2 it is described. In Secs. 2.2.4 and 2.2.3 calculations of the condensation fraction of particles and transition temperature are described respectively. In Sec. 2.2.5 the density profile of particles is determined.

2.2.1 The Bose Distribution

In thermodynamic equilibrium for non-interacting bosons, the mean occupation number of single particle state υ is given by the Bose distribution function [35];

$$f^0(\in_\upsilon) = \frac{1}{e^{(\in_\upsilon - \mu)/kT} - 1} \tag{2.8}$$

where, $\in_\upsilon$ shows the energy of single particle state for the particular trapping potential under consideration. T is the temperature and k is the Boltzmann constant. μ denotes the chemical potential. It is determined as a function of N (total number of particles) and T (temperature) by the condition that the total number of particles be equal to the sum of the occupancies of the individual levels [31].

In thermodynamics, chemical potential μ is a measure of the potential that a substance has to produce in order to alter a system. Particles tend to move from higher chemical potential to lower chemical potential [32].

Chemical potential can be studied in terms of fugacity and it is defined the quantity $\zeta = \exp(\mu/kT)$. If the energy of lowest single-particle state is taken zero, the fugacity is less than unity above the transition temperature and equal to unity in the condensed state.

When the vapor pressure is not too high, the fugacity is approximately equal to the vapor pressure, so the fugacity of a real gas is formally defined by an equation analogous to the relation between the chemical potential and the pressure of an ideal gas $(\zeta = \exp(\mu/kT))$ [33].

In Bose-Einstein statistics, the average occupancy of each $\in_\upsilon$ energy quantum states was given by Bose distribution function in equation 1. In this equation, the term of minus one (-1) on the denominator is most important point of the equation. If the energy spectrum of bosons from ground state is listed, it can be obtained;

$$\in_0 < \in_1 < \in_2 \ldots.. \qquad (2.9)$$

Though the minimum energy of the ground state is taken $\in_0 = 0$, average occupation number of particles $\mathrm{f}^0(\in_\upsilon)$ cannot be equal to minus value so in the Bose gases, the expression of $\exp(-\mu/kT)$ or μ must be like this [34];

$$exp\,(-\mu/kT) < 1 \qquad (2.10)$$

$$-\infty < \mu \leq 0 \qquad (2.11)$$

It is known that at high temperatures chemical potential is much less than the energy of the lowest single particles state $(\in_{min})$ and average occupation number of any state is much less than unity. But when the temperature is lowered, chemical potential rises and average occupation number increase. However the chemical potential cannot exceed $\in_{min}$, otherwise the Bose distribution function would be negative and unphysical. Consequently the average occupation number of any excited single particle state can be expressed in Eq. (2.8).

In the following Figure 1 the distribution function is shown as a function of energy for various values of fugacity [30].

$$\zeta = 1 \qquad \zeta = exp(\mu/kT) \qquad \mu = 0 \tag{2.12}$$

$$\zeta = 0.5 \qquad \zeta = exp(\mu/kT) \qquad \mu = -0{,}69kT \tag{2.13}$$

$$\zeta = 0.25 \qquad \zeta = exp\left(\frac{\mu}{kT}\right) \qquad \mu = -1{,}39kT \tag{2.14}$$

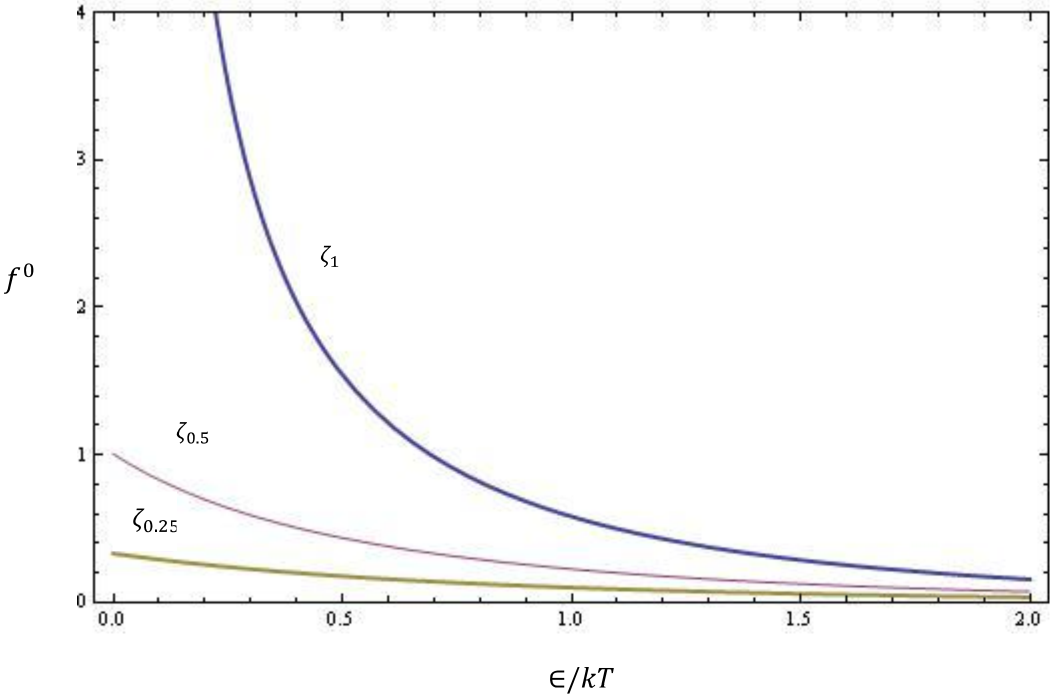

Figure 2.5 The Bose distribution function.

The Bose distribution function f^0 is as a function of energy for different value of the fugacity. The blue one $\zeta = 1$ corresponds to temperature below the transition temperature. The purple one $\zeta = 0.5$ shows that the $\mu = -0{,}69kT$ and the green one shows the $\mu = -1{,}39kT$ also in the two values of fugacity it can be seen that temperature increases so occupation number of the particle decreases.

2.2.2 Density of States

If the thermodynamic properties of gases studied, sums at all levels are replaced with integrals and density of state is used to smooth out details of the level structure. This method is unsuccessful for a Bose-Einstein condensed systems, because the contribution from the ground state is not correctly explained. However it gives a good approximation to contribution from excited states, and these smoothed densities of states are calculated for a number of different situations.

One dimension density of states can be obtained but firstly phase space should be explained after that in three dimensions it should be obtained.

First, let us consider a particle in a one dimensional coordinate system in the classical mechanics. If Hamiltonian *H(q , p)* is given, by using Hamiltonian equation solution of *q(t)* and *p(t)* can be obtained

The two dimensional space which have the axes of *p* and *q* is called phase space as shown in Figure 2.6. Micro state of a particle at time *t* is a point corresponding values of *p(t)* and *q(t)* in phase space. If time *t* changes, *p(t)* and *q(t)* changes and the point representing micro state in the phase space moves on the a orbit.

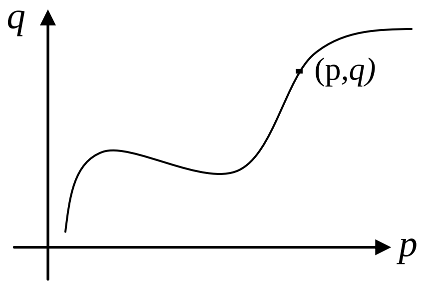

Figure 2.6 Phase space

If the Hamiltonian of harmonic oscillator in the phase space is written, it will be like form;

$$H(p,q) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 = \in \qquad (2.15)$$

Eq. (2.15) is a ellipse equation and the diameter of the ellipse varies depending on the value of $\in$. So in the phase space the harmonic oscillator draws elliptical orbits as shown in Figure 2.7

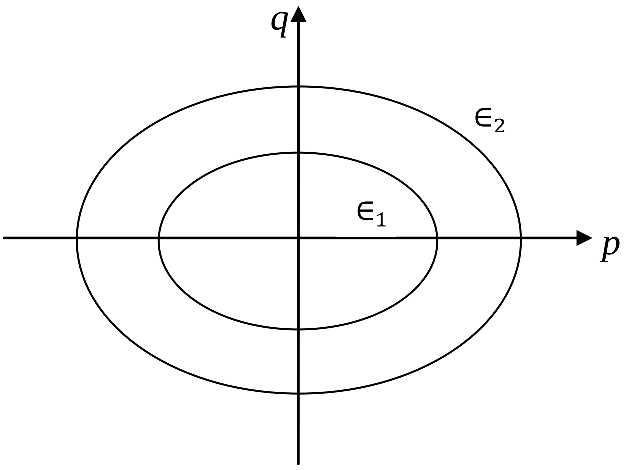

Figure 2.7 The orbits of Hamiltonians of two harmonic oscillators in the phase space

When the micro-states of classical systems are searched, there is a serious problem; because the position and momentum of a particle take continuous values, in the region where the motion become, the number of the micro-state is infinite. For example, if the energy of particles changes between $\in_1$ and $\in_2$, it can be written

$$\in_1 \leq H(p,q) \leq \in_2 \tag{2.16}$$

and there are infinite points between ellipses $\in_1$ and $\in_2$. When the number of micro-state is infinite, it is not possible to make statistical analysis. But the uncertainty principle of quantum mechanics can be used to for this situation. According to the uncertainty principle, the product of Δq uncertainty of the position with of Δp uncertainty of the momentum must be at least as much as h (Planck’s constant) [30]

$$\Delta p . \Delta q \geq h \tag{2.17}$$

$$h = 2\pi\hbar \tag{2.18}$$

then, if in the phase space surface element *dq.dp* is smaller than value of h (Planck's constant), the surface element cannot be evaluated and it is unphysical. In the surface element *dq.dp,* surface area covered by micro-state is h, so the number of micro-states is given in the one dimension by [30]

$$G(\in)=\int \frac{dpdq}{h} \tag{2.19}$$

also, in three dimensions it can be given

$$G(\in)=\int \frac{(dpdq)^3}{h^3} \tag{2.20}$$

so, the number of state can be finite value. In these equations Planck's constant h can be written in terms of reduced Planck's constant or Dirac constant and it is equal to the Planck's constant divided by 2π and is denotes $\hbar$ (h-bar)

$$h=2\pi\hbar \tag{2.21}$$

In three dimension, for a free particle in a particular internal state, there is on average one quantum state per volume $(2\pi\hbar)^3$ of phase space. The region of momentum space for which the magnitude of momentum is less than p has a volume $4\pi p^3/3$ equal to that of a sphere of radius p and, since the energy of a particle of momentum p is given $\in_p = p^2/2m$, the number of micro-states $G(\in)$, with energy less than $\in$ is given by [32];

$$G(\in)=\int \frac{(dpdq)^3}{(2\pi\hbar)^3} \tag{2.22}$$

$(dp)^3$ is the volume of momentum,

$$(dp)^3 = \frac{4}{3}\pi p^3 \quad and \quad p = \sqrt{2m \in} \tag{2.23}$$

$$(dp)^3 = \frac{4}{3}\pi(2\pi \in)^{3/2} \tag{2.24}$$

$(dq)^3$ is the volume of system, and it is equal to V

If the number of states $G(\in)$ is re-written, in terms of *dp* and *dq,* it is obtained this form,

$$G(\epsilon)=V\frac{4}{3}\frac{\pi(2\pi\epsilon)^{3/2}}{(2\pi\hbar)^3} \tag{2.25}$$

Quite generally, the number of states with energy between $\in$ and $\in + d\in$ is given by $g(\in)d\in$, where $g(\in)$ is the density of states. Therefore;

$$g(\in) = \frac{dG(\in)}{d \in} \tag{2.26}$$

If Eq. (2.25) put in the Eq. (2.26), Eq. (2.27) is obtained;

$$g(\in) = \frac{d}{d \in}\left(V\frac{4}{3}\frac{\pi(2\pi\epsilon)^{3/2}}{(2\pi\hbar)^3}\right) \tag{2.27}$$

$$g(\in) = \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3} \in^{1/2} \tag{2.28}$$

In Eq. (2.28) density of states were obtained in three dimension systems for free particles, also in *d*-dimension the corresponding results can be given;

$$g(\in) \propto \in^{\left(\frac{d}{2}-1\right)} \tag{2.29}$$

Now, let us consider a particle in the anisotropic harmonic oscillator potential and in the three dimensions this potential can be written;

$$V(r) = \frac{1}{2}m(\omega^2 x^2 + \omega^2 y^2 + \omega^2 z^2) \tag{2.30}$$

where, ω_i (i =1,2,3) is classical oscillation frequencies and *x*, *y* and *z* are positions in three dimension systems.

