

การแก้ปัญหาของโบนอนที่มีประจุที่ถูกกักแบบไม่ขึ้นกับทิศทางโดยการอินทิเกรตตามวิถี



นายชาคริต นวลฉิมพลี

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต

สาขาวิชาฟิสิกส์ ภาควิชาฟิสิกส์

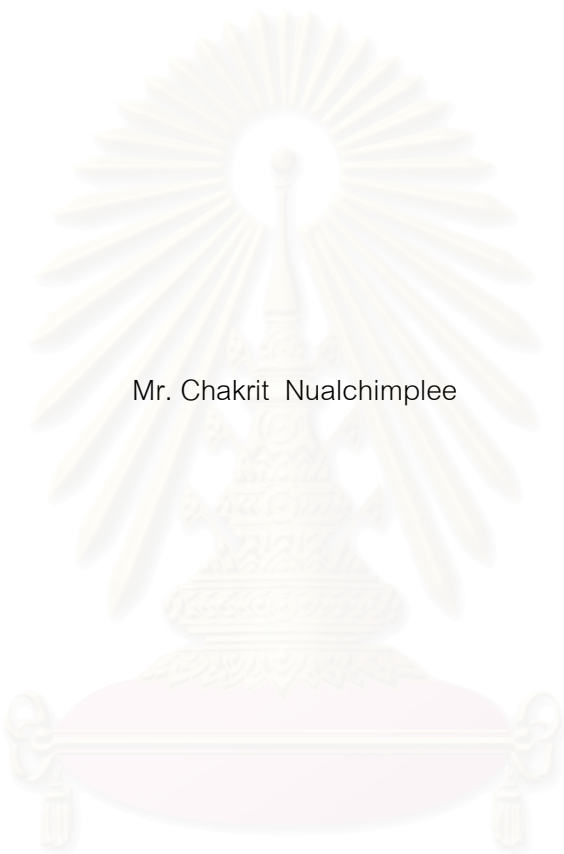
คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย

ปีการศึกษา 2544

ISBN 974-17-0273-6

ลิขสิทธิ์ของจุฬาลงกรณ์มหาวิทยาลัย

PATH INTEGRATION APPROACH TO CHARGED BOSONS IN AN ISOTROPIC TRAP



Mr. Chakrit Nualchimplee

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science in Physics

Department of Physics
Faculty of Science
Chulalongkorn University
Academic Year 2001
ISBN 974-17-0273-6

Thesis Title Path Integration Approach to Charged Bosons in an Isotropic Trap
By Mr. Chakrit Nualchimplee
Field of Study Physics
Thesis Advisor Professor Virulh Sa-yakanit, F.D.

Accepted by the Faculty of Science, Chulalongkorn University in Partial
Fulfillment of the Requirements for the Master 's Degree

..... Deputy Dean for Administrative Affairs
(Associate Professor Pipat Karntiang, Ph.D.) Acting Dean, Faculty of Science

THESIS COMMITTEE

..... Chairman
(Assistant Professor Pisistha Ratanavararaksa, Ph.D.)

..... Thesis Advisor
(Professor Virulh Sa-yakanit, F.D.)

..... Member
(Associate Professor Mayuree Natenapit, Ph.D.)

..... Member
(Rujikorn Dhanawittayapol, Ph.D.)

นาย ชาคกริต นวลฉิมพลี : การแก้ปัญหาของโบซอนที่มีประจุที่ถูกกักแบบไม่ขึ้นกับทิศทางโดยการอินทิเกรตตามวิถี (PATH INTEGRATION APPROACH TO CHARGED BOSONS IN AN ISOTROPIC TRAP) อ. ที่ปรึกษา : ศ. ดร. วิรุพห์ สายคณิต, 83 หน้า. ISBN 974-17-0273-6.

วิทยานิพนธ์ฉบับนี้นำเสนอ การศึกษาโบซอนที่มีประจุที่ถูกกักแบบไม่ขึ้นกับทิศทางโดยประยุกต์ใช้วิธีการอินทิเกรตตามวิถีแบบพายน์แมน ซึ่งค่าขอบเขตบนของพลังงานสถานะพื้นสามารถคำนวณได้โดยการประยุกต์เทคนิคการอินทิเกรตตามวิถีแบบแปรผัน นอกจากนี้ได้คำนวณเมตริกซ์ความหนาแน่นโดยการประมาณ และคำนวณฟังก์ชันคลื่นด้วย และได้เปรียบเทียบพลังงานสถานะพื้นกับผลที่ได้จากวิธีการของกินส์เบิร์ก – ปีเตเยฟสกี – กรอสส์ ซึ่งพบว่าผลการคำนวณที่ได้สอดคล้องกัน นอกจากนี้เมื่อละทิ้งผลจากศักย์กักขังคูลอมบ์ ที่เกิดในพลังงานสถานะพื้นในกรณีของศักย์กักขังคูลอมบ์ เราจะพบพลังงานสถานะพื้นของศักย์คูลอมบ์เป็นตามที่คาดหมายไว้

สถาบันวิทยบริการ จุฬาลงกรณ์มหาวิทยาลัย

ภาควิชา ฟิสิกส์
สาขาวิชา ฟิสิกส์
ปีการศึกษา 2544

ลายมือชื่อนิสิต

ลายมือชื่ออาจารย์ที่ปรึกษา

4172268023: MAJOR PHYSICS

KEY WORD: BOSE – EINSTEIN CONDENSATION / CHARGED BOSONS / PATH INTEGRATION
 CHAKRIT NUALCHIMPLEE: PATH INTEGRATION APPROACH TO
 CHARGED BOSONS IN AN ISOTROPIC TRAP. THESIS ADVISOR:
 PROF. VIRULH SA-YAKANIT, F.D., 83 pp. ISBN 974-17-0273-6.

In this thesis, the case of charged bosons confined in an isotropic magnetic trap is studied by using Feynman path integration. We show that the upper bound of the ground state energy can be evaluated by applying the variational path integral technique. Consequently, the approximated density matrix and wavefunction are obtained. The ground state energy is then compared with the result obtained by Ginzburg – Pitaevskii – Gross approach. It is shown that our result agrees with such an approach. Furthermore, from our result, when we neglect the effect of screened Coulomb potential in the ground state energy of the screened Coulomb case, the ground state energy of the Coulomb potential arises as expected.



สถาบันวิทยบริการ
 จุฬาลงกรณ์มหาวิทยาลัย

Department of Physics

Field of study: Physics

Academic year 2001

Student's signature.....

Advisor's signature.....

Acknowledgements

The author would like to express his deep gratitude to his advisor Professor Virulh Sa-yakanit for his valuable advice, discussion and help. Thanks also go without saying to the thesis committee, Assistant Professor Pisistha Ratanavararaksa, Associate Professor Mayuree Natenapit, Dr. Rujikorn Dhanawittayapol for their reading and criticizing the manuscript.

Thanks are also due to Mr. Kobchai Tayanasant and Mr. Boonlit Krunavakarn for their uncountable advice, suggestion and assistance in calculating many parts of the thesis. He is grateful to Mr. Natthapon Nakpathomkun, Mr. Sarun Phibanchon and Mr. Sorakrai Srisuphaphon for their valuable suggestion.

Sincerely, he would like to thank Dr. Thiranee Khumlumlert, Mr. Chanruangrith Channok, Miss Suwicha Wannawichian, Miss Kamonporn Klappong, Mr. Pornjuk Srepusharawoot and Mr. Yuttakan Ratthanachai for their assistance in typing many parts of the thesis. Special thanks are given to Miss Pennapa Didkaew for her warmly helping and supporting.

Finally, he would like to show invaluable appreciation to his parents, Mr. Chao and Mrs. Namkang Nualchimplee for their heartening all the time.

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Contents

Abstract in Thai	iv
Abstract in English	v
Acknowledgements	vi
Contents	vii
List of Figures	ix
Chapter 1 Introduction	1
Chapter 2 Feynman Path Integrals	9
2.1 Feynman Propagator	9
2.2 Propagator from Schrödinger Equation	12
2.3 Variational Path Integration	20
Chapter 3 Bose-Einstein Condensation: Ginzburg-Pitaevskii-Gross Approach	22
3.1 Ginzburg-Pitaevskii-Gross Equation: Time-independent Case	23
3.2 Gross-Pitaevskii Equation: Time-dependent Case	27
3.3 Free Bose Gas: Non-interacting Case	28
3.4 Ground State Energy from the Thomas-Fermi Approximation	31
3.5 Ground State Energy of Neutral Bosons: Short-range Interaction Case	33
3.6 Ground State Energy of Charged Bosons: Long-range Interaction Case	36
Chapter 4 Results	39
4.1 Ground State Energy with Coulomb Potential	39
4.2 Ground State Energy with Screened Coulomb Potential	53

Contents (cont.)