It is known that the energy levels $\in (n_1 n_2 n_3)$ are given [35];

$$\in (n_1, n_2, n_3) = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1 + \left(n_2 + \frac{1}{2}\right)\hbar\omega_2 + \left(n_3 + \frac{1}{2}\right)\hbar\omega_3 \tag{2.31}$$

Where, n_1, n_2 and n_3 are positive integer.

Same procedure can be applied for a particles in the anisotropic harmonic potential system to determine the number of states $G(\in)$ for free particles in the three dimensions. Firstly, the number of states $G(\in)$ with energy less than a given value $\in$ can be treated. For large energies compared with $\hbar\omega_i$, as continuous variables n_i is treated and zero-point motion is neglected. Therefore a coordinate system is defined with axes of $\in = \hbar\omega_i n_i$ and in this coordinate system surface which is constant the total energy $\in = \in_1 + \in_2 + \in_3$, occurs a plane. Then $G(\in)$ is proportional to the volume in the first octant bounded by the plane and is defined so the number of states can be obtained this form [35];

$$G(\in) = \frac{\in^3}{6\hbar^3\omega_1\omega_2\omega_3} \tag{2.32}$$

From $g(\in) = dG(\in)/(d\in)$, density of states is obtained;

$$g(\in) = \frac{d}{d\in}\left(\frac{\in^3}{6\hbar^3\omega_1\omega_2\omega_3}\right) \tag{2.33}$$

$$g(\in) = \frac{\in^2}{2\hbar^3\omega_1\omega_2\omega_3} \tag{2.34}$$

so, for a particle sin the three dimension anisotropic potential corresponding results can be given $g(\in) \propto \in^{(\mathrm{d}-1)}$ [35].

Density of states in three dimensions;

For free particle $$g(\in) = \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3} \in^{1/2} \tag{2.35}$$

For anisotropic potential $$g(\in) = \frac{\in^2}{2\hbar^3\omega_1\omega_2\omega_3} \tag{2.36}$$

were obtained.

It can be seen that density of states varies as power of the energy.

To calculate easily the thermodynamic properties of systems, density of states can be written following form [35].

$$\mathrm{g}(\in) = \mathrm{C}_\alpha \in^{\alpha-1} \tag{2.37}$$

Where C_α is constant and for free particle in Eq. (2.28) and for harmonic oscillator potential in Eq. (2.34) may be read off.

For free particle;

$$\alpha = \frac{3}{2} \qquad g(\in) = C_{3/2} \in^{3/2-1} \qquad C_\alpha = C_{3/2} = \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3} \tag{2.38}$$

For anisotropic potential;

$$\alpha = 3 \qquad g(\in) = C_3 \in^{3-1} \qquad C_\alpha = C_3 = \frac{1}{2\hbar^3\omega_1\omega_2\omega_3} \tag{2.39}$$

2.2.3 Transition Temperature

As the highest temperature where occupation number of the lowest single particle state appears, the transition temperature T_c is defined. When the number of particles N is enough large, zero point energy in Eq. (2.31) can be neglected, thus the lowest energy $\in_{\min}$ may be zero.

Under such situation, according to density of states and distribution function which is defined in Eq. (2.37) and Eq. (2.8) respectively, transition temperature can be obtained.

The number of particles in the excited states is given by; [37]

$$N_{ex} = \int_0^\infty d \in g(\in) f^0(\in) \tag{2.40}$$

This achieves its greatest value for $\mu = 0$ and the transition temperature T_c is determined by condition that the total number of particles can be accommodated in excited states, that is;

$$N = N_{ex}(T_c, \mu = 0) = \int_0^\infty d \in g(\in) f^0(\in) \tag{2.41}$$

$$g(\in) = C_\alpha \in^{\alpha-1}$$

$$f^0(\in) = \frac{1}{e^{(\in-\mu)/kT} - 1}$$

$$N = N_{ex}(T_c, \mu = 0) = \int_0^\infty d \in C_\alpha \in^{\alpha-1} \frac{1}{e^{(\in-\mu)/kT} - 1} \tag{2.42}$$

When Eq. (2.41) is written in terms of the dimensionless variables $x = \in / kT_c$, it can be obtained the result is given in Eq. (2.45).

$$xkT_c = \in \tag{2.43}$$

$$kT_c dx = d \in \tag{2.44}$$

$$\mathrm{N} = \mathrm{N}_{\mathrm{ex}}(\mathrm{T}_c, \mu = 0) = \int_0^\infty \mathrm{dx}\,(\mathrm{kT_c})\,\mathrm{C}_\alpha\,(\mathrm{xkT_c})^{\alpha-1}\frac{1}{\mathrm{e}^\alpha - 1}$$

$$\mathrm{N} = \mathrm{N}_{\mathrm{ex}}(\mathrm{T}_c, \mu = 0) = \int_0^\infty \mathrm{dx}\,(\mathrm{kT_c})^\alpha\,\mathrm{C}_\alpha\frac{\mathrm{x}^{\alpha-1}}{\mathrm{e}^\alpha - 1}$$

$$\mathrm{N} = \mathrm{N}_{\mathrm{ex}}(\mathrm{T}_c, \mu = 0) = (\mathrm{kT_c})^\alpha\,\mathrm{C}_\alpha\int_0^\infty \mathrm{dx}\frac{\mathrm{x}^{\alpha-1}}{\mathrm{e}^\alpha - 1} \tag{2.45}$$

$$\int_0^\infty \mathrm{dx}\frac{\mathrm{x}^{\alpha-1}}{\mathrm{e}^\alpha - 1} = \Gamma(\alpha)\zeta(\alpha) \tag{2.46}$$

In Eq. (2.45) the side of integral can be defined in terms of the gamma function $\Gamma(\alpha)$ and the Riemann zeta function $\zeta(\alpha)$. In evaluating the integral in Eq.(2.45) Bose function is expanded in power of e^{-x} and equation $\int_0^\infty \mathrm{dx}\mathrm{x}^{\alpha-1}\mathrm{e}^{-\mathrm{x}} = \Gamma(\alpha)$ is used.[35]

In the following Table (2.1) lists $\Gamma(\alpha)$ and $\zeta(\alpha)$ for selected values of α.

Table 2.1 The Gamma function and Riemann zeta function for various values of α [35].

α	$\Gamma(\alpha)$	$\zeta(\alpha)$
1	1	∞
1,5	$\sqrt{\pi}/2 = 0{,}886$	2,612
2	1	$\pi^2/6 = 1{,}645$
2,5	$3\sqrt{\pi}/4 = 1{,}329$	1,341
3	2	1,202
3,5	$15\sqrt{\pi}/8 = 3{,}323$	1,127
4	6	$\pi^4/90 = 1{,}082$

Eq. (2.45) can be written in terms of Eq. (2.46), and result is given;

$$N = N_{ex}(T_c, \mu = 0) = \ (kT_c)^{\alpha}\ C_{\alpha}\Gamma(\alpha)\zeta(\alpha) \tag{2.47}$$

so transition temperature can be written like;

$$kT_c = \frac{N^{1/\alpha}}{(C_{\alpha}\Gamma(\alpha)\zeta(\alpha))^{1/\alpha}} \tag{2.48}$$

for a three dimensional harmonic oscillator potential α is equal to 3 and C_3 is given by Eq. (2.39), the transition temperature is given by;

$$kT_c = \frac{N^{1/3}}{(C_3\Gamma(3)\zeta(3))^{1/3}} \tag{2.49}$$

$$kT_c = \frac{2^{1/3}\hbar(\omega_1\omega_2\omega_3)^{1/3}N^{1/3}}{(\Gamma(3)\zeta(3))^{1/3}} = 0{,}94\hbar(\omega_1\omega_2\omega_3)^{1/3}N^{1/3} \tag{2.50}$$

Where product of $(\omega_1\omega_2\omega_3)^{1/3}$ can be written in terms of geometric mean of them.

$$\bar{\omega} = (\omega_1\omega_2\omega_3)^{1/3} \tag{2.51}$$

so, result is given;

$$kT_c = 0{,}94\hbar\bar{\omega}N^{1/3} \tag{2.52}$$

Eq. (2.52) may be written in the useful form

$$kT_c = 4{,}5\left(\frac{\bar{f}}{100}\right)N^{1/3}\ \ nK \tag{2.53}$$

where, $\bar{f} = \bar{\omega}2\pi$.

For a uniform Bose gas in a three dimensional box of volume V, α is equal to 3/2 and $C_{3/2}$ is given by Eq. (2.38) thus the transition temperature is given by;

$$kT_c = \frac{N^{2/3}}{\left(C_{3/2}\Gamma\left(\frac{3}{2}\right)\zeta(\frac{3}{2})\right)^{2/3}} \tag{2.54}$$

$$kT_c = \frac{\left(\sqrt{2}\pi^2\hbar^3\right)^{2/3}}{(Vm^{3/2})^{2/3}}\frac{N^{2/3}}{\left(\Gamma\left(\frac{3}{2}\right)\zeta(\frac{3}{2})\right)^{2/3}} \tag{2.55}$$

$$kT_c = \frac{N^{2/3}}{V^{2/3}}\frac{\left(\sqrt{2}\right)^{2/3}\pi^{4/3}\hbar^2}{m}\frac{1}{\left(\sqrt{\pi}/2\right)(2{,}612))^{2/3}} \tag{2.56}$$

$$kT_c = 3{,}31\frac{\hbar^2 n^{2/3}}{m} \tag{2.57}$$

where, $n = N/V$ is the number density.

For a free particle in two dimensions, because d is equal to 2 α is equal to 1 and the Eq. (2.45) diverges. Thus in two dimensional box Bose-Einstein may occur only at zero temperature. But in two dimensional harmonic oscillator potential, Bose gas can condense at non-zero temperature [35].

2.2.4 Condensate Fraction

Below the transition temperature the number N_{ex} of particles in excited states is given by Eq. (2.40) with $\mu = 0$.

$$N_{ex} = \int_0^\infty d\in C_\alpha \in^{\alpha-1}\frac{1}{e^{\in/kT}-1} \tag{2.58}$$

In Sec. 2.3.3 in order to find the transition temperature, it can be supposed that the total number of particles became in excited states and chemical potential which is equal to zero is taken, so results are given in Eq. (2.47) [35].

$$N = \; C_{\alpha}\Gamma(\alpha)\zeta(\alpha)(kT_c)^{\alpha} \tag{2.59}$$

In Eq. (2.58) below the transition temperature T_{c} the number N_{ex} of particles in excited states can be written in the form;

$$N_{ex} = \; C_{\alpha}\Gamma(\alpha)\zeta((\alpha)(kT)^{\alpha} \tag{2.60}$$

Note that this result does not depend on the total number of particles.

If Eqs. (2.59) and (2.60) are used to find condensate fraction, it can be written;

$$\frac{N_{ex}}{N} = \frac{C_{\alpha}\Gamma(\alpha)\zeta((\alpha)(kT)^{\alpha}}{C_{\alpha}\Gamma(\alpha)\zeta((\alpha)(kT_c)^{\alpha}} \tag{2.61}$$

$$\frac{N_{ex}}{N} = \left(\frac{T}{T_c}\right)^{\alpha} \tag{2.62}$$

In condensate the number of particles is so given by;

$$N_0(T) = N - N_{ex}(T) \tag{2.63}$$

If Eq. (2.62) is used to in Eq. (2.63), it is obtained by;

$$N_0(T) = N - N\left(\frac{T}{T_c}\right)^{\alpha}$$

$$N_0(T) = N\left[1 - \left(\frac{T}{T_c}\right)^{\alpha}\right] \tag{2.64}$$

For free particles in a volume V, α is equal to 3/2 so the occupancy of the condensate can be written from Eq. (2.64).

$$N_0(T) = N\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right] \tag{2.65}$$

For a three dimensional harmonic oscillator potential α is equal to 3 the number of particles in condensate is;

$$N_0(T) = N\left[1 - \left(\frac{T}{T_c}\right)^{3}\right] \tag{2.66}$$

The transition temperature T_c which is given Eq. (2.48) is suit in all cases for the appropriate value of α [35].

2.2.5 Density Profile

The cold clouds of atoms that are investigated at μK (micro-kelvin) temperatures contain about order of $10^4 – 10^7$ atoms. Due to a lot of reasons, it is possible to apply the techniques of low temperature physics to these systems. First, there are rather few atoms, second the system are metastable so one cannot allow them to come into equilibrium with another body, and third the system have a lifetime which is of order second to minutes. So among the quantities that can be measured is the density profile. One way to do this is made by using some experimental procedure. During the experimental procedure, the distributions of particles which become in the cold atomic cloud do not only depend on early density distribution of particles but also depend on beginning the velocity distribution of particles. [35]

In the ground state of the system, all atoms are condensed in the lowest single particle quantum state and the density distribution n(r) shows the shape of the ground state wave function $\emptyset_0(r)$ for a particle in the trap since, for non-interacting particles, the density is given by;

$$n(r) = N|\emptyset_0(r)|^2 \tag{2.67}$$

where, N is the number of particles. For anisotropic harmonic oscillator the ground state wave function is given this form; [35]

$$\emptyset_0(r) = \frac{1}{\pi^{3/4}(a_1 a_2 a_3)^{1/2}} \exp\left(-\frac{x^2}{2a_1^2} - \frac{y^2}{2a_2^2} - \frac{z^2}{2a_3^2}\right) \tag{2.68}$$

where, the widths a_i of the wave function in the three directions are given by $a_i = \hbar/m\omega_i$.

Thus, density distribution is anisotropic and if the three frequencies ω_1, ω_2 and ω_3 are not all equal, the greatest begin associated with the lowest frequency.

Eq. (2.68) can be written in momentum space by using Fourier transform Eq. (2.69).

$$\emptyset_0(p) = \int_{-\infty}^{+\infty} dx \emptyset_0\,(r) e^{-ipr} \tag{2.69}$$

$$\emptyset_0(p) = \int_{-\infty}^{+\infty} dxdydz\, \emptyset_0\,(x)\, \emptyset_0(y)\, \emptyset_0(z) e^{-ipx} e^{-ipy} e^{-ipz} \tag{2.70}$$

Thus, ground state wave function is obtained in the momentum space like form;

$$\emptyset_0(p) = \frac{1}{\pi^{3/4}(c_1 c_2 c_3)^{1/2}}\, exp\left(-\frac{p_x^2}{2c_1^2} - \frac{p_y^2}{2c_2^2} - \frac{p_z^2}{2c_3^2}\right) \tag{2.71}$$

Where, $c_i^2 = m\hbar\omega_i$ and it can be written like form $c_i = \hbar/a_i = \sqrt{m\hbar\omega_i}$.

The density in momentum space corresponding to Eq. (2.67) is given by;

$$n(p) = N|\emptyset_0(p)|^2 \tag{2.72}$$

$$n(p) = \frac{N}{\pi^{3/4}(c_1 c_2 c_3)^{1/2}}\, exp\left(-\frac{p_x^2}{2c_1^2} - \frac{p_y^2}{2c_2^2} - \frac{p_z^2}{2c_3^2}\right) \tag{2.73}$$

Eq. (2.73) has the form of a Maxwell distribution with different temperatures for three directions.

$$T_i = \frac{\hbar\omega_i}{2k} \tag{2.74}$$

As seen in following Eq. (2.75) Maxwell distribution is given;

$$f_p(p_x, p_y, p_z) = \left(\frac{1}{2mkT\pi}\right)^{3/2} exp\left(-\frac{p_x^2 + p_y^2 + p_z^2}{2mkT}\right) \tag{2.75}$$

Spatial distribution is anisotropic, so the momentum distribution also depends on direction. According to the uncertainty principle, a narrow spatial distribution correspond to a broad momentum distribution, as seen in the Fourier transform Eq. (2.71) in which the width c_i are proportional to the square root of the oscillator frequencies.

When the gas behaviors classical gas in the well above Bose-Einstein condensation temperature, it can be looked the differences between classical distribution which are corresponded to density and momentum distribution. Density distribution classically is proportional with $exp(-V(r)/kT)$ and results are given;

$$n(r) = \frac{N}{\pi^{3/4}(R_1 R_2 R_3)^{1/2}}\, exp\left(-\frac{x^2}{R_1^2} - \frac{y^2}{R_2^2} - \frac{z^2}{R_3^2}\right) \tag{2.76}$$

where, R_i is width spatial distribution, and it is given by;

$$R_i^2 = \frac{2kT}{m\omega_i} \tag{2.77}$$

These widths depend on temperature. Note that, the ratio of R_i/a_i which is bigger than value one, is equal to the $(2kT/\hbar\omega_i)^{1/2}$ under the typically experimental situations. As a result of semi-classical behaviors situations are provided and it can be concluded that the thermal cloud is wider than the part of condense. Below critical temperature T_c the part of condenses appears as a sharp peak in the spatial distribution. According to thermal distribution when the temperature decreases, the weight of peak increases. Above T_c the density *n*(p) in the momentum space is isotropic in equilibrium, since it is determined only by the temperature and the particle mass, and in the classical limit it is given by;

$$n(p) = Cexp\left(-\frac{p^2}{2mkT}\right) \tag{2.78}$$

where, *C* constant is independent of momentum. If thermal cloud grows up more than initial size of it, the cloud which made up depends on the isotropy of velocity distribution and then it gets shape of spherical symmetry [35].

CHAPTER 3

THE INTERACTING BOSE GASES

3.1 THEORY OF CONDENSATE STATES

In the present section, the structure of Bose-Einstein condensation state in the presence of interactions will be considered. This topic is based on the Gross-Pitaevskii equation which describes the zero temperature properties of the non-uniform Bose gas when scattering length a is much less than mean inter-particle distance. This equation also called the non-linear Schrödinger equation and non-linear term of the equation will be defined in the next subsection.

Firstly, in section 3.1.1 Bogoluibov approximations will be defined. This theory that is discussed by Bogoluibov provides a good approximation to search the behaviors of a system consist of interacting bosons by using perturbation theory.

In section 3.1.2 Gross-Pitaevskii equation is derived at zero temperature by treating the interaction between particles in terms of Bose field operator $\widehat{\Psi}$. In section 3.1.2.1 for the ground state energy, in the time-independent Gross-Pitaevskii equation, Thomas-Fermi approximation obtained by neglecting the term of kinetic energy will be described.

3.1.1 Bogoliubov Approximation and Mean Field Theory

The mean field theory of the interacting bosons systems with multi-particles at zero temperature first time is discussed by Bogoliubov. In 1947 Bogoliubov improved a approximation to search the behaviors of a system consist of interacting bosons by using perturbation theory. Although this theory gives good results for low density and weak interacting systems, for systems which become inter-atomic effective interactions this theory is not good approximation. The theory of Bogoliubov is one of the commonly used methods to examine the properties of Bose-Einstein condensation (Edwards and his friends 1996, Du Bois and Glyde 2003) [36]

The Hamiltonian of the N interacting bosons with each other trapped by external potential is given by [35];

$$\hat{H} = \int d^3r \hat{\Psi}^{\dagger}(r)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r)\right]\hat{\Psi}(r) + \frac{1}{2}\int d^3r \int d^3r'\, \hat{\Psi}^{\dagger}(r)\hat{\Psi}^{\dagger}(r')V_{int}(r,r')\hat{\Psi}(r')\hat{\Psi}(r) \tag{3.1}$$

Where $\hat{\Psi}(r)$ and $\hat{\Psi}^{\dagger}(r)$ are the field operators of bosons, and they are respectively the annihilation and creation operators for a particle at position r. $V_{int}(r,r')$ is the inter-atomic interaction potential between two particles.

The thermodynamic properties and ground states of the system can be directly calculated by using the Hamiltonian in Eq. (3.1). But, such calculations are very hard (Krauth 1996). For these type interaction systems the mean field approximation has been developed and it has been used to accurate solution of the multi-particle Schrödinger equations.

The idea, which defines dilute a Bose gas with mean field approximation, is suggested by Bogoliubov in 1947. The field operators can be written [36];

$$\hat{\Psi} = \sum_{\alpha} \psi_{\alpha}(r) a_{\alpha} \tag{3.2}$$

Where, $\psi_{\alpha}(r)$ is single particle wave function and a_{α} is the annihilation operator. The bosonic annihilation and creation operators, a_{α} and $a_{\alpha}{}^{\dagger}$ are defined in Fock space through the relations [36];

$$a_{\alpha}{}^{\dagger}\left|n_0, n_1, \dots, n_{\alpha}, \dots\right\rangle = \sqrt{n_{\alpha}+1}\left|n_0, n_1, \dots, n_{\alpha}+1, \dots\right\rangle \tag{3.3}$$

$$a_{\alpha}\left|n_0, n_1, \dots, n_{\alpha}, \dots\right\rangle = \sqrt{n_{\alpha}}\left|n_0, n_1, \dots, n_{\alpha}-1, \dots\right\rangle \tag{3.4}$$

Where, n_α are the eigenvalue of the operator $n_\alpha = {a_\alpha}^\dagger a_\alpha$ giving number of atoms in the single particle α state. They obey the usual commutation rules.

$$\left[{a_\alpha}^\dagger, a_\beta\right] = \delta_{\alpha,\beta} \tag{3.5}$$

$$\left[a_\alpha, a_\beta\right] = 0 \tag{3.6}$$

$$\left[{a_\alpha}^\dagger, {a_\beta}^\dagger\right] = 0 \tag{3.7}$$

Where $\delta_{\alpha,\beta}$ is called Kronecher delta or Kronecher's delta and it is a function of two variables, usually integers. The function is 1 if the variables are equal and 0 otherwise. It can be defined by;

$$\delta_{\alpha,\beta} = \begin{cases} 0, & if \quad \alpha \neq \beta \\ 1, & if \quad \alpha = \beta \end{cases} \tag{3.8}$$

Bose-Einstein condensation occurs when the number of atoms n_0 of a particular single-particle state becomes very: $n_0 \equiv N_0 \gg 1$ and the ratio N_0/N remains finite in the thermodynamic limit $N \to \infty$. In this limit the states with N_0 and $N_0 \mp 1 \approx N$ correspond to the same physical configuration and consequently the operators a_0 and ${a_0}^\dagger$ can be treated like complex number: $a_0 = {a_\alpha}^\dagger = \sqrt{N_0}$. For a uniform gas in a volume V, Bose-Einstein condensation occurs in the single particle state $\Psi_0 = 1/\sqrt{V}$ having zero momentum and this mean that the field operator having zero momentum and this mean $\hat{\Psi}(r)$ can be decomposed $\hat{\Psi}(r) = \sqrt{N_0/V} + \Psi'(r)$. By treating the operator $\hat{\Psi}'(r)$ as a small perturbation; Bogoliubov developed the "first-order" theory for the excitations of interacting Bose gasses. [35]

The generalization of the Bogoliubov prescription to the case of non-uniform and time-dependent configurations is given by [36];

$$\hat{\Psi}(r,t) = \psi(r,t) + \Psi'(r,t) \tag{3.9}$$

where, Heisenberg representation is used for the field operators. Also $\psi(r,t)$ is a complex function defined as expectation value of the field operator;

$$\psi(r,t) = \langle \hat{\Psi}(r,t) \rangle \tag{3.10}$$

Beside the condensation density is obtained with;

$$n_0(r,t) = |\psi(r,t)|^2 \tag{3.11}$$

The function $\psi(r,t)$ is defined as wave function of the condensation and $\Psi'(r,t)$ which defines the fluctuation in the condensate is a small perturbation term [36].

3.1.2 Gross-Pitaevskii Equation

In the first experiments, alkali atoms which are in the form of a quite dilute gas clouds were used. In these systems the interparticle distance between atoms is bigger than the distance of interaction between atoms. In the weak interactive dilute gases, the interaction of two particles that are defined with s-wave scattering length is expected to be the dominant. Gross-Pitaevskii theory describes the mean field theory of the Bose-Einstein condensation in the situation that has the low density and too much condensed atoms. This theory was improved by Gross (1961) and by Pitaevskii (1961) by using different techniques independently each other. In the literature, G.P. (Gross-Pitaevskii) equation has been used to examine lots of properties of boson gases trapped by isotropic (Fabrocini and Polls 1999, Du Bois and Glyde 2003) and anisotropic traps (Dalfavo and Strigari 1996, Du Bois and Glyde 2001)

In Eq. (3.1) the second quantized Hamiltonian in terms of the Bose field operator $\hat{\Psi}$ can be written again;

$$\begin{aligned}\hat{H} = \int d^3r \hat{\Psi}^\dagger(r) H_0 \hat{\Psi}(r) \\ + \frac{1}{2}\int d^3r \int d^3r' \, \hat{\Psi}^\dagger(r)\hat{\Psi}^\dagger(r') V_{int}(r,r') \hat{\Psi}(r')\hat{\Psi}(r)\end{aligned} \tag{3.12}$$

where, $V_{int}(r,r')$ is the interaction potential acting between the bosons and $H_0 = -\hbar^2/2m\,\nabla^2 + V_{ext}(r)$ is the single particle Hamiltonian, where m is the particle mass and $V_{ext}(r)$ is the external potential acting on the system. The operator $\hat{\Psi}^\dagger(r)$ and $\hat{\Psi}(r)$ represents the creation and annihilation of a boson at position r, and satisfy the crucial Bose commutation rules that will be given below.