Chapter 5 Discussion and Conclusion	61
References	64
Vitae	70



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

List of Figures

Figure	Page
Figure 2.1	Diagram showing how the path integrals can be constructed.....12
Figure 2.2	Diagram showing a path deviating from the classical path.....18



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Chapter 1

Introduction

The Bose-Einstein Condensation(BEC) [1-4] is one of the most remarkable phenomena in quantum many-body system. The condensation is a logical consequence of the Bose-Einstein statistics: a gas of non-interacting bosonic atoms, below a certain temperature, suddenly develops a macroscopic population in the lowest energy quantum mechanical state.

According to quantum mechanics, all particles belong to one of two kinds, bosons or fermions, named after the scientists who first introduced them, S.N. Bose and E. Fermi. Bosons are particles which have integer spin; the angular momentum of the particle is 0, 1, 2, 3, and so on, in units of the reduced Planck constant $\hbar = h/2\pi$. Fermions are particles which have half-integral spin: 1/2, 3/2, 5/2, and so on, in the same units.

Moreover, another major different between bosons and fermions is that fermions are subject to the Pauli exclusion principle, while bosons are not. Put in simple term, this means that no two fermions can be in the same state at the same time, while bosons do not suffer from such a restriction. On the contrary, they have a tendency to accumulate in the same state. Fermions are repelled by each other, while bosons are attracted under the effect of the so-called exchange force. There are some classic examples. Both photons and phonons are examples of bosons, while protons, neutrons and electrons are examples of fermions.

Furthermore, we have known from quantum statistics that at ultra-low temperature the de Broglie wavelength, λ_{db} , of atoms becomes extremely large, then they begin to feel that they are not isolated, even at low density. It is

as if the atoms had long tentacles that allow them to probe their environment and notice the presence of other atoms. One of two things can then happen, depending upon whether the atoms are bosons or fermions: Fermions start to repel each other so as to make to sure that no two of them are in the same state. Bosons, on the other hand, begin to attract each other, attempting to all occupy the same state. At absolute zero temperature, all atoms eventually condense into the lowest energy state. This is the phenomenon of Bose-Einstein condensation.

Basically, we can say that Bose-Einstein condensation is a phase transition that occurs when a collection of identical bosons is cooled to the point that their quantum mechanical de Broglie wave overlaps. The basic physics of this phase transition is worked out in every text in statistical mechanics [5]. But the most important point is that Bose-Einstein condensation occurs only at quite low temperatures. The de Broglie wavelength, λ_{db} , is equal to \hbar/p , where \hbar is Planck constant and p is the momentum of the particle. At temperature T , typical value of p will be $(2mk_B T)^{\frac{1}{2}}$, where m is the mass of the particle and k_B is Boltzmann's constant. The precise condition for Bose-Einstein condensation to occur is that

$$n\lambda_{db}^3 = n \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{\frac{3}{2}} = 2.612 \quad (1.1)$$

where n is the number density of the particles.

Originally, in 1925, Bose-Einstein condensation was predicted by Einstein that a non-interacting gas of atoms (bosons) would undergo a phase transition at low temperature, when a macroscopic number of atoms occupy the lowest energy level (in a uniform ideal Bose gas, this is the zero momentum single-particle state). His work was inspired by a novel derivation of the Planck distribution for photons by Bose in 1924.

For many years, however, Bose-Einstein condensation had been regarded as a mathematical artifact. Until 1938, the theory of Bose-Einstein condensation was first applied to superfluid liquid helium [6,7] and shortly thereafter was used to explain superconductivity in metals at low temperature [8]. These two branches of condensed matter physics have been enormously important research since their inception.

Subsequently, in the 1970's, efforts started to observe Bose-Einstein condensation in a dilute vapor of spin-polarized hydrogen [9], whose inter-atomic interaction is sufficiently weak and well understood. However, Bose-Einstein condensation in the hydrogen gas was not achieved for a long time, because of the existence of inelastic inter-atomic collisions, which cause trap loss and heating. Nevertheless, several of the key ideas that led to success in alkali atoms in 1995 grew out of the pioneering work on hydrogen gas in the 1970's.

Afterwards, in 1993, the evidence of Bose-Einstein condensation in a gas of excitons in a semi-conductor host has been observed [10]. Although the interactions in these systems are weak, little information about them is known, and thus it is difficult to understand the net effect of Bose-Einstein condensation in the exciton gas. Furthermore, attention has also focused on the alkali atoms: Li, Na, K, Rb and Cs. The atoms are bosons, with an even number of neutrons. Moreover, by combinations of various new technologies developed in atomic physics such as laser cooling and trapping [11], evaporation cooling and magnetic trap have made it possible to observe Bose-Einstein condensation of alkali atoms in controllable situations. The essential idea behind laser cooling is that when an atom absorbs a photon, it slows down.

In 1995, Bose-Einstein condensation was observed in a series of experi-

ments on vapors of ^{87}Rb [12], ^7Li [13, 14], and ^{87}Na [15] in which the atoms were confined in magnetic traps and cooled down to extremely low temperature of the order of $10^{-6} - 10^{-7}$ K [16-19]. Moreover, in 1998, Bose-Einstein condensation of spin-polarized hydrogen atoms was also finally observed [20]. Now, more than twenty groups have succeeded in observing Bose-Einstein condensation [21-24].

Alkali atoms are perfect for Bose-Einstein condensation studies. They have a magnetic moment, and hence can be trapped by magnetic field. They essentially have a one-electron structure. They are thus simple atoms, and have been well studied by atomic physicists. One can easily selectively flip the spin of higher energy trapped atoms. These hot atoms are then quickly ejected from the magnetic trap and the remaining atoms quickly thermalize to a lower temperature. This evaporate cooling is very efficient and quickly brings one into the temperature region required for Bose-Einstein condensation.

It is useful to mention a few experimental fact about the magnetic traps currently in use. As it turns out, these traps are well described as a harmonic potential

$$V_{ex}(\vec{r}) = \begin{cases} \frac{m\omega^2 r^2}{2} & (\text{isotropic}) \\ \frac{m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)}{2} & (\text{anisotropic}) \end{cases} \quad (1.2)$$

Most current traps are either:

$$\text{pancakes ,} \quad \omega_z \gg \omega_x \quad (= \omega_y) \quad (1.3)$$

$$\text{cigars ,} \quad \omega_z \ll \omega_x \quad (= \omega_y) \quad (1.4)$$

and the trap frequencies are of the order $\omega \sim 2\pi \times 100$ Hz. In 1995, the first condensates were small $\sim 10^3$ atoms and $T_{BEC} \sim 100$ nK. However in 1999, the condensates can be quite large $\sim 10^8$ atoms at $T_{BEC} \sim \mu\text{K}$. These have size \sim many microns, which can be easily seen optically when the condensates are small,

the trap is turned off and cloud allowed to expand, and then measured by optical methods. The results are simple to analyze if gas is non-interacting. However, more analysis is needed to include the effects of interaction during expansion.

In addition, observation of Bose-Einstein condensation in cooled and trapped dilute gases of alkali atoms and spin polarized atomic hydrogen has generated a renewed theoretical interest in understanding such systems. In a mean field approach, which is valid in the limit $\rho a^3 \ll 1$ where ρ is density of atoms and a is the s-wave scattering length, ground state of these systems can be described by Ginzburg-Pitaevskii-Gross equation [25]. Various numerical procedures and approximate analytical methods have been used to solve the Ginzburg-Pitaevskii-Gross equation. Among these variational scheme proposed by Gordon Baym and C.J. Pethick [26] to explain the experimental observations of ^{87}Rb is particularly appealing. In this approach the trial wavefunction was taken to be of the form of ground state of the trap potential, modeled by an anisotropic harmonic oscillator potential. Thus the wavefunction is represented by a three dimensional Gaussian with axial and transverse frequencies as variational parameters. This form of wavefunction, however, is valid only when the number of atoms in the trap is very small. As the number increases, the repulsive interaction between the atoms tends to expand the condensate and flatten the density profile in the central region of the trap where the density is maximum. Of these two effects, only expansion of the condensate can be described adequately by the Gaussian trial wavefunction. On the other hand, in the limit of very large number of atoms in the trap, an essentially exact expression for the ground state wavefunction can be described by the Thomas-Fermi approximation [27], by neglecting the kinetic energy term in the Ginzberg-Pitaevskii-Gross equation. It is also important to

note that the Thomas-Fermi wavefunction does not describe the surface region properly which significantly affects some relevant physical observables, e.g., the aspect ratio.

In addition the inter-particle interaction in the work of Gordon Baym and C.J. Pethick are of finite range (short-range) and well approximated by the delta function. Furthermore the long-range interaction are also considered which it is the problem of charged boson. Inter-particle interactions of charged bosons system are long-range and approximated by Coulomb potential. The problem of charged bosons is rather academic, but turns out to be quite interesting because its concept can be used in various branches of condensed matter and plasma physics.

Moreover, charged boson problem recently became of particular interest motivated by the bipolaron theory of high-temperature superconductivity [28]. Initially, in 1955, Schafroth [29] demonstrated that an ideal gas of charged bosons exhibits the Meissner-Ochsenfeld effect below the ideal Bose-gas condensation temperature. Later on, in 1961, Foldy [30] studied the theory of a homogeneous plasma of charged bosons by using the Bogoliubov [31] approach. Until 1995 that Bose-Einstein condensation was observed. Then the properties of the ground state energy of charged bosons became more important, and it was studied by using Ginzburge-Pitaevskii-Gross equation which is based on mean field theory. There are numerical procedure and approximate analytical method that have been used to solve the Ginzburge-Pitaevskii-Gross equation. The important numerical procedure is the work of Yeong E. Kim and Alexander L. Zubarev [32] to approximate the ground state energy of charge bosons, but this procedure is valid when the number of atoms in the system is large. In addition, the impor-

tant approximated analytical method is the work of Takeya Tsurumi, Hirofumi Morise and Miki Wadati [33]. By using variational technique, they can approximate the ground state energy of charged bosons, and can show that the ground state energy of long-range interacting bosons under traps is stable.

Unfortunately, up to the present there is no experimental evidence of Bose-Einstein condensation for bosonic atoms with charges. In the future, new technology may make it possible to observe this Bose-Einstein condensation for bosonic atoms with charges, and after that the ground state energy of charged bosons will be proved. Although the directly experimental proof is not yet realized, the concept may still be useful in condensed matter physics, especially bipolaron theory of high temperature superconductivity, and the theory of plasma physics such as a plasma in the core of white dwarfs [34].

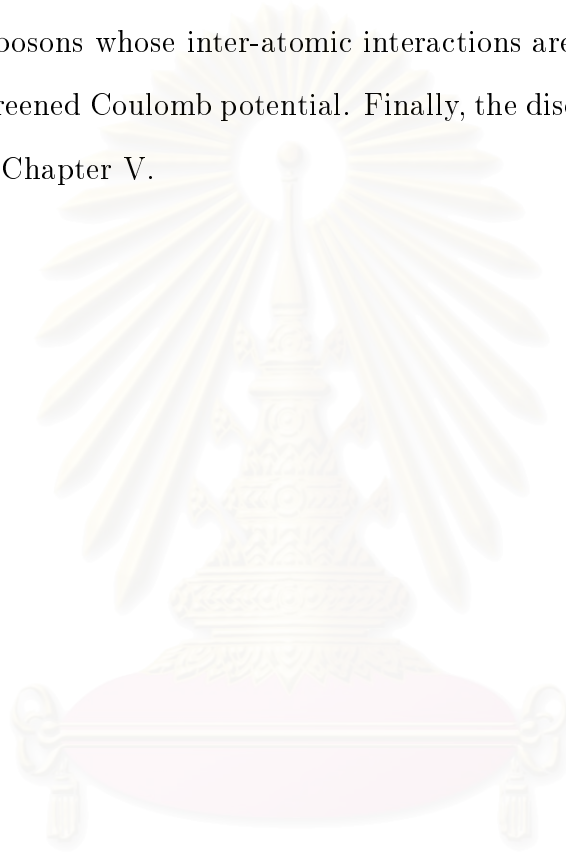
Since the concept of charged bosons is important in various branches of physics, the propose of this thesis is to evaluate the ground state energy of charged bosons in an isotropic trap whose inter-atomic interaction is approximated by Coulomb and Screened Coulomb potential using the method of the variational Feynman path integration developed by R.P. Feynman [35], and then compare the result with the result from the Ginzburg-Pitaevskii-Gross approach.

Since the problem of charged bosons will be formulated in the form of Feynman path integrals, Chapter II is devoted to the construction of the basic ideas of the Feynman path integrals, and the discussion of how the variational Feynman path integral can be used to evaluate the ground state energy of the quantum systems.

Then, Chapter III is devoted to the review of the current research in the evaluation of the ground state energy for bosonic atoms with and without charges

by using the Ginzburg-Pitaevskii-Gross approach; the basic ideas of the Ginzburg-Pitaevskii-Gross equation are also presented. Moreover, the lower and the upper limit of the ground state energy of Bose-Einstein condensation is presented by using the evaluation of the ideal Bose gas (non-interacting Bose gas) model and the Thomas-Fermi approximation respectively.

Next, Chapter IV is devoted to the calculation of the ground state energy of charged bosons whose inter-atomic interactions are approximated by the Coulomb and Screened Coulomb potential. Finally, the discussion and conclusion are presented in Chapter V.



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Chapter 2

Feynman Path Integrals

Since we will formulate the problem of charged bosons in an isotropic traps in the form of Feynman path integrals [44], we will devote this chapter to introduce the basic ideas of Feynman path integrals. We present in this chapter the mathematical formulation of the propagator in the form of a path integral. Moreover, we will discuss how the variational path integration which can be used to estimate the upper bound of the ground state energy of our system.

2.1 Feynman Propagator

If a particle moves from one to another point there are many possible path which the particle can take. In classical mechanics, when we consider the particle as a point, there is a principle of least action which expresses the condition that determines a particular path from all of the possible paths. For simplicity, we will restrict ourselves to the case of a particle moving in one dimension. Thus the position at any time can be specified by coordinate x which is a function of time. The path thus means a function $x(t)$.

If a particle starts from the point x_a at an initial time, t_a , and then moves to the end point, x_b , at the end time, t_b , there are many possible paths in the area of interest, in which the particle can move. For each path, the action S ,

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t) dt, \quad (2.1)$$

where L is the Lagrangian for the system.

The principle of least action states that the particular path $x(t)$ along which the particle actually travels corresponds to the extremum value of S . In other words, the value of S is unchanged to the first order if the path $x(t)$ is the classical path.

Quantum mechanics deals with probabilities, that is, we cannot specify the position of a particle but we can only know the probability of its being found in a given place. The probability of a particle being found to have a position $x(t)$ is the absolute square of a probability amplitude. The probability amplitude is associated with the entire motion of a particle as a function of time, rather than simply with the position of the particle at a particular time. Thus consider the path along which the particle move from a to b , we must specify how much each trajectory contributes to the probability amplitude $K(b, a)$. It is not just the particular path of extreme action which contributes; rather, it is the case of the all of paths contribute. The contribution $\phi[x(t)]$ from a single path depends on the classical action for that path in the units of \hbar ,

$$\phi[x(t)] = (\text{const}) \exp \left[\frac{i}{\hbar} S\{x(t)\} \right]. \quad (2.2)$$

The amplitude $K(b, a)$ is the sum over all trajectories between the end points of a and b of the contributions $\phi[x(t)]$,

$$K(b, a) = \sum_{\text{all paths from } a \text{ to } b} \phi[x(t)], \quad (2.3)$$

hence, from Eqs.(2.2) and (2.3), we obtain

$$K(b, a) = \sum_{\text{all paths from } a \text{ to } b} (\text{const}) \exp \left[\frac{i}{\hbar} S\{x(t)\} \right]. \quad (2.4)$$

We have thus described the physical ideas concerned in the construction of the amplitude for a particle to reach a particular point in space and time by

closely following its motion in getting there. So if we want to find the probability amplitude of the particle going from a to b , we have to carry out the sum in Eq. (2.4), but the number of paths from a to b is infinite, so Eq. (2.4) is very difficult to work with. Another method and more efficient method of computing the sum over all paths will be described now.