The gas is sufficiently dilute that the atomic interactions are dominated by low energy, two-body s-wave collisions. These are essentially elastic, hard sphere collisions between two atoms, and can be modeled in terms of pseudo-potential [40].

$$V_{int}(r,r') = g\delta(r'-r) \tag{3.13}$$

where, $g = 4\pi\hbar^2 Na/m$ with a the s-wave scattering length. Also $\delta(r'-r)$ is the delta function.

$$\sum_{r'=-\infty}^{\infty} k_{r'}\,\delta(r'-r) = k_r \tag{3.14}$$

Also, if delta function over all space is integrated, it is given by;

$$\int_{-\infty}^{\infty} dr'\,\Psi(r')\delta(r'-r) = \Psi(r) \tag{3.15}$$

So, Eq. (3.12) can be written in terms of Eq. (3.13)

$$\begin{aligned}\hat{H} = \int d^3r\hat{\Psi}^\dagger(r)H_0\,\hat{\Psi}(r) \\ +\frac{1}{2}\int d^3r\int d^3r'\,\hat{\Psi}^\dagger(r)\hat{\Psi}^\dagger(r')V_{int}(r,r')\hat{\Psi}(r')\hat{\Psi}(r)\end{aligned} \tag{3.16}$$

So, Eq. (3.16) can be written in terms of the properties of delta function;

$$\hat{H} = \int d^3r \hat{\Psi}^\dagger(r) H_0 \hat{\Psi}(r) + \frac{g}{2}\int d^3r \ \hat{\Psi}^\dagger(r)\hat{\Psi}(r) \int d^3r' \, \hat{\Psi}^\dagger(r')\delta(r'-r)\hat{\Psi}(r') \tag{3.17}$$

So, Eq. (3.17) can be written in terms of integrated delta function over all space

$$\hat{H} = \int d^3r \hat{\Psi}^\dagger(r) H_0 \hat{\Psi}(r) + \frac{g}{2}\int d^3r \ \hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r) \tag{3.18}$$

where, the dependence on r' has now been conveniently integrated out.

By using the Bose commutation relations [40];

$$\left[\hat{\Psi}(r'), \hat{\Psi}^\dagger(r)\right] = \ \delta(r'-r) \tag{3.19}$$

$$\left[\hat{\Psi}(r'), \hat{\Psi}(r)\right] = \ \left[\hat{\Psi}^\dagger(r'), \hat{\Psi}^\dagger(r)\right] = 0 \tag{3.20}$$

After that, the second quantize Hamiltonian in Eq. (3.18) can be written in terms of Heisenberg's time evolution equation;

$$i\hbar \frac{d\hat{\Psi}(r')}{dt} = \left[\hat{\Psi}(r'), \hat{H}\right] \tag{3.21}$$

And, the results of commutation relations between $\hat{\Psi}(r')$ and $\hat{H}$ is given by;

$$i\hbar \frac{d\hat{\Psi}(r')}{dt} = \hat{\Psi}(r') \, \hat{H} - \hat{H} \, \hat{\Psi}(r') \tag{3.22}$$

$$
\begin{aligned}
i\hbar\frac{d\hat{\Psi}(r')}{dt} = \hat{\Psi}(r')\int d^3r\hat{\Psi}^\dagger(r)H_0\,\hat{\Psi}(r) \\
+\frac{g}{2}\hat{\Psi}(r')\int d^3r\;\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r) \\
-\int d^3r\hat{\Psi}^\dagger(r)H_0\,\hat{\Psi}(r)\hat{\Psi}(r') \\
-\frac{g}{2}\int d^3r\;\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\,\hat{\Psi}(r')
\end{aligned}
\tag{3.23}
$$

Eq. (3.23) can be written in terms of commutation relation in Eq. (3.19);

$$
\begin{aligned}
i\hbar\frac{d\hat{\Psi}(r')}{dt} = \int d^3r\left(\delta(r'-r)+\hat{\Psi}^\dagger(r)\hat{\Psi}(r')\right)\,H_0\,\hat{\Psi}(r) \\
+\frac{g}{2}\int d^3r\;\left(\delta(r'-r)+\hat{\Psi}^\dagger(r)\hat{\Psi}(r')\right)\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r) \\
-\int d^3r\left(\hat{\Psi}(r')\hat{\Psi}^\dagger(r)-\delta(r'-r)\right)H_0\,\hat{\Psi}(r) \\
-\frac{g}{2}\int d^3r\;\hat{\Psi}^\dagger(r)\;\left(\hat{\Psi}(r')\hat{\Psi}^\dagger(r)-\delta(r'-r)\right)\hat{\Psi}(r)\hat{\Psi}(r)
\end{aligned}
\tag{3.24}
$$

$$
\begin{aligned}
i\hbar\frac{d\hat{\Psi}(r')}{dt} = \int d^3r\delta(r'-r)\,H_0\hat{\Psi}(r)+\int d^3r\,\hat{\Psi}^\dagger(r)\hat{\Psi}(r')\,H_0\,\hat{\Psi}(r) \\
+\frac{g}{2}\int d^3r\;\delta(r'-r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r) \\
+\frac{g}{2}\int d^3r\,\hat{\Psi}^\dagger(r)\hat{\Psi}(r')\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r) \\
-\int d^3r\hat{\Psi}(r')\hat{\Psi}^\dagger(r)H_0\hat{\Psi}(r)+\int d^3r\,\delta(r'-r)H_0\,\hat{\Psi}(r) \\
-\frac{g}{2}\int d^3r\;\hat{\Psi}^\dagger(r)\,\hat{\Psi}(r')\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r) \\
+\frac{g}{2}\int d^3r\,\hat{\Psi}^\dagger(r)\delta(r'-r)\hat{\Psi}(r)\hat{\Psi}(r)
\end{aligned}
\tag{3.25}
$$

$$
\begin{aligned}
i\hbar\frac{d\hat{\Psi}(r')}{dt} &= \int d^3r\delta(r'-r)H_0\hat{\Psi}(r) + \int d^3r\delta(r'-r)H_0\hat{\Psi}(r) \\
&\quad + \int d^3r\left(\hat{\Psi}^\dagger(r)\,\hat{\Psi}(r') - \hat{\Psi}(r')\hat{\Psi}^\dagger(r)\right)H_0\hat{\Psi}(r) \\
&\quad + g\int d^3r\ \delta(r'-r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r)
\end{aligned}
\tag{3.26}
$$

$$
\begin{aligned}
i\hbar\frac{d\hat{\Psi}(r')}{dt} &= \int d^3r\delta(r'-r)H_0\hat{\Psi}(r) \\
&\quad + g\int d^3r\ \delta(r'-r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r)\hat{\Psi}(r)
\end{aligned}
\tag{3.27}
$$

$$
i\hbar\frac{d\hat{\Psi}(r')}{dt} = H_0\hat{\Psi}(r') + g\hat{\Psi}^\dagger(r')\hat{\Psi}(r')\hat{\Psi}(r')
\tag{3.28}
$$

Since the condensate state involves the macroscopic occupation of a single state it is appropriate to decompose the Bose field operator in terms of a macroscopically-populated mean field term in Eq. (3.10) $\psi(r') = \langle\hat{\Psi}(\mathrm{r}')\rangle$ and a fluctuation term $\hat{\Psi}'(\mathrm{r}')$ in Eq. (3.9).

$$
\hat{\Psi}(\mathrm{r}') = \psi(r') + \hat{\Psi}'(\mathrm{r}')
\tag{3.29}
$$

Then, taking only the leading order terms in ψ, Eq. (3.28) leads to the time-dependent Gross-Pitaevskii equation,

$$
i\hbar\frac{d\psi(r,t)}{dt} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r) + g|\psi(r,t)|^2\right)\psi(r,t)
\tag{3.30}
$$

The equation known as Gross-Pitaevskii (GP) equation was derived by Gross (1961 and 1963) [23-24] and Pitaevskii (1961) [25]. Its validity is based on the condition that s-wave scattering length be much smaller than the average distance between atoms and that the number of atoms in the condensate be much larger than 1. The GP equation can be used, at low temperature, to explore the macroscopic behavior of the system, characterized by variation of the order parameter over distance larger than the mean distance between atoms.

The ground state can be easily obtained within the formalism of mean field theory. For this one can write the condensate wave function as $\psi(r,t) = \psi(r)\exp{(-i\mu t/\hbar)}$, where μ is the chemical potential and ψ is real and normalized to the total number of particles. $\int dr|\psi(r)|^2 = N_0 = N$. The time-independent GP equation becomes,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r) + g|\psi(r)|^2\right)\psi(r) = \mu\psi(r) \tag{3.31}$$

This has the form of a non-linear Schrödinger equation in which the potential acting on particles is the sum of the external potential V_{ext} and a non-linear term $g|\psi(r)|^2$ that takes into account the mean field produced by the other bosons. Note that the eigenvalue is the chemical potential, not the energy per particle as it is for the usual (linear) Schrödinger equation. For non-interacting particles all in the same state the chemical potential is equal to the energy per particle, but for interacting particles it is not.

3.1.2.1 The Thomas-Fermi Approximation

For sufficiently large clouds, an accurate expression for the ground-state energy may be obtained by neglected the kinetic energy term in the time-independent Gross-Pitaevskii equation. A better approximation for the condensate wave function for large numbers of atoms may be obtained by solving the Gross-Pitaevskii equation, neglecting the kinetic energy term from the start. In Eq. (3.31) GP equation can be written in terms of this approximation [35].

$$(V_{ext}(r) + g|\psi(r)|^2)\psi(r) = \mu\psi(r) \tag{3.32}$$

where, μ is the chemical potential and condensation density n(r) can be written again in terms of the absolute square of the wave function of the condensation in Eq. (3.11);

$$n(r) = |\psi(r)|^2 \tag{3.33}$$

$$|\psi(r)|^2 = \frac{(\mu - V_{ext}(r))}{g} \tag{3.34}$$

This equation has the solution in the region where the right hand side is positive while $\psi = 0$ outside this region. The boundary of the cloud is therefore given by;[35]

$$V(r) = \mu \tag{3.35}$$

The physical content of this approximation is that the energy to add a particle at any point in the cloud is the same everywhere. This energy is given by the sum of the external potential $V(r)$ and an interaction contribution $n(r)g$ which is the chemical potential of a uniform gas having a density equal to the local density $n(r)$. Since this approximation is reminiscent of the Thomas-Fermi approximation in the theory of atoms, it is generally referred to by the same name. For atoms, the total electrostatic potential takes the place of trapping potential and the local Fermi energy that of the mean-field energy $g|\psi|^2 = gn$.