We choose a subset of all paths by first separating the independent time into small interval, ϵ . This gives us a set of successive times t_1, t_2, t_3, \dots between t_a and t_b , where $t_{i+1} = t_i + \epsilon$. At each time, t_i , we select some special point x_i and constructing a path by connecting all of the points, so we set the form of them to be a line. This processes are shown in Figure 2.1. It is possible to define a sum over all paths constructed in this manner by taking a multiple integral over all values of x_i for i from 1 to $n - 1$, where

$$n\epsilon = t_b - t_a, t_0 = t_a, t_n = t_b$$

$$x_0 = x_a, x_n = x_b$$

By using this method, Eq. (2.4) become

$$K(b, a) = \int \int \dots \int (\text{const}) \exp \left[\frac{i}{\hbar} S\{x(t)\} \right] dx_1 dx_2 \dots dx_{n-1}. \quad (2.5)$$

We do not integrate over x_0 or x_n because these are the fixed end point x_a and x_b . In order to achieve the correct measure, Eq. (2.5) must be taken in the limit of $\epsilon \rightarrow 0$ and some normalizing factor A^{-n} which depends on ϵ must be provided in order that the limit of Eq. (2.5) becomes

$$K(b, a) \approx \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \int \dots \int (\text{const}) \exp \left[\frac{i}{\hbar} S\{x(t)\} \right] \frac{dx_1}{A} \frac{dx_2}{A} \dots \frac{dx_n}{A} \quad (2.6)$$

Eq. (2.6) can also be written in a less restrictive notation as

$$K(b, a) \approx N \int \int \dots \int (\text{const}) \exp \left[\frac{i}{\hbar} S\{x(t)\} \right] D(\text{path}) \quad (2.7)$$

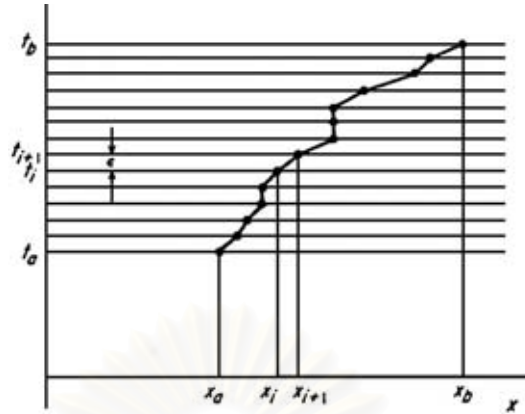


Figure 2.1: Diagram showing how the path integrals can be constructed.

This is called a path integral and the amplitude $K(b, a)$ is known as the Feynman propagator.

2.2 Propagator from Schrödinger Equation

So far, we have followed Feynman's argument in writing down the propagator in the form of path integral. It will now be shown that the propagator in this form can also be derived directly from the Schrödinger equation. The time-dependent Schrödinger equation is

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] \Psi(\vec{x}, t) = 0. \quad (2.8)$$

We can define the one-electron Green Function of this equation as the solution of

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H} \right] G(\vec{x}, \vec{x}'; t, t') = \delta(\vec{x} - \vec{x}') \delta(t - t'). \quad (2.9)$$

Thus the Green function can be written in matrix form as

$$G(\vec{x}, \vec{x}'; t, t') = \langle \vec{x} | \exp\left\{ -\frac{i}{\hbar} \hat{H}(t - t') \right\} | \vec{x}' \rangle. \quad (2.10)$$

Let us divide the time interval $t - t'$ into n equal small subintervals, so that $t - t' = n\epsilon$. By making use of the identity

$$\exp\left(-\frac{i\epsilon\hat{H}n}{\hbar}\right) = \lim_{\epsilon \rightarrow 0} \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right)^n, \quad (2.11)$$

Eq. (2.20) becomes to

$$G(\vec{x}, \vec{x}'; t, t') = \lim_{\epsilon \rightarrow 0} \langle \vec{x} | \underbrace{\left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) \dots \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right)}_{n \text{ factors}} | \vec{x}' \rangle. \quad (2.12)$$

According to of quantum mechanics we can insert a complete set of states between each pair of factors in Eq. (2.12):

$$\begin{aligned} G(\vec{x}, \vec{x}'; t, t') &= \lim_{\epsilon \rightarrow 0} \int \int \dots \int \langle \vec{x} | \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) | \vec{x}_{n-1} \rangle d\vec{x}_{n-1} \\ &\quad \cdot \langle \vec{x}_{n-1} | \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) | \vec{x}_{n-2} \rangle d\vec{x}_{n-2} \dots \\ &\quad \cdot \langle \vec{x}_2 | \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) | \vec{x}_1 \rangle d\vec{x}_1 \langle \vec{x}_1 | \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) | \vec{x}' \rangle \end{aligned} \quad (2.13)$$

We now consider the Hamiltonian of the system in the position representation

$$\hat{H} = \frac{P^2}{2m} + V(\vec{x}), \quad (2.14)$$

where P is the momentum operator. Then

$$\begin{aligned} \langle \vec{x}_{i+1} | \left(1 - \frac{i\epsilon\hat{H}}{\hbar}\right) | \vec{x}_i \rangle &= \int \langle \vec{x}_{i+1} | \vec{p} \rangle d\vec{p} \langle \vec{p} | 1 - \frac{i\epsilon}{\hbar} \left\{ \frac{p^2}{2m} + v(\vec{x}) \right\} | \vec{x}_i \rangle \\ &= \int \langle \vec{x}_{i+1} | \vec{p} \rangle d\vec{p} \langle \vec{p} | \vec{x}_i \rangle \cdot \left[1 - \frac{i\epsilon}{\hbar} \left\{ \frac{p^2}{2m} + V(\vec{x}) \right\} \right] \end{aligned} \quad (2.15)$$

From quantum mechanics, the momentum eigenfunction $\langle \vec{x} | \vec{p} \rangle$ for a free particle is

$$\langle \vec{x} | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left(\frac{i}{\hbar} \vec{p} \cdot \vec{x}\right). \quad (2.16)$$

Therefore

$$\begin{aligned} \langle \vec{x}_{i+1} | \left(1 - \frac{i\epsilon \hat{H}}{\hbar} \right) | \vec{x}_i \rangle &= \frac{1}{(2\pi\hbar)^{3/2}} \int \exp \left\{ \frac{i}{\hbar} (\vec{x}_{i+1} - \vec{x}_i) \cdot \vec{p} \right\} \\ &\cdot \left[1 - \frac{i\epsilon}{\hbar} \left\{ \frac{p^2}{2m} + v(\vec{x}) \right\} \right] d\vec{p}. \end{aligned} \quad (2.17)$$

We now replace $1 - \frac{i\epsilon}{\hbar} \left\{ \frac{p^2}{2m} + V(\vec{x}) \right\}$ by the corresponding exponential, the error introduced here is $O(\epsilon^2)$, so that the total error from all the n factors can be neglected. Eq. (2.17) becomes to

$$\begin{aligned} \langle \vec{x}_{i+1} | \left(1 - \frac{i\epsilon \hat{H}}{\hbar} \right) | \vec{x}_i \rangle &= \frac{1}{(2\pi\hbar)^3} \int \exp \left[-\frac{i\epsilon}{\hbar} \left\{ \frac{p^2}{2m} - \frac{(\vec{x}_{i+1} - \vec{x}_i) \cdot \vec{p}}{\epsilon} \right\} \right] d\vec{p} \\ &\cdot \exp \left\{ -\frac{i\epsilon}{\hbar} V(\vec{x}) \right\} \\ &= \frac{1}{(2\pi\hbar)^3} \int \exp \left[-\frac{i\epsilon}{2m\hbar} \left\{ p^2 - \frac{2m(\vec{x}_{i+1} - \vec{x}_i) \cdot \vec{p}}{\epsilon} \right. \right. \\ &\quad \left. \left. + \left(\frac{m}{\epsilon} (\vec{x}_{i+1} - \vec{x}_i) \right)^2 - \left(\frac{m}{\epsilon} (\vec{x}_{i+1} - \vec{x}_i) \right)^2 \right\} \right] d\vec{p} \\ &\cdot \exp \left\{ -\frac{i\epsilon}{\hbar} V(\vec{x}) \right\} \\ &= \frac{1}{(2\pi\hbar)^3} \int \exp \left[-\frac{i\epsilon}{2m\hbar} \left\{ \vec{p} - \frac{m}{\epsilon} (\vec{x}_{i+1} - \vec{x}_i) \right\}^2 \right] d\vec{p} \\ &\cdot \exp \left\{ \frac{i\epsilon}{2m\hbar} \left(\frac{m}{\epsilon} (\vec{x}_{i+1} - \vec{x}_i) \right)^2 \right\} \cdot \exp \left\{ -\frac{i\epsilon}{\hbar} V(\vec{x}) \right\}. \end{aligned} \quad (2.18)$$

So,

$$\begin{aligned} \langle \vec{x}_{i+1} | \left(1 - \frac{i\epsilon \hat{H}}{\hbar} \right) | \vec{x}_i \rangle &= \frac{1}{(2\pi\hbar)^3} \left(\frac{2m\pi\hbar}{i\epsilon} \right)^{3/2} \cdot \exp \left\{ \frac{im}{2\hbar\epsilon} (\vec{x}_{i+1} - \vec{x}_i)^2 - \frac{i\epsilon}{\hbar} V(\vec{x}) \right\} \\ &= \left(\frac{m}{2\pi\hbar i\epsilon} \right)^{3/2} \cdot \exp \left[\frac{i\epsilon}{\hbar} \left\{ \frac{m}{2} \left(\frac{\vec{x}_{i+1} - \vec{x}_i}{\epsilon} \right)^2 - V(\vec{x}) \right\} \right] \end{aligned} \quad (2.19)$$

Substituting Eq. (2.19) into Eq. (2.13), we obtain

$$G(\vec{x}, \vec{x}'; t, t') = \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \int \dots \int \exp \left[\frac{i\epsilon}{\hbar} \sum_{i=0}^{n-1} \left\{ \frac{m}{2} \left(\frac{\vec{x}_{i+1} - \vec{x}_i}{\epsilon} \right)^2 - V(\vec{x}) \right\} \right] \cdot \frac{d\vec{x}_1}{A} \frac{d\vec{x}_2}{A} \dots \frac{d\vec{x}_{n-1}}{A} \quad (2.20)$$

where $\frac{1}{A} = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{3/2}$, $\vec{x}_n = \vec{x}$, $\vec{x}_0 = \vec{x}'$. In an obvious notation

$$G(\vec{x}, \vec{x}'; t, t') = \frac{1}{A} \int \int \dots \int \exp \left[\frac{i}{\hbar} \int_{t'}^t \left\{ \frac{m}{2} \dot{\vec{x}}^2 - V(\vec{x}) \right\} dt \right] \frac{d\vec{x}_1}{A} \frac{d\vec{x}_2}{A} \dots \frac{d\vec{x}_{n-1}}{A} \quad (2.21)$$

It can be shown that the time-dependent Green function (Eq. (2.20)) of Schrödinger equation has exactly the same form as the Feynman propagator, (Eq. (2.6)). The latter can be written in this form by using the argument discussed at the beginning of this chapter. As a simple example of how to obtain $G(\vec{x}, \vec{x}'; t, t')$ written in the form of Eq. (2.21), let us consider the case of a free electron.

For a free electron $L = \frac{m}{2} \dot{\vec{x}}^2$, by using Eq. (2.20) we obtain

$$G(\vec{x}, \vec{x}'; t, t') = \lim_{\epsilon \rightarrow 0} \frac{1}{A} \int \int \dots \int \exp \left[\frac{i\epsilon}{\hbar} \sum_{i=0}^{n-1} \frac{m}{2} \left(\frac{\vec{x}_{i+1} - \vec{x}_i}{\epsilon} \right)^2 \right] \cdot \frac{d\vec{x}_1}{A} \frac{d\vec{x}_2}{A} \dots \frac{d\vec{x}_{n-1}}{A}. \quad (2.22)$$

The calculation is carried out by direct integrations as follows. Since

$$\int_{-\infty}^{\infty} \exp \left\{ a(\vec{x}_0 - \vec{x}_1)^2 + b(\vec{x}_2 - \vec{x}_1)^2 \right\} d\vec{x}_1 = \left(-\frac{\pi}{a+b} \right)^{3/2} \exp \left\{ \frac{ab}{a+b} (\vec{x}_2 - \vec{x}_0)^2 \right\}, \quad (2.23)$$

we have

$$\begin{aligned} & \left(\frac{m}{2\pi i \hbar \epsilon} \right)^3 \int_{-\infty}^{\infty} \exp \left\{ \frac{im}{2\hbar \epsilon} [(\vec{x}_1 - \vec{x}_0)^2 + (\vec{x}_2 - \vec{x}_1)^2] \right\} d\vec{x}_1 \\ &= \left(\frac{m}{2\pi i \hbar \epsilon} \right)^3 \left(\frac{\pi i \hbar \epsilon}{m} \right)^{3/2} \exp \left\{ \frac{im}{2\hbar(2\epsilon)} (\vec{x}_2 - \vec{x}_0)^2 \right\} \\ &= \left(\frac{m}{2\pi i \hbar(2\epsilon)} \right)^{3/2} \exp \left\{ \frac{im}{2\hbar(2\epsilon)} (\vec{x}_2 - \vec{x}_0)^2 \right\}. \end{aligned} \quad (2.24)$$

Multiplying the result by $\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-1/2} \exp\left\{\frac{im}{2\hbar\epsilon}(\vec{x}_3 - \vec{x}_2)^2\right\}$ and integrating over \vec{x}_2 , we obtain

$$\begin{aligned}
& \frac{1}{A} \int \int \exp\left[\frac{im}{2\hbar\epsilon}\{(\vec{x}_1 - \vec{x}_0)^2 + (\vec{x}_2 - \vec{x}_1)^2 + (\vec{x}_3 - \vec{x}_2)^2\}\right] \frac{d\vec{x}_1}{A} \frac{d\vec{x}_2}{A} \\
&= \int \left(\frac{m}{2\pi i\hbar(2\epsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar(2\epsilon)}(\vec{x}_2 - \vec{x}_0)^2\right] \cdot \left(\frac{m}{2\pi i\hbar(2\epsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar\epsilon}(\vec{x}_3 - \vec{x}_2)^2\right] d\vec{x}_2 \\
&= \left(\frac{m}{2\pi i\hbar(2\epsilon)}\right)^{3/2} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{3/2} \left(-\frac{2\pi\hbar(2\epsilon)}{3im}\right)^{3/2} \exp\left[\frac{im}{2\hbar(3\epsilon)}(\vec{x}_3 - \vec{x}_0)^2\right] \\
&= \left(\frac{m}{2\pi i\hbar(3\epsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar(3\epsilon)}(\vec{x}_3 - \vec{x}_0)^2\right]. \tag{2.25}
\end{aligned}$$

In this way a recurring process is established by which, after $(n - 1)$ steps, we obtain

$$G_0(\vec{x}, \vec{x}'; t) = \left(\frac{m}{2\pi i\hbar(n\epsilon)}\right)^{3/2} \exp\left[\frac{im}{2\hbar(n\epsilon)}(\vec{x}_n - \vec{x}_0)^2\right]$$

. Since $n\epsilon = t$, $\vec{x}_n = \vec{x}$ and $\vec{x}_0 = \vec{x}'$, then

$$G_0(\vec{x}, \vec{x}'; t) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \exp\left[\frac{im}{2\hbar t}(\vec{x} - \vec{x}')^2\right]. \tag{2.26}$$

The method of direct integration can be carried out only for this simple case of a free electron. For other case, the path integral is more difficult to work out. Therefore, a different way to solve this difficult problem is required.

First, we begin with the general form of the Feynman path integral

$$K(b, a) = N \int D[\vec{x}(t)] \exp\left[\frac{i}{\hbar}S(\vec{x}(t))\right]. \tag{2.27}$$

We known from classic physics that the action S is extremized and then it furnishes us the classical path completely fixed. Therefore, any path $\vec{x}(t)$ can be expressed as the sum of the classical path, $\vec{x}_c(t)$, and a new variable $\vec{y}(t)$. That is

$$\vec{x}(t) = \vec{x}_c(t) + \vec{y}(t) \tag{2.28}$$

and it is clear that the path differential $D[\vec{x}(t)]$ can be replaced by $D[\vec{y}(t)]$. This means that besides defining a point on the path by its distance $\vec{x}(t)$ from an arbitrary coordinate axis, we now give the meaning of it by its deviation $\vec{y}(t)$ from the classical path, as shown in Figure 2.2. The crucial conditions which the deviations, $\vec{y}(t)$ have to satisfy are

$$\vec{y}(0) = \vec{y}(T) = 0. \quad (2.29)$$

In this situation, we begin from the time $t = 0$ to the time at $t = T$. Generally, the Lagrangian will be the quadratic form

$$L = a(t)\dot{\vec{x}}^2(t) + b(t)\dot{\vec{x}}(t)\vec{x}(t) + c(t)\vec{x}^2(t) + d(t)\dot{\vec{x}}(t) + e(t)\vec{x}(t) + f(t). \quad (2.30)$$

Hence, the action S can be expressed as

$$\begin{aligned} S[\vec{x}(t)] &= S[\vec{x}_c(t) + \vec{y}(t)] \\ &= \int_0^T \left[a(t) \left\{ \dot{\vec{x}}_c^2(t) + 2\dot{\vec{x}}_c(t)\dot{\vec{y}}(t) + \dot{\vec{y}}^2(t) \right\} + \dots + f(t) \right] dt. \end{aligned} \quad (2.31)$$