In the Thomas-Fermi approximation the extension of the cloud in the three directions is given by the three semi-axes R_i obtained by inserting Eq. (3.36) anisotropic three dimensional harmonic potential into Eq. (3.35)

$$V(x, y, z) = \frac{1}{2}m(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2) \tag{3.36}$$

$$R_i = \frac{2\mu}{m\omega_i^2} \tag{3.37}$$

The lengths R_i may be evaluated in terms of trap parameters once the chemical potential has been determined. The normalization conditions on ψ, Eq. (3.38) yields a relation between the chemical potential μ and the total number of particles N. For a harmonic trap with a potential given by Eq. (3.36) it can be obtained;

$$N = \int dr|\psi(r)|^2 \tag{3.38}$$

$$N = \int dr \frac{(\mu - V_{ext}(r))}{g} \tag{3.39}$$

$$N = \int dr \frac{\mu}{g} - \int \frac{1}{g} V_{ext}(r) dr \tag{3.40}$$

$$N = \frac{8\pi}{15} \left(\frac{2\mu}{m\bar{\omega}^2}\right)^{3/2} \frac{\mu}{g} \tag{3.41}$$

as may be seen by scaling each spatial coordinate by $(2\mu/m\omega_i^2)^{1/2}$ and integrating over the interior of the unit sphere. Solving Eq. (3.41) for μ following relation between μ and $\hbar\bar{\omega}$:

$$\mu = \frac{15^{2/5}}{2} \left(\frac{Na}{\bar{a}}\right)^{2/5} \hbar\bar{\omega} \tag{3.42}$$

where, $\bar{\omega} = (\omega_1\omega_2\omega_3)^{1/3}$ is the geometric mean of the three oscillator frequencies and $\bar{a} = \sqrt{\hbar/m\bar{\omega}}$ is the widths of the wave function or the characteristic length. [36]

The quantity $\bar{R} = (R_1R_2R_3)^{1/3}$ is a convenient measure of the spatial extent of the cloud. By combining Eq. (3.37) and Eq. (3.42) it can be obtained [36];

$$\bar{R} = \left(\left(\frac{2\mu}{m\omega_1^2}\right)^{1/2} \left(\frac{2\mu}{m\omega_2^2}\right)^{1/2} \left(\frac{2\mu}{m\omega_3^2}\right)^{1/2} \right)^{1/3} \tag{3.43}$$

$$\bar{R} = \left(\frac{2}{m}\sqrt{\frac{2}{m}}\,\mu\sqrt{\mu}\,\frac{1}{\omega_1\omega_2\omega_3} \right)^{1/3} \tag{3.44}$$

$$\bar{R} = 15^{1/5}\left(\frac{Na}{\bar{a}}\right)^{1/5}\bar{a} \tag{3.45}$$

With the replacement of the value of μ in Eq. (3.44), last equation (3.45) can be obtained and this equation implies a relation between $\bar{a}$ that is characteristic length and $\bar{R}$ that is a convenient measure of the spatial extent of the cloud obtained in terms of μ.

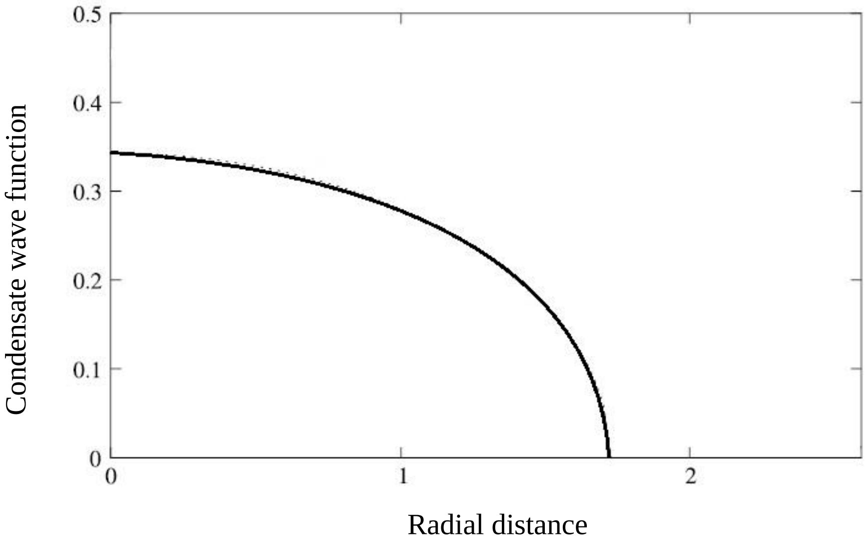

Figure 3.1 The form of the Thomas-Fermi approximation wave function [35].

The form of the Thomas-Fermi approximation wave function is given by in Eq. (3.34) and chemical potential is determined by normalization condition in Eq. (3.38) so, plot of wave function can be drawn in terms of harmonic oscillator length units in this form.

CHAPTER 4

CALCULATIONS

4.1 INTRODUCTION

The time-independent Gross-Pitaevskii equation for a dilute assembly of bosons at *T=0* is given in Eq. (3.31). This equation has the form of non-linear Schrödinger equation for condensed neutral atoms in the different potential and it can be written under different potential. Firstly we start to solve this equation for harmonic potential and then this equation will have been solved for different two potentials that are not investigated in literature up to now.

G-P equation has following form in the external potential.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V_{ext}(r)\psi(r) + Ng|\psi(r)|^2\psi(r) = \mu\psi(r) \tag{4.1}$$

Where, $\psi(r)$ is the Bose-Einstein condensation wave function, m is the mass of single atom, N is the number of atom in the condensate and g value characterizes the atom-atom interaction and it is given by;

$$g = \frac{4\pi\hbar^2 a}{m} \tag{4.2}$$

where, a is the scattering length. This interaction is valid at sufficiently low energies and for s-wave interaction between atoms. For the purpose of this discussion, that a is taken as positive [41].

In the three dimensional space differential volumes unit is equal to $r^2 sin\theta dr d\theta d\varphi$ and because in Eq. (4.1) the norm of $\psi(r)$ wave function must be finite, a transformation should be made [26];

$$\psi(r) = A\frac{\emptyset(r)}{r} \tag{4.3}$$

Bose-Einstein ground state wave function is spherically symmetric, thus it can be write the form of the Eq. (4.3)

where, A is the normalization. Eq. (4.3) can be inserted in Eq. (4.1) but firstly Laplacian operator in Eq. (4.1) should be defined in the three dimensional spherical coordinate.

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{4.4}$$

In Eq. (4.1) ground state wave function only depend on radial part of operator, thus in Eq. (4.4) second and third part is going to zero so, result is given by;

$$\nabla^2\psi(r) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi(r)}{\partial r}\right) \tag{4.5}$$

So, Eq. (4.3) is inserted in Eq. (4.5), Laplacian operator has following form,

$$\nabla^2\psi(r) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\left(A\frac{\emptyset(r)}{r}\right)\right) \tag{4.6}$$

$$\nabla^2\psi(r) = \frac{1}{r}A\frac{d^2\emptyset(r)}{dr^2} \tag{4.7}$$

So, Eq. (4.1) can be written in terms of Eq. (4.3) and Eq. (4.7) and it is given by,

$$-\frac{\hbar^2}{2m}\frac{1}{r}A\frac{d^2\emptyset(r)}{dr^2} + V_{ext}(r)A\frac{\emptyset(r)}{r} + Ng\left|A\frac{\emptyset(r)}{r}\right|^2 A\frac{\emptyset(r)}{r} = \mu A\frac{\emptyset(r)}{r} \tag{4.8}$$

In Eq. (4.8) A and r are reduced and it is given;

$$-\frac{\hbar^2}{2m}\frac{d^2\emptyset(r)}{dr^2}+V_{ext}(r)\emptyset(r)+NgA^2\left|\frac{\emptyset(r)}{r}\right|^2\emptyset(r)=\mu\emptyset(r) \tag{4.9}$$

Eventually, we have obtained a suitable form to apply different potentials. Firstly we handle the harmonic potential for the solution of Gross-Pitaevskii equation after than anharmonic and morse potentials.

4.2 SOLUTION OF GROSS-PITAEVSKII EQUATION FOR DIFFERENT POTENTIALS

4.2.1 Harmonic Oscillator Potential

Last form of Gross-Pitaevskii equation Eq. (4.9) can be investigated in terms of harmonic potential $V_{ext}(r)={}^{1}/_{2}\,m\omega^2r^2$.

To obtain an equation suitable for numerical work, we transform to dimensionless length unit by letting

$$r=\alpha x \tag{4.10a}$$

$$dr=\alpha dx \tag{4.10b}$$

$$\frac{d^2}{dr^2}=\frac{1}{\alpha^2}\frac{d^2}{dx^2} \tag{4.10c}$$

Eq. (4.9) is written in terms of Eqs. (4.10a), (4.10b) and (4.10c) also $V_{ext}(r)=\frac{1}{2}m\omega^2r^2$ is taken and it has following form,

$$-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\frac{d^2\emptyset(x)}{dx^2}+\frac{1}{2}m\omega^2\alpha^2x^2\emptyset(x)+NgA^2\left|\frac{\emptyset(x)}{\alpha x}\right|^2\emptyset(x)=\mu\emptyset(x) \tag{4.11}$$

To get the dimensionless form of Eq. (4.11) we use the transformation given below,

$$\alpha = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \tag{4.12}$$

$$r = \left(\frac{\hbar}{2m\omega}\right)^{1/2} x \tag{4.13}$$

Also, β value is selected as the dimensionless energy,

$$\beta = \frac{2m\alpha^2\mu}{\hbar^2} = \frac{\mu}{\hbar\omega} \tag{4.14}$$

where, according to [26], the value of chemical potential is taken $\mu = \beta\hbar\omega$ so $\mu = 4.3\hbar\omega$, and with same procedure it can be taken like form,

$$\gamma = \frac{2mg}{\hbar^2} = 8\pi a \tag{4.15}$$

where, a is the scattering length and its numerical value is about 3nm also for the solution of our calculation is taken $N{\sim}10^5$ in a trap of frequency 10 Hz. This is a reasonable case that one might expect to realize in the case of alkali-metal atoms, say Cs (Cesium) [26]

Finally, we have obtained dimensionless form of the Eq. (4.11),

$$\frac{d^2\emptyset(x)}{dx^2} + \left[\beta - \frac{x^2}{4} - NA^2\gamma\left(\frac{\emptyset(x)}{x}\right)^2\right]\emptyset(x) = 0 \tag{4.16}$$

Now we can consider Eq. (4.16) as $x \to 0$. The non-linear term inside the square brackets approaches a constant in this limit because of the regularity of the wave function at $x = 0$. Thus we should write the value of wave function at $x = 0$ to solve in terms of second order Runge-Kutta method.

For $x = 0$, Eq. (4.16) has following form.

$$\frac{d^2\emptyset(x)}{dx^2} + \left[\beta - NA^2\gamma\left(\frac{\emptyset(x)}{x}\right)^2\right]\emptyset(x) = 0 \tag{4.17}$$

So, the wave function can be written first two terms of Taylor series at $x = 0$,

$$\emptyset(x) \approx \emptyset(0) + \emptyset'(0)x \tag{4.18}$$

For $x = 0$, we can say that $\emptyset(0) = 0$

For $x = 0$, in Eq. (4.18) $\emptyset'(0)$ is a constant and if Eq. (4.17) can be written in terms of Eq. (4.18) and it is solved at $x = 0$, $\emptyset'(0)$ can be obtained like form,

$$\emptyset'(0) = \left[\frac{\beta}{NA^2\gamma + 1}\right]^{1/2} \tag{4.19}$$

where, the numerical value of initial conditions for harmonic potential and other initial conditions have like form,

$$\emptyset(0) = 0 \qquad\qquad \emptyset'(0) = 2.07155 \tag{4.20}$$

By using Eq. (4.1) G-P Equation, Eq. (4.16) was obtained and for $x = 0$, initial conditions in Eqs. (4.19) and (4.20) were obtained [26].

Another property of the condensate wave function is its mean square radius. In the any experiment, we suppose that there are a lot of particles which are represented by same wave function in the x-axis direction. We can make a lot of measurement to find the position of particles. Although the wave functions of particles are same each other, the position of particles that are measured in all measurement will be different. So it will be important to know the expected value of positions of atoms.

In the Bose-Einstein condensation movement of any particles do not leave other ones therefore in the condensate the movement of all the atoms not take into account separately but take into consideration like movement of a single large atom and movement of any particles is represented by same wave function.

In this case for BEC expected value of position will be important. In addition, the uncertainty around the expected value of position that is the standard deviation defined in the calculation of the probability for position, mean square of position will be important in quantum mechanics.

So we can define the mean square of position following form,

$$\langle r^2 \rangle = \int r^2 \, |\psi(r)|^2 r^2 sin\theta dr d\theta d\varphi \tag{4.21a}$$

$$\langle r^2 \rangle = \frac{4\pi}{N} \int r^4 \, |\psi(r)|^2 dr \tag{4.21b}$$

We can write the x in terms of r, according to Eqs. (4.10a) and (4.13),

$$\langle x^2 \rangle = \frac{4\pi}{N} (\alpha)^5 \int x^4 \, |\psi(x)|^2 dx \tag{4.22}$$

Where, $\alpha = \left(\frac{\hbar}{2m\omega}\right)^{1/2}$ for harmonic potential and it has following form;

$$\langle x^2 \rangle = \frac{4\pi}{N} \left(\frac{\hbar}{2m\omega}\right)^{5/2} \int x^4 \, |\psi(x)|^2 dx \tag{4.23}$$

After the calculations and definitions of system are made, we can obtain the solutions of Gross-Pitaevskii equation by using Wolfram Mathematica 8.0 programs.