It is obvious that the integral of all terms involving exclusively $\vec{x}_c(t)$ is exactly the classical action and the integral of all terms that are linear in $\vec{y}(t)$ precisely vanishes. So, all the remaining terms in the integral are the second-order terms in $\vec{y}(t)$ only. That is

$$S[\vec{x}(t)] = S_{cl}[\vec{x}_c(t)] + \int_0^T \left[a(t)\dot{\vec{y}}^2(t) + b(t)\dot{\vec{y}}(t)\vec{y}(t) + c(t)\vec{y}^2(t) \right] dt \quad (2.32)$$

From Eq. (2.32), the propagator or the Green's function can be rewritten

as

$$\begin{aligned} K(b, a) &= N \int D[\vec{y}(t)] \exp \left[\frac{i}{\hbar} \left(S_{cl}[\vec{x}_c(t)] + \int_0^T dt \left\{ a(t)\dot{\vec{y}}^2(t) + b(t)\dot{\vec{y}}(t)\vec{y}(t) + c(t)\vec{y}^2(t) \right\} \right) \right] \\ &= \exp \left\{ \frac{i}{\hbar} S_{cl}[\vec{x}_c(t)] \right\} N \int D[\vec{y}(t)] \exp \left[\frac{i}{\hbar} \int_0^T dt \left\{ a(t)\dot{\vec{y}}^2(t) + b(t)\dot{\vec{y}}(t)\vec{y}(t) + c(t)\vec{y}^2(t) \right\} \right] \end{aligned} \quad (2.33)$$

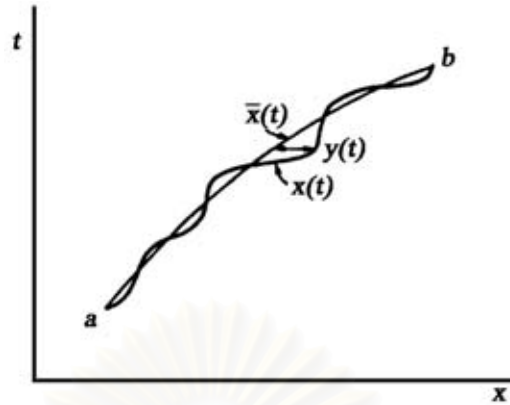


Figure 2.2: Diagram showing a path deviating from the classical path.

For the quadratic Lagrangian, customarily, the propagator can be written as

$$K(b, a) = F(T) \exp \left\{ \frac{i}{\hbar} S_d[\bar{x}_c(t)] \right\}, \quad (2.34)$$

where

$$F(T) = N \int D[\vec{y}(t)] \exp \left[\frac{i}{\hbar} \int_0^T dt \left\{ a(t) \dot{\vec{y}}^2(t) + b(t) \dot{\vec{y}}(t) \vec{y}(t) + c(t) \vec{y}^2(t) \right\} \right] \quad (2.35)$$

is a prefactor.

Next, we show that the method can be used to the problem of a one-dimensional harmonic oscillator of which the Lagrangian is

$$L[x(t), \dot{x}(t)] = \frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2. \quad (2.36)$$

We obtain the equation of motion by applying the Euler-Lagrange equation to the Lagrangian

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0$$

thus we have

$$\ddot{x}_c + \omega^2 x_c = 0 \quad (2.37)$$

and the solution of Eq. (2.37), with boundary conditions $x(0) = x'$ and $x(T) = x$, is

$$x_c(t) = \frac{x - x' \cos \omega T}{\sin \omega t} \sin \omega t + x' \cos \omega t. \quad (2.38)$$

Therefore, the corresponding action can be expressed as

$$\begin{aligned} S_{cl}[x_c(t)] &= \int_0^T \frac{m}{2} \left[\dot{x}_c^2(t) - \omega^2 x_c^2(t) \right] dt \\ &= \frac{m}{2} \left[\dot{x}_c(T)x_c(T) - \dot{x}_c(0)x_c(0) - \int_0^T x_c [\ddot{x}_c - \omega^2 x_c] dt \right]. \end{aligned}$$

Using Eq. (2.37), we have

$$S_{cl}[x_c(t)] = \frac{m}{2} [\dot{x}_c(T)x_c(T) - \dot{x}_c(0)x_c(0)]. \quad (2.39)$$

Substituting Eq. (2.38) into Eq. (2.39), we have

$$S_{cl}[x_c(t)] = \frac{m\omega}{2 \sin \omega T} \left[\cos \omega T (x^2 x'^2) - 2xx' \right] \quad (2.40)$$

that is the classical action of the harmonic oscillator. From Eqs. (2.34) and (2.40), we obtain, to complete the propagator we must to find the prefactor, $F(T)$. Hence, from Eq. (2.37), we begin with

$$F(T) = N \int D[y(t)] \exp \left[\frac{i}{\hbar} \int_0^T dt \frac{m}{2} \{ \dot{y}^2 - \omega^2 y^2 \} \right] \quad (2.41)$$

with the boundary conditions $y(0) = y(T) = 0$.

By expressing $y(t)$ in the form of a Fourier series,

$$y(t) = \sum_n a_n \sin \frac{n\pi t}{T}, \quad (2.42)$$

it is obvious that we can change the integration variables from y 's to the new variables a_n 's, and then with the use of the identity

$$\lim_{N \rightarrow \infty} \prod_{n=1}^N \left(1 - \left(\frac{\omega T}{n\pi} \right)^2 \right)^{-1/2} = \sqrt{\frac{\omega T}{\sin \omega T}} \quad (2.43)$$

we obtain the result as

$$F(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}}. \quad (2.44)$$

Finally, the time-independent propagator or Green's function of the harmonic oscillator is

$$K(b, a) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp \left\{ \frac{im\omega}{2\hbar \sin \omega T} \left[\cos \omega T (x^2 + x'^2) - 2xx' \right] \right\}. \quad (2.45)$$

2.3 Variational Path Integration

In this section the variational path integration approach is described. By constructing an appropriate action with some variational parameters, we can use the path integral of this action to estimate the upper bound of the ground state energy. To be more clearly, consider the density matrix in the form of the sum over energy eigenstates.

$$\rho(\vec{x}_2, \vec{x}_1; \beta) = \sum_n \psi_n^*(\vec{x}_2) \psi_n(\vec{x}_1) \exp[-E\beta]. \quad (2.46)$$

As the imaginary time goes to infinity, i.e., temperature goes to zero, the higher order terms of the summation decay more rapidly than the first leading term or the term involving the ground state energy. So we can write

$$\rho \xrightarrow{\beta \rightarrow \infty} \exp(-E_0\beta). \quad (2.47)$$

Whenever we choose any trial action namely S_1 , where we can find its density matrix exactly, we can write the path integral

$$\begin{aligned} \rho &= \int D[x(t)] e^S \\ &= \int D[x(t)] e^{(S-S_1)} e^{S_1} \\ &= \langle e^{S-S_1} \rangle \int D[x(t)] e^{S_1} \end{aligned} \quad (2.48)$$

where we average with weighting factor e^{S_1} defined by

$$\langle F \rangle = \frac{\int D[x(t)] e^{S_1} F}{\int D[x(t)] e^{S_1}}. \quad (2.49)$$

In order to evaluate the energy as in Eq. (2.47), we must write the density matrix in the exponential form. To do this we apply the inequality

$$\langle e^F \rangle \gg \exp \langle F \rangle$$

called the Feynman-Jansen inequality. The density matrix in Eq. (2.47) can be approximated as

$$\rho \gg \exp \langle S - S_1 \rangle \int D[x(t)] e^{S_1}. \quad (2.50)$$

Remember that the path integral of S_1 gives the ground state energy as

$$\rho_1 \approx \exp(-E_1 \beta). \quad (2.51)$$

Then Eq. (2.50) can be written as

$$e^{-(E_0 \beta)} \gg e^{\langle S - S_1 \rangle} e^{-E_1 \beta}. \quad (2.52)$$

Hence

$$E_0 \ll E_1 - \frac{\langle S - S_1 \rangle}{\beta}. \quad (2.53)$$

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Chapter 3

Bose-Einstein Condensation: Ginzburg-Pitaevskii-Gross Approach

In this chapter we present the basic equation describing Bose-Einstein condensation and review recent researches which evaluate the ground state energy of bosonic atoms with and without charges by using the Ginzburg-Pitaevskii-Gross approach.