We use the Runge-Kutta method for second order differential equation to Eq. (4.16).

As a result, the ground state wave function of condensate under harmonic potential with initial conditions has been obtained for $\psi(x) = A\, \emptyset(x)/x$ and numerical values which are used in this calculation are taken from the [26].

Figure 4.1 gives probability density of bosons particle $|\psi(x)|^2 = A^2|\emptyset(x)|^2/x^2$ at $T = 0$ and at position x under harmonic potential.

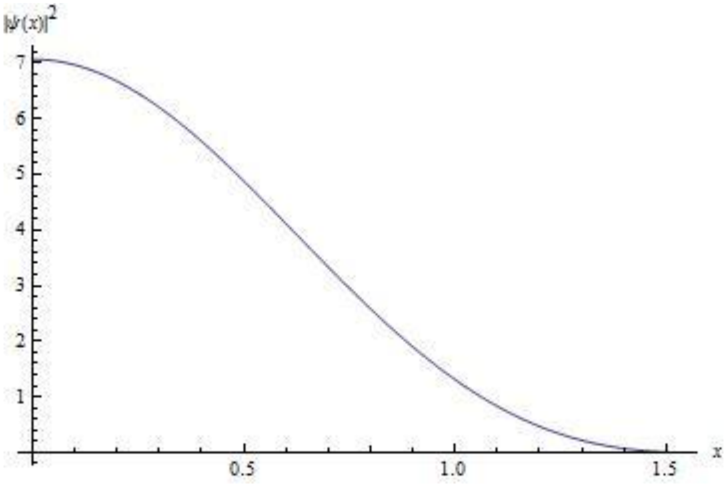

Figure 4.1 Harmonic potential probability density.

Figure 4.1 at absolute zero temperature under harmonic potential large fraction of bosons became in the centre of potential and according to changing distance it is decreasing.

In section 3.1.2 we defined that, eigenvalue is chemical potential in Gross-Pitaevskii equation, not the energy per particle as it is for the usual Schrödinger equation. For non-interacting particle all in the same state the chemical potential is equal to the energy per particle, for interacting particle it is not. That is, there is a relation chemical potential and number of particles and it can be defined statistical law $\delta E = \mu \delta N$ [32]. The effect of changing chemical potential to the position of the atoms in the condensate is seen in Figure 4.2.

For decreasing value of the chemical potential, it seen that the probability density of particle in condensate state decrease. If the getting value of the chemical potential $\mu = 4.3\hbar\omega$ in Figure 4.1 is reduced with step by step $0.2\hbar\omega$, Figure 4.2 is obtained.

In the following table 4.1 these data are given and associated with these data, probability density and mean square radius are calculated.

Table 4.1 For different value of chemical potential, probability density of boson particle and mean square radius are given.

$\beta = \mu/\hbar\omega$	$\lvert\psi(0)\rvert^2$	$\langle x^2 \rangle$	$\beta = \mu/\hbar\omega$	$\lvert\psi(0)\rvert^2$	$\langle x^2 \rangle$
2,1	2.14799	0.00078	3,3	4.1217	0.00151
2,3	2.37175	0.00081	3,5	4.6144	0.00169
2,5	2.63402	0.00096	3,7	5.1572	0.00189
2,7	2.93748	0.00107	3,9	5.7487	0.00211
2,9	3.28494	0.00120	4,1	6.3859	0.00234
3,1	3.67897	0.00135	4,3	7.0636	0.00259

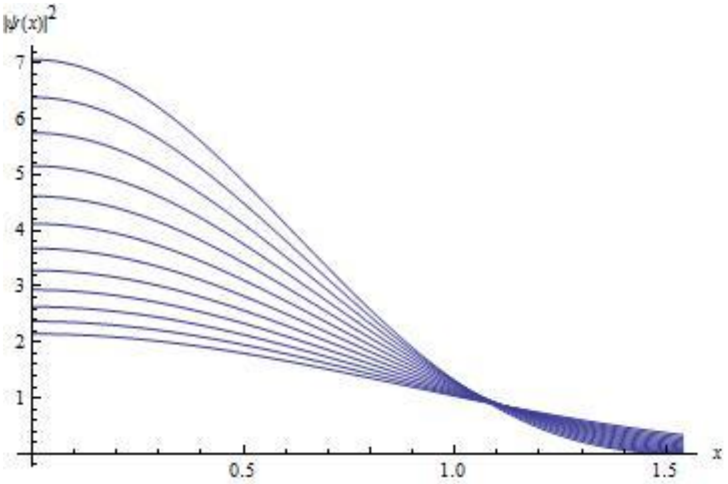

Figure 4.2 Harmonic potential probability density, for changing value of chemical potentials. From (top curve) $4.3\hbar\omega$ to (bottom curve) $2.1\hbar\omega$ chemical potential respectively.

This graph is obtained by using the data given in Table 4.1. For increasing values of the chemical potential the number of particles that become in the center and join the condensation increase.

4.2.2 Anharmonic Oscillator Potential

So far, numerical solution for time-independent Gross-Pitaevskii equation is made for harmonic potential. All calculations which are made for harmonic potential can be made again for both anharmonic and morse potentials.

We can handle time-independent Gross-Pitaevskii equation for anharmonic potential.

Before it is taken numerical solution of Gross-Pitaevskii equation for anharmonic potential, we should make some dimensionless.

Firstly, Eq. (4.9) can be written again for anharmonic potential,

$$V_{ext} = \frac{1}{2} m\omega^2 r^2 + cr^4 \tag{4.24}$$

Where, c is the coupling constant of the quartic term and it can be very small values. Large enough values of r the quartic potential cr^4 eventually supersedes, the harmonic potential $\frac{1}{2}m\omega^2 r^2$ and it can no longer be consider weak.

Gross-Pitaevskii equation under anharmonic potential is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2\emptyset(r)}{dr^2} + \left(\frac{1}{2}m\omega^2 r^2 + cr^4\right)\emptyset(r) + NgA^2\left|\frac{\emptyset(r)}{r}\right|^2 \emptyset(r) = \mu\emptyset(r) \tag{4.25}$$

We transform to dimensionless length unit by Eqs. (4.10a), (4.10b) and (4.10c) so, it has following form.

$$\begin{gathered}-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\frac{d^2\emptyset(x)}{dx^2} + \left(\frac{1}{2}m\omega^2\alpha^2 x^2 + c\alpha^4 x^4\right)\emptyset(x)\\ +NgA^2\left|\frac{\emptyset(x)}{\alpha x}\right|^2 \emptyset(x) = \mu\emptyset(x)\end{gathered} \tag{4.26}$$

After reductions are made, some terms have following form,

$$\alpha = \left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{4.27a}$$

$$z = \frac{2\hbar c}{m^2\omega^3} \tag{4.27b}$$

$$\gamma = \frac{2mg}{\hbar^2} = 8\pi a \tag{4.27c}$$

$$\beta = \frac{2\mu}{\hbar\omega} \tag{4.27d}$$

Finally, to solve a suitable equation is obtained with these terms,

$$\frac{d^2\emptyset(x)}{dx^2} + \beta\emptyset(x) - (x^2 + zx^4)\emptyset(x) + \gamma N A^2 \left|\frac{\emptyset(x)}{x}\right|^2 \emptyset(x) = 0 \tag{4.28}$$

Now we can consider Eq. (4.28) as $x \to 0$. The non-linear term inside the square brackets approach a constant in this limit because of the regularity of the wave function at $x = 0$. In Eq. (4.28) the term of $(x^2 + zx^4)$ is going to zero while x is going to zero, so with same procedure in harmonic oscillator calculations, initial conditions Eq. (4.20) can be obtained again and same numerical values can be applied.[26]

The mean square radius defined in Eq. (4.22) for harmonic, it can be written again in terms of $\alpha = \sqrt{\frac{\hbar}{m\omega}}$ for anharmonic potential.

$$\langle x^2 \rangle = \frac{4\pi}{N}\left(\frac{\hbar}{m\omega}\right)^{5/2} \int x^4\, |\psi(x)|^2 dx \tag{4.29}$$

After the calculation and definitions of system, we can be obtained the ground state wave function of condensate under anharmonic potential. In this solution wave function is $\psi(x) = A\,\emptyset(x)/x$ and following Figure 4.3 gives probability density of bosons particle $|\psi(x)|^2 = A^2|\emptyset(x)|^2/x^2$ at $T = 0$, and at position x under anharmnic potential.

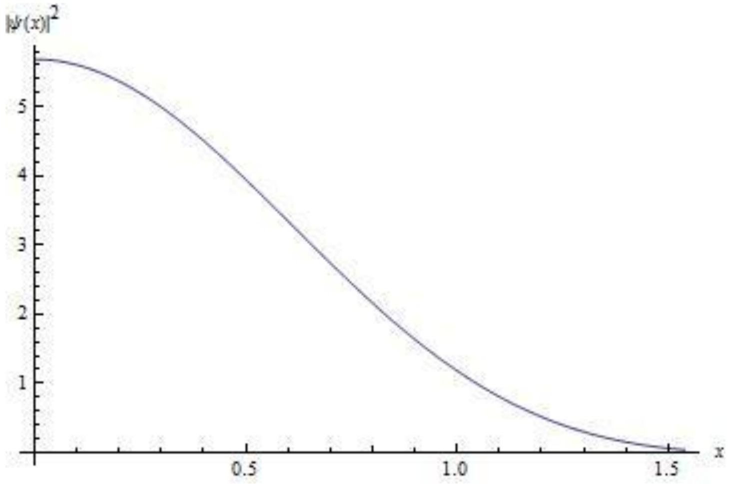

Figure 4.3 Anharmonic potential probability density

Figure 4.3 at absolute zero temperature under anharmonic potential large fraction of bosons became in the centre of potential and according to changing distance it is decreasing.

Numerical values which have been used in harmonic potential solutions can be used for anharmonic solutions too, in Figure 4.4 so we can obtain following Table 4.2.

Table 4.2 For different value of chemical potential, probability density of boson particle and mean square radius are given.

$\beta = 2\mu/\hbar\omega$	$\lvert\psi(0)\rvert^2$	$\langle x^2\rangle$	$\beta = 2\mu/\hbar\omega$	$\lvert\psi(0)\rvert^2$	$\langle x^2\rangle$
2,1	1.4814	0.00308	3,3	3.0415	0.00632
2,3	1.6498	0.00343	3,5	3.4577	0.00719
2,5	1.8496	0.00384	3,7	3.9286	0.00817
2,7	2.0848	0.00433	3,9	4.4567	0.00926
2,9	2.3591	0.00490	4,1	5.0429	0.01048
3,1	2.6766	0.00556	4,3	5.6865	0.01182

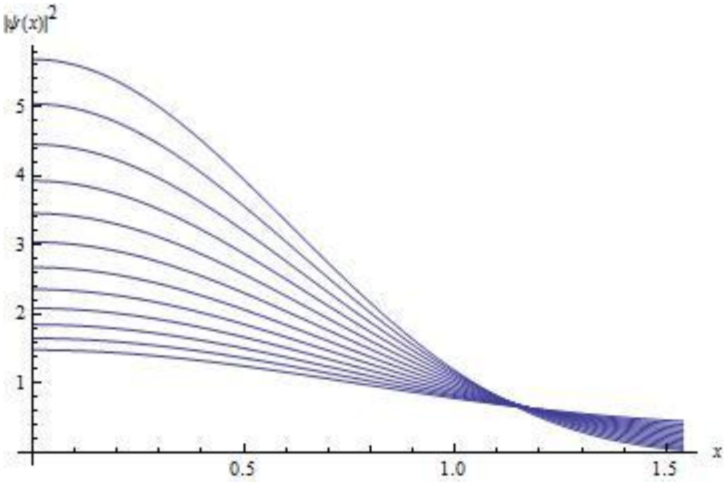

Figure 4.4 Anharmonic potential probability density for changing value of chemical potentials. From (top curve) $4.3\hbar\omega$ to (bottom curve) $2.1\hbar\omega$ chemical potential respectively.

This graph is obtained by using the data given in Table 4.2. Same situation with harmonic potential can be seen in Figure 4.4, for increasing values of the chemical potential the number of particles that become in the center and join the condensation increase.

4.2.3 Morse Potential

Another interesting potential in this study is morse potential which is a convenient model for the potential of a diatomic molecule. It is a better approximation for the vibrational structure of molecule than harmonic oscillator because it explicitly includes the effects of bond breaking, such as the existence of unbound states. It also accounts for the anharmonicty of real bonds and the non-zero transition probability for overtone and combination bands. The morse potential can also be used to model other interactions such as the interaction between an atom and surface. The morse potential energy function is of the form $V(r) = D(1 - exp\ b(-r + r_e))^2$,

Here r is the distance between the atoms. r_e is the equilibrium bond distance so we can get zero it. D is the well depth and b controls the width of the potential.

Since the zero of potential energy is arbitrary, the equation for morse potential can be rewritten any number of ways by adding or subtracting a constant value. When it is used to model the atom surface interaction, the morse potential is usually written in the following form,

$$V_{ext}(r) = D(exp(-2br) - 2exp\ (-br)), \tag{4.30}$$

Eq. (4.9) can be written for Eq. (4.30) again and letting $b = 1$,

$$-\frac{\hbar^2}{2m}\frac{d^2\emptyset(r)}{dr^2} + D(e^{-2r} - 2e^{-r})\emptyset(r) + NgA^2\left|\frac{\emptyset(r)}{r}\right|^2 \emptyset(r) = \mu\emptyset(r) \tag{4.31}$$

We transform to dimensionless length unit by Eqs. (4.10a), (4.10b) and (4.10c) so, it has following form for $b = 1$. So Eq. (4.31) can be written following form.

$$\begin{gathered}-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\frac{d^2\emptyset(x)}{dx^2} + D(e^{-2\alpha x} - 2e^{-\alpha x})\emptyset(x) \\ +NgA^2\left|\frac{\emptyset(x)}{\alpha x}\right|^2 \emptyset(x) = \mu\emptyset(x)\end{gathered} \tag{4.32}$$

After reductions are made, some terms have following form,

$$\alpha = \left(\frac{\hbar}{2mD}\right)^{1/2} \tag{4.33a}$$

$$r = \left(\frac{\hbar}{2mD}\right)^{1/2} x \tag{4.33b}$$

Also, β and γ can be written, and same values of Eqs. (4.14) and (4.15) can be got,

$$\beta = \frac{2m\alpha^2\mu}{\hbar^2} = \frac{\mu}{D} \tag{4.34a}$$

$$\gamma = \frac{2mg}{\hbar^2} = 8\pi a \tag{4.34b}$$

The chemical potential $\mu = \beta D = 4.3D$ and $D = 1$,

Finally, to solve a suitable form of equation is obtained,

$$\frac{d^2\emptyset(x)}{dx^2} + \left[\beta - (e^{-2\alpha x} - 2e^{-\alpha x}) - NA^2\gamma\left(\frac{\emptyset(x)}{x}\right)^2\right]\emptyset(x) = 0 \qquad (4.35)$$

Also, same procedure for harmonic potential can be made $x \to 0$ and numerical values of initial conditions have the form,

$$\emptyset'(0) = \left[\frac{\beta + 1}{NA^2\gamma + 1}\right]^{1/2} = 2{,}30125 \qquad (4.36a)$$

$$\emptyset(0) = 0 \qquad (4.36b)$$

The mean square radius defined in Eq. (4.22), it can be written again in terms of $\alpha = \left(\frac{\hbar}{2mD}\right)^{1/2}$ for morse potential.

$$\langle x^2\rangle = \frac{4\pi}{N}\left(\frac{\hbar}{2mD}\right)^{5/2}\int x^4\,|\psi(x)|^2 dx \qquad (4.37)$$

After the calculation and definitions of system, we can be obtained the ground state wave function of condensate for morse potential. In this solution wave function is $\psi(x) = A\,\emptyset(x)/x$ and following Figure 4.5 gives probability density of bosons particle $|\psi(x)|^2 = A^2|\emptyset(x)|^2/x^2$ at $T = 0$, and at position x under morse potential.

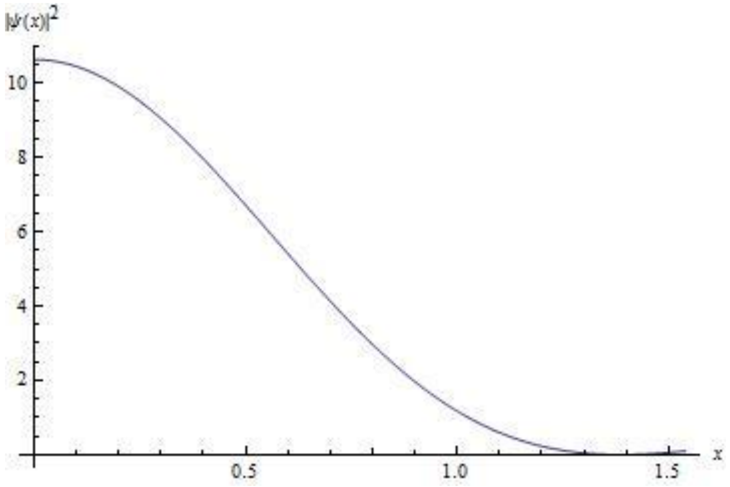

Figure 4.5 Morse potential probability density.

Figure 4.5 at absolute zero temperature under morse potential large fraction of bosons became in the centre of potential and according to changing distance it is decreasing.

Numerical values which have been used both in harmonic potential and anharmonic potential solutions can be used too for morse potential solutions, in Figure 4.6 so we can obtained following Table 4.3 for $D = 1$.

Table 4.3 For different value of chemical potential, probability density of boson particle and mean square radius are given.

$\beta = \mu/D$	$\lvert\psi(0)\rvert^2$	$\langle x^2\rangle$	$\beta = \mu/D$	$\lvert\psi(0)\rvert^2$	$\langle x^2\rangle$
2,1	3.620	0.00133	3,3	6.965	0.00256
2,3	4.056	0.00149	3,5	7.670	0.00281
2,5	4.542	0.00166	3,7	8.401	0.00308
2,7	5.078	0.00186	3,9	9.147	0.00336
2,9	5.662	0.00208	4,1	9.896	0.00363
3,1	6.293	0.00231	4,3	10.635	0.00390

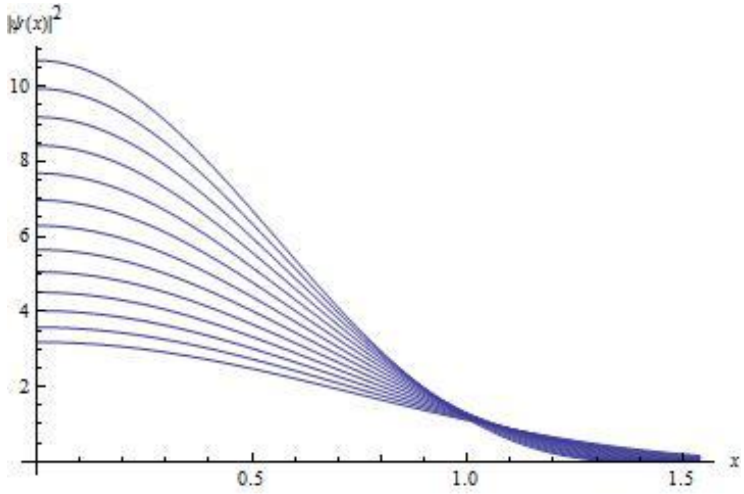

Figure 4.6 Morse potential probability density for changing value of chemical potentials. From (top curve) $4.3\hbar\omega$ to (bottom curve) $2.1\hbar\omega$ chemical potential respectively.

This graph is obtained by using the data given in Table 4.3. Same situation with harmonic potential and anharmonic potential can be seen in Figure 4.4, for increasing values of the chemical potential the number of particles that become in the center and join the condensation increase.

4.3 THOMAS-FERMI APPROXIMATION

4.3.1 Harmonic Oscillator Potential

Thomas-Fermi approximation was defined in section 3.1.2.1 for sufficiently large clouds, an accurate expression for the ground-state energy may be obtained by neglected the kinetic energy term in the time-independent Gross-Pitaevskii equation. A better approximation for the condensate wave function for large numbers of atoms may be obtained by solving the Gross-Pitaevskii equation, neglecting the kinetic energy term. As defined in this section Eq. (3.34) is written again for harmonic potential $V_{ext} = \frac{1}{2}m\omega^2 r^2$, it can be obtained following form, [26]

$$|\psi(r)|^2 = \frac{\left(\mu - \frac{1}{2}m\omega^2 r^2\right)}{g} \tag{4.38}$$

Also, condensate density and number of particle have following form,

$$n(r) = |\psi(r)|^2 \tag{4.39a}$$

$$N(r) = \int |\psi(r)|^2 \, dV \tag{4.39b}$$

Eq. (4.38) has the solution in the region where the right hand side is positive while $\psi = 0$ outside this region. The boundary of the cloud is therefore given by;

$$V(r) = \mu \tag{4.40}$$

as may be seen by scaling each spatial coordinate by $(2\mu/m\omega_i^2)^{1/2}$ and according to solution of Eq. (4.39b) chemical potential can be obtained like form, [26]

$$\mu = \left[\frac{15Ng}{8\pi}\right]^{\frac{2}{5}} \left(\frac{1}{2}m\omega^2\right)^{3/5} \tag{4.41}$$

By using Eq. (4.38) and Eq. (4.41) we can obtain following graph for harmonic potential. This graph shows the probability density of this approximation for harmonic potential.

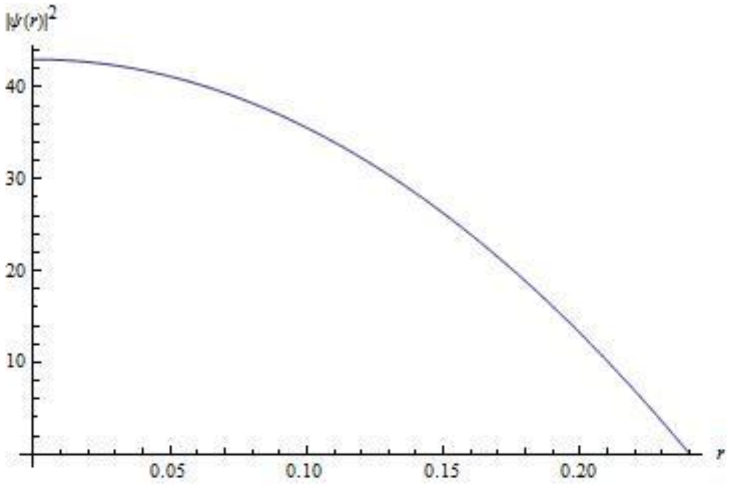

Figure 4.7 Thomas-Fermi approximation probability density of bosons particles for harmonic potential.

In Figure 4.7 by using Thomas-Fermi approximation the probability density versus position plotted for the system with large number of particles. In this graph, particles are spread over a large proportion and majority of them are not distributed over the center of system like exact solution in Figure 4.1.

After, Figure 4.7 is obtained; by using Eq. (4.41) number of particle versus chemical potential can be plotted in Figure 4.8 [26].

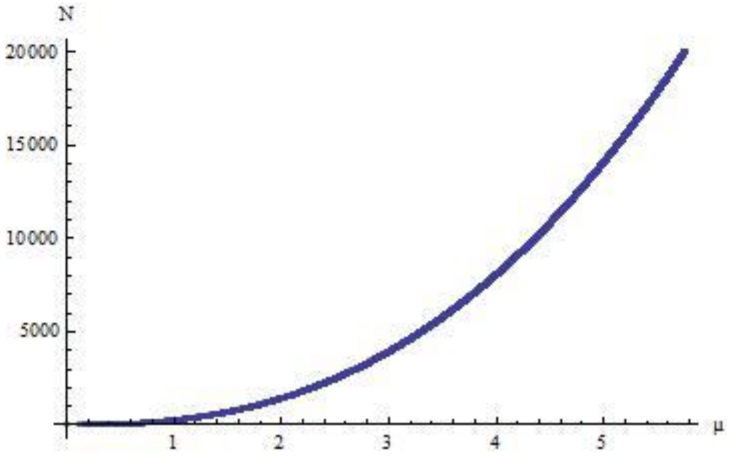

Figure 4.8 A plot of the number of condensate atoms as a function of the chemical potential for harmonic potential.