In section 3.1, we will derive the Ginzburg-Pitaevskii-Gross equation, which is based on the Hartree approximation and essentially equivalent to the time-independent nonlinear Schrödinger equation. In section 3.2, we consider the time-dependent case. To derive the equation of motion for the condensate, we begin with the second-quantized formulation. By employing the mean field approach, we obtain the so-called Gross-Pitaevskii equation or equivalently the time-dependent nonlinear Schrödinger equation.

In section 3.3, we discuss the Bose-Einstein condensation of a free gas, or non-interacting gas, under harmonic potentials. The results are simple to analyze. In section 3.4, we give some details to calculate the ground state energy of the condensate under the three-dimensional Thomas-Fermi approximations. In the Thomas-Fermi approximation, the kinetic term in the Ginzburg-Pitaevskii-Gross equation is neglected due to the assumption of the Thomas-Fermi approximation stated that the number of atoms in the system is very large and hence the potential terms in the Ginzburg-Pitaevskii-Gross equation are dominated. Moreover, we find that the non-interacting gas model gives the lower limit of the ground state energy, on the other hand, the Thomas-Fermi approximation gives

the upper limit.

In section 3.5, we review of the recent researches which evaluate the ground state energy of neutral bosonic atoms confined in magnetic trap by variational method which proposed by Gordon Baym and C.J. Pethick. Then we can find that the inter-atomic interaction in this method are finite range or short-range and well approximated by the delta function.

Finally in section 3.6 we review the work of Takeya Tsurumi, Hirofumi Moris and Miki Wadati [33]. They evaluated the ground state energy of charge bosons confined in anisotropic trap. The inter-atomic interaction are long-rang interaction and well approximated by coulomb potential, and we find that the result is stable.

3.1 Ginzburg-Pitaevskii-Gross Equation: Time-independent Case

In this section, we derive the Ginzburg-Pitaevskii-Gross equation based on the Hartree approximation, [36]-[38], which is essentially equivalent to the time-independent nonlinear Schrödinger equation.

Firstly, we consider N identical bosonic particles whose inter-atomic interactions are of finite range, trapped in an external potential $V(\vec{r})$. We assume that the gas is sufficiently dilute and at very low temperature. In such a situation, two-body interaction dominates and the s-wave part plays a central role. We may replace the scattering from an inter-atomic potential of finite range by the hard sphere potential of diameter a , which is identical to s-wave scattering length in this case. Then, the Hamiltonian operator of the system of hard spheres can be given in certain approximations by the pseudopotential Hamiltonian operator [39],

$$H = \sum_{i=1}^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V(\vec{r}_i) \right) + \frac{1}{2} \sum_{i \neq j} U_0 \delta(\vec{r}_i - \vec{r}_j) \frac{\partial}{\partial r_{ij}} r_{ij}, \quad (3.1)$$

where m is the mass of bosonic particle, and

$$\nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}, \quad (3.2)$$

$$r_{ij} = |\vec{r}_i - \vec{r}_j|, \quad (3.3)$$

$$U_0 = 4\pi\hbar^2 a/m. \quad (3.4)$$

The magnetic trap is well approximated by a harmonic potential,

$$V(\vec{r}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad (3.5)$$

with $(\omega_x, \omega_y, \omega_z)$ being trap frequencies.

In the ground state of the system, almost all bosons may occupy the lowest single-particle state because of sufficiently weak inter-atomic interactions. Thus, following the Hartree approximation, we write the ground state wavefunction, $\Phi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$, in terms of the product of N single-particle state wavefunctions, $g(\vec{r})$:

$$\Phi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i=1}^N g(\vec{r}_i) \quad (3.6)$$

where $g(\vec{r})$ is normalized as

$$\langle g|g \rangle \equiv \int d\vec{r} |g(\vec{r})|^2 \equiv 1, \quad (3.7)$$

and thus the norm of the wavefunction Φ_0 , defined by $\langle \Phi_0 | \Phi_0 \rangle$,

$$\langle \Phi_0 | \Phi_0 \rangle \equiv \int d\vec{r}_1 \dots \int d\vec{r}_N |\Phi_0(\vec{r}_1, \dots, \vec{r}_N)|^2 = \left(\int d\vec{r} |g(\vec{r})|^2 \right)^N, \quad (3.8)$$

is equal to unity. From Eqs. (3.1) and (3.6), we have

$$\langle \Phi_0 | H | \Phi_0 \rangle = \sum_{i=1}^N \int d\vec{r}_1 \dots \int d\vec{r}_N \Phi_0^* \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V(\vec{r}_i) \right) \Phi_0$$

$$\begin{aligned}
& + \frac{U_0}{2} \sum_{i \neq j} \int d\vec{r}_1 \dots \int d\vec{r}_N \Phi_0^* \delta(\vec{r}_i - \vec{r}_j) \frac{\partial}{\partial r_{ij}} (r_{ij} \Phi_0) \\
& = N \int d\vec{r} g^*(\vec{r}) \left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) g(\vec{r}) \\
& = + \frac{N(N-1)}{2} U_0 \int d\vec{r}_1 \int d\vec{r}_2 g^*(\vec{r}_2) g^*(\vec{r}_1) \delta(\vec{r}_1 - \vec{r}_2) \\
& \quad \cdot \frac{\partial}{\partial r_{12}} [r_{12} g(\vec{r}_1) g(\vec{r}_2)], \tag{3.9}
\end{aligned}$$

where the superscript * means the complex conjugate and

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \tag{3.10}$$

In Eq. (3.9), if the product of two single-state wavefunctions $g(\vec{r}_1)g(\vec{r}_2)$ is not singular at $r_{12} = 0$, the operator $(\partial/\partial r_{12})(r_{12})$ can be set equal to unity, which gives

$$\begin{aligned}
\langle \Phi_0 | H | \Phi_0 \rangle & = N \int d\vec{r} g^*(\vec{r}) \left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) g(\vec{r}) \\
& \quad + \frac{N(N-1)}{2} U_0 \int d\vec{r} \int d\vec{r}' g^*(\vec{r}') g^*(\vec{r}) \delta(\vec{r} - \vec{r}') g(\vec{r}) g(\vec{r}') \\
& = N \int d\vec{r} \left[g^*(\vec{r}) \left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) g(\vec{r}) + \frac{N-1}{2} U_0 |g(\vec{r})|^4 \right] \tag{3.11}
\end{aligned}$$

We minimize the functional $\langle \Phi_0 | H | \Phi_0 \rangle$ (3.11) under the constraint:

$$\langle \Phi_0 | \Phi_0 \rangle = 1. \tag{3.12}$$

To find the constrained extremum of $\langle \Phi_0 | H | \Phi_0 \rangle$, we set the variation of a functional $\langle \Phi_0 | H | \Phi_0 \rangle - \mu \langle \Phi_0 | \Phi_0 \rangle$ equal to zero,

$$\frac{\delta}{\delta g^*(\vec{r})} \left(\langle \Phi_0 | H | \Phi_0 \rangle - \mu \langle \Phi_0 | \Phi_0 \rangle \right) = 0, \tag{3.13}$$

where μ is a Lagrange's multiplier. Substituting Eqs. (3.8) and (3.11) into Eq. (3.13), we obtain

$$\frac{-\hbar^2}{2m} \nabla^2 g(\vec{r}) + V(\vec{r}) g(\vec{r}) + (N-1) U_0 |g(\vec{r})|^2 g(\vec{r}) = \mu g(\vec{r}). \tag{3.14}$$

Introducing a wavefunction $\Psi(\vec{r})$,

$$\Psi(\vec{r}) \equiv N^{1/2}g(\vec{r}). \quad (3.15)$$

we get

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + V(\vec{r})\Psi(\vec{r}) + \left(1 - \frac{1}{N}\right)U_0|\Psi(\vec{r})|^2\Psi(\vec{r}) = \mu\Psi(\vec{r}) \quad (3.16)$$

with

$$\langle\Psi|\Psi\rangle \equiv \int d\vec{r}|\Psi(\vec{r})|^2 = N. \quad (3.17)$$

The wavefunction Ψ has many names: an order parameter, a macroscopic wavefunction and a Bose-Einstein condensation wavefunction. For sufficiently large N , we can neglect the $1/N$ -order term appearing on the left hand side of Eq. (3.6). Thus

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + V(\vec{r})\Psi(\vec{r}) + U_0|\Psi(\vec{r})|^2\Psi(\vec{r}) = \mu\Psi(\vec{r}). \quad (3.18)$$

We refer to Eq. (3.18) as the Ginzburg-Pitaevskii-Gross equation with an external potential term. This equation may also be referred to as the time-independent nonlinear Schrödinger equation.