This graph the number of condensate atoms as a function of the chemical potential and it is obtained by using Thomas-Fermi approximation. As seen in Figure 4.8 the number of condensate atoms increased in direct proportion to the increased of chemical potential.

4.3.2 Anharmonic Potential

After Figures 4.7 and 4.8 were obtained for harmonic potential, for systems which have increasing the number of particles, Thomas-Fermi approximation wave function can be obtained under anharmonic potential too. According to the approximation, Eq. (3.34) can be written again for Eq. (4.24) and chemical potential can be obtained again the name of Eqs. (4.39a), (4.39b) and (4.40). According to Eq. (4.40) chemical potential can be scaled spatial coordinate by $\frac{1}{2}\left(\frac{-m\omega^2+\sqrt{16\mu c+m^2\omega^4}}{c}\right)^{1/2}$ which are boundary conditions of potential. Also chemical potential can be obtained with same procedure in the harmonic potential solution but mathematical results give us very large roots in program so it is not given in here.

Finally, we can plot the Gross-Pitaevskii equation for Thomas-Fermi approximation under anharmonic potential. This graph is the probability density of this approximation for anharmonic potential.

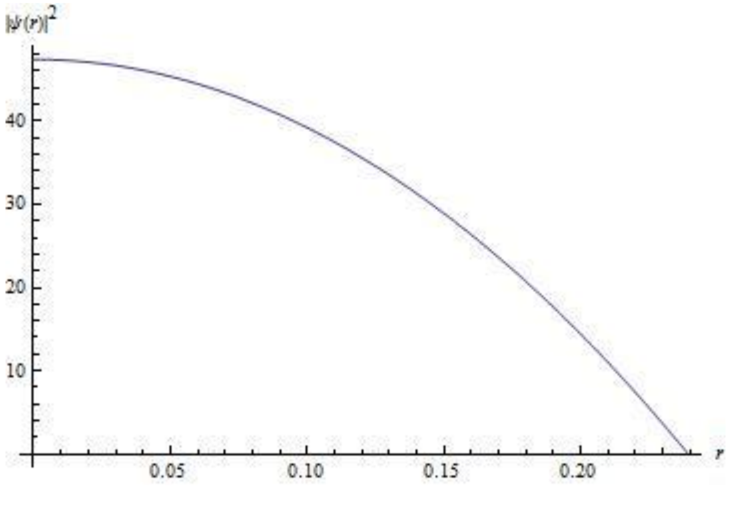

Figure 4.9 Thomas-Fermi approximation probability density of bosons particles for anharmonic potential.

In Figure 4.9 by using Thomas-Fermi approximation the probability density versus position plotted for the system with large number of particles. In this graph, particles are spread over a large proportion and majority of them are not distributed over the center of system like exact solution in Figure 4.3.

After, Figure 4.9 is obtained; by using root of chemical potential which is found by the mathematical program for Thomas-Fermi approximation under anharmonic potential number of particle versus chemical potential can be plotted in Figure 4.10.

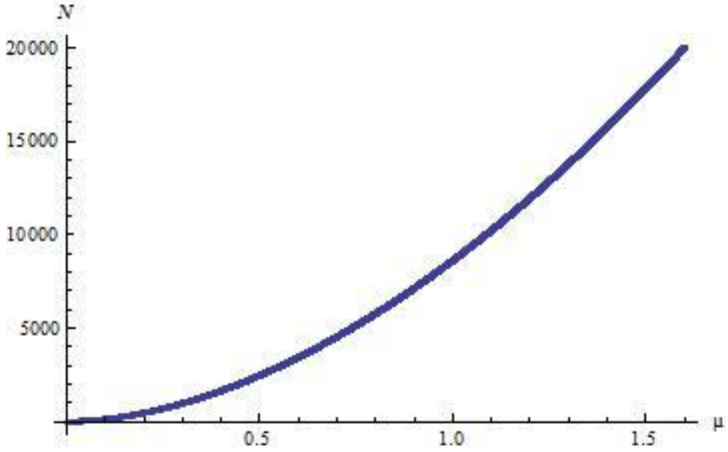

Figure 4.10 A plot of the number of condensate atoms as a function of the chemical potential for anharmonic potential.

This graph the number of condensate atoms as a function of the chemical potential and it is obtained by using Thomas-Fermi approximation. As seen in Figure 4.10 the number of condensate atoms increased in direct proportion to the increased of chemical potential

4.3.3 Morse Potential

After Thomas-Fermi approximation wave functions both harmonic and anharmonic potentials were obtained, for systems which have increasing the number of particles, Thomas-Fermi approximation can be obtained for morse potential too with same procedure. According to this approximation Eq. (3.34) can be written again for morse potential Eq. (4.30) and chemical potential can be obtained again the name of Eqs. (4.39a), (4.39b) and (4.40). According to Eq. (4.40) chemical potential can be scaled spatial coordinate by $log\left(\frac{-D\sqrt{D^2+D\mu}}{\mu}\right)/b$ which are boundary conditions of potential. Also chemical potential can be obtained with same procedure in the both harmonic potential solution and anharmonic potential solution but mathematical results give us very large roots in program so we cannot write here.

Finally we can plot the Gross-Pitaevskii equation for Thomas-Fermi approximation under morse potential. This graph is the probability density of this approximation for anharmonic potential with same procedure both harmonic and anharmonic potential.

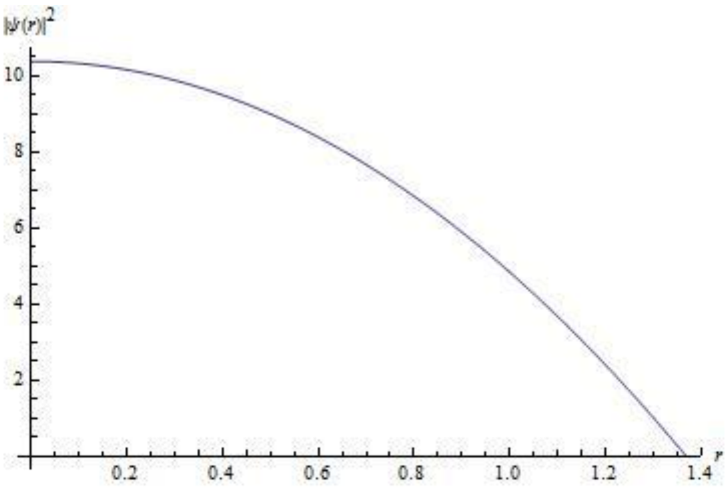

Figure 4.11 Thomas-Fermi approximation probability density of bosons particles for morse potential.

In Figure 4.11 by using Thomas-Fermi approximation the probability density versus position plotted for the system with large number of particles. In this graph, particles are spread over a large proportion and majority of them are not distributed over the center of system like exact solution in Figure 4.5.

After, Figure 4.11 is obtained; by using root of chemical potential which is found by the mathematical program for Thomas-Fermi approximation under morse potential number of particle versus chemical potential can be plotted in Figure 4.12.

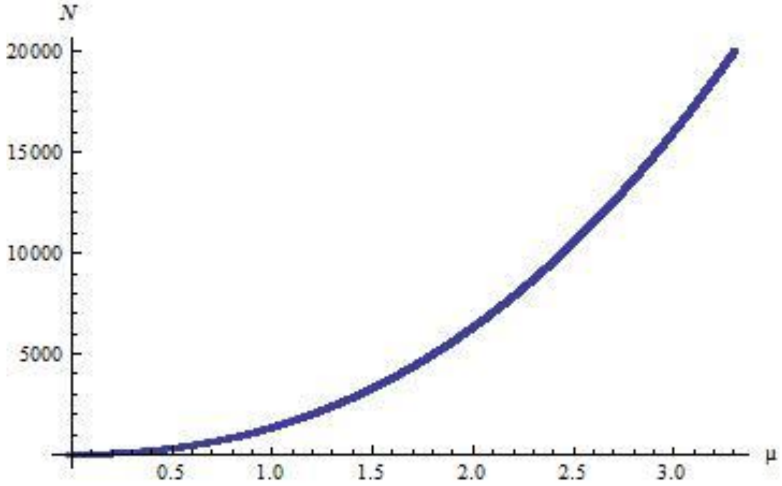

Figure 4.12 A plot of the number of condensate atoms as a function of the chemical potential for morse potential.

This graph the number of condensate atoms as a function of the chemical potential and it is obtained by using Thomas-Fermi approximation. As seen in Figure 4.12 the number of condensate atoms increased in direct proportion to the increased of chemical potential.

CHAPTER 5

CONCLUSION

Bose-Einstein condensation is a phase transition at absolute zero temperature. While a system which comprises alkali bosons gas atoms shows behavior of classical gas at high temperature limits, the system with decreasing temperature gas shows behavior of quantum gas and at absolute zero temperature Bose-Einstein condensation occurs. In this situation particles that become in this system occupy the ground energy state. The motions of particles are not distinguished from each other and all of them begin to behave as the movement of a single particle so as a result of such situation the particles which becomes in the system can be represented with one condensate wave function. The equation which describes such a system and wave function is the solution of Gross-Pitaevskii equation or in other words non-linear Schrödinger equation.

In this thesis, Gross-Pitaevskii equation is handled for different potentials. First potential is harmonic oscillator potential and the solution of this potential is investigated in literature [26]. The other two potentials are anharmonic and morse potentials.

In the solution of the literature for harmonic potential by using the same numerical data with Runge-Kutta method condensate wave function are obtained. By using this solution, change in condensate probability density of particles are shown in Figure 4.1. This graph is represented probability density versus width of potential. With same procedure, both anharmonic and morse potential are drawn to obtained condensate probability density in Figures 4.3 and 4.5 respectively. In the center of potential, it is observed that there is an increase in the number of particles participating condensation in these three graphs. Also in these graphs, a decrease in the number of particles towards the boundary of potential can be seen.

As we defined in section 4.2.1, it can be seen that when the chemical potential decreases, the number of particles which participating in condensation decreases too in the system. This situation can be seen for harmonic oscillator potential in Figure 4.2, for anharmonic potential in Figure 4.4 and for morse potential in Figure 4.6. These figures are drawn for all potential from larger chemical potential to low chemical potential. For these potentials, it is seen that number of particles that become in the center of potential decreases towards from high to low chemical potentials. It is concluded that chemical potential and number of particles participating in condensation is proportional to each other. Also in the these three graphs, it is seen that if the chemical potential is low, particles become on a large extent in the each region of potential but in the large value of chemical potential, particles concentrate towards to center of potential on the large scale. The solution of Gross-Pitaevskii equation that is probability density of condensation is obtained both different potentials and different chemical potentials.

By using Thomas-Fermi approximation for these three potentials probability density of condensation are obtained and their graphs are given in Figure 4.7, Figure 4.9 and Figure 4.11 respectively. Because this approximation is used for larger number of particles, numerical value of chemical potential are not used like in the exact solutions, it is derived as a function of number particle from Eq. (3.34) for all potentials. In the approximation these graphs show similarity with graphs of exact solutions. While an increase in the number of particles is observed in the center of potentials, particles distribute with small change towards the boundary of potential and it is zero in the boundary. If we consider these there graphs there are most number of particles in the center of morse potential contrary to harmonic and anharmonic potential, also it can be seen that morse potential have similar density distribution with exact solution of morse potential when it is used same boundary of potential.

It can be seen that whereas the majority of particles participating condensation accumulate in the center of potential, the minority of particles participating condensation accumulate in the boundary of potential in the both exact solution and Thomas-Fermi approximation solution of Gross-Pitaevskii equation for the these three potentials. Particles also distribute almost equal ratio in these potentials for Thomas-Fermi approximation and it shows similar distribution with the exact solutions in the solution of low chemical potential but note that only graphically representation shows similarity boundary values of potential are different except morse potential.

In Thomas-Fermi approximation, graphs of probability density for each three potentials are obtained by using Eq. (3.34) and Eq. (3.38) and for each potential, chemical potential is defined as a function number of particles. According to these functions the graph of chemical potential versus number of particles are obtained for harmonic potential and they are given in Figure 4.8, for anharmonic potential in Figure 4.10 and for morse potential in Figure 4.12. It can be seen in each graph, an increase of number of particles cause an increase of chemical potential

These investigations help us understand the behavior of alkali bosons gases atoms at absolute zero temperature. We have analyzed two potential additionally to harmonic oscillator potential.

There are important physical results of Bose-Einstein condensation. All atoms reaching ground energy state and behave like single particle so Bose-Einstein condensation explains quantum processes in macroscopic scale.

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