From Eqs. (3.11) and (3.15), the ground state energy of the system, E , is

$$\begin{aligned} E &= N \int d\vec{r} \left[\frac{\hbar^2}{2m} |\nabla g(\vec{r})|^2 + V(\vec{r})|g(\vec{r})|^2 + (N-1)\frac{U_0}{2}|g(\vec{r})|^4 \right] \\ &= \int d\vec{r} \left[\frac{\hbar^2}{2m} |\nabla\Psi(\vec{r})|^2 + V(\vec{r})|\Psi(\vec{r})|^2 + \left(1 - \frac{1}{N}\right)\frac{U_0}{2}|\Psi(\vec{r})|^4 \right], \end{aligned} \quad (3.19)$$

which we call the Ginzburg-Pitaevskii-Gross energy functional with an external potential term. On the other hand, multiplying the both sides of Eq. (3.16) by $\Psi^*(\vec{r})$ and integrating it, we get

$$\begin{aligned} N\mu &= \int d\vec{r} \left[\frac{\hbar^2}{2m} |\nabla\Psi|^2 + V(\vec{r})|\Psi|^2 + \left(1 - \frac{1}{N}\right)U_0|\Psi|^4 \right] \\ &= E + \left(1 - \frac{1}{N}\right)\frac{U_0}{2} \int d\vec{r}|\Psi|^4. \end{aligned} \quad (3.20)$$

It is clear that μ , introduced as a Lagrange's multiplier, has a meaning of the chemical potential of the system.

3.2 Gross-Pitaevskii Equation: Time-dependent Case

In this section, we consider the time-dependent case, $\Psi = \Psi(\vec{r}, t)$. To derive the equation of motion of Ψ , we use the second-quantized formation. Let $\hat{\Psi}(\vec{r}, t)$ and $\hat{\Psi}^+(\vec{r}, t)$ denote the bosonic annihilation and creation operators, respectively. The (equal-time) commutation relations among the operators are

$$\left[\hat{\Psi}(\vec{r}, t), \hat{\Psi}(\vec{r}', t) \right] \equiv \hat{\Psi}(\vec{r}, t)\hat{\Psi}(\vec{r}', t) - \hat{\Psi}(\vec{r}', t)\hat{\Psi}(\vec{r}, t) = 0, \quad (3.21)$$

$$\left[\hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \right] = \delta(\vec{r} - \vec{r}'), \quad (3.22)$$

and the second-quantized Hamiltonian of the system, \hat{H} , can be written as

$$\hat{H} \equiv \int d\vec{r} \left[\frac{\hbar^2}{2m} \nabla \hat{\Psi}^+ \cdot \nabla \hat{\Psi} + V(\vec{r}) \hat{\Psi}^+ \hat{\Psi} + \frac{U_0}{2} \hat{\Psi}^+ \hat{\Psi}^+ \hat{\Psi} \hat{\Psi} \right]. \quad (3.23)$$

The time-evolution of the operator $\hat{\Psi}(\vec{r}, t)$ obeys the Heisenberg equation,

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi} = [\hat{\Psi}, \hat{H}]. \quad (3.24)$$

Substituting the Hamiltonian (3.23) into Eq. (3.24) and using the commutation relations (3.21) and (3.22) we get

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi} = \frac{-\hbar^2}{2m} \nabla^2 \hat{\Psi} + V(\vec{r}) \hat{\Psi} + U_0 \hat{\Psi}^+ \hat{\Psi} \hat{\Psi}. \quad (3.25)$$

We denote an expectation value by $\langle \cdot \rangle$. The Heisenberg equation for the bosonic operator (3.25) gives

$$i\hbar \frac{\partial}{\partial t} \langle \hat{\Psi} \rangle = \frac{-\hbar^2}{2m} \nabla^2 \langle \hat{\Psi} \rangle + V(\vec{r}) \langle \hat{\Psi} \rangle + U_0 \langle \hat{\Psi}^+ \hat{\Psi} \hat{\Psi} \rangle. \quad (3.26)$$

According to the mean field theory [16, 40], we may replace the expectation values of the bosonic annihilation and creation operators by the condensate wavefunction $\hat{\Psi}(\vec{r}, t)$ and its complex conjugate $\Psi^*(\vec{r}, t)$ respectively,

$$\langle \hat{\Psi}(\vec{r}, t) \rangle = \Psi(\vec{r}, t), \quad \langle \hat{\Psi}^\dagger(\vec{r}, t) \rangle = \Psi^*(\vec{r}, t). \quad (3.27)$$

For the third term in the right hand side of Eq. (3.26) takes the following approximated form,

$$\langle \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \rangle \approx \langle \hat{\Psi}^\dagger \rangle \langle \hat{\Psi} \rangle \langle \hat{\Psi} \rangle = |\Psi(\vec{r}, t)|^2 \Psi(\vec{r}, t). \quad (3.28)$$

Substituting (3.27) and (3.28) into Eq. (3.26), we get

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}) \Psi(\vec{r}, t) + U_0 |\Psi(\vec{r}, t)|^2 \Psi(\vec{r}, t). \quad (3.29)$$

which is called the Gross-Pitaevskii equation with an external potential or the (time-dependent) nonlinear Schrödinger equation. The Eq. (3.29) can be written in a variational form,

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial \Psi^*} E[\Psi], \quad (3.30)$$

where the function $E[\cdot]$ is defined by Eq. (3.29) with the $1/N$ -order term deleted.

We note that, by setting

$$\Psi(\vec{r}, t) = \exp(-i\mu t) \Psi(\vec{r}),$$

in Eq. (3.29), we obtain the Ginzburg-Pitaevskii-Gross Eq. (3.18) again.

3.3 Free Bose Gas: Non-Interacting Case

In this section, we discuss the Bose-Einstein condensation of a free gas under harmonic potentials. The N -body Hamiltonian (first quantization) is

$$\begin{aligned} H &= \sum_{j=1}^N H_j \\ &= \sum_{j=1}^N \left[\frac{1}{2m} (p_{jx}^2 + p_{jy}^2 + p_{jz}^2) + \frac{m}{2} (\omega_x^2 x_j^2 + \omega_y^2 y_j^2 + \omega_z^2 z_j^2) \right], \end{aligned} \quad (3.31)$$

where $\vec{p}_j \equiv (p_{jx}, p_{jy}, p_{jz})$ is the momentum operator of particle j , and $\vec{p}_j \equiv -i\hbar \frac{\partial}{\partial \vec{r}_j}$.

Since there is no interaction among particles, the eigenstates are expressed as

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{j=1}^N \phi(\vec{r}_j), \quad (3.32)$$

where the single-particle state wavefunction $\phi(\vec{r})$ satisfies

$$\left[\frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \right] \phi(\vec{r}) = \epsilon \phi(\vec{r}). \quad (3.33)$$

The eigenvalues of Eq. (3.33) is well-known;

$$\epsilon_{n_x n_y n_z} = \left(n_x + \frac{1}{2} \right) \hbar \omega_x + \left(n_y + \frac{1}{2} \right) \hbar \omega_y + \left(n_z + \frac{1}{2} \right) \hbar \omega_z, \quad (3.34)$$

where $n_x, n_y, n_z = 0, 1, 2, \dots$

We adopt the grand canonical ensemble. The total particle number N and the total energy E is given by

$$N = \sum_{n_x, n_y, n_z} \left[\exp \beta (\epsilon_{n_x n_y n_z} - \mu) - 1 \right]^{-1} \quad (3.35)$$

$$E = \sum_{n_x, n_y, n_z} \epsilon_{n_x n_y n_z} \left[\exp \beta (\epsilon_{n_x n_y n_z} - \mu) - 1 \right]^{-1} \quad (3.36)$$

where $\beta = (k_B T)^{-1}$ and μ is the chemical potential. For later discussion, we shift the chemical potential as $\mu - \hbar(\omega_x + \omega_y + \omega_z)/2 \rightarrow \mu$. At very low temperature, Eq. (3.35) is written in the following form,

$$N = N_0 + N, \quad (3.37)$$

where

$$N_0 = 1/(e^{-\beta\mu} - 1), \quad (3.38)$$

$$N = \sum_{n_x, n_y, n_z \neq 0} \left[\exp \beta (n_x \hbar \omega_x + n_y \hbar \omega_y + n_z \hbar \omega_z) - 1 \right]^{-1}. \quad (3.39)$$

Discussions, here and in what follows, are essentially the same as those for free boson gas in a box. The Bose-Einstein condensation is the situation where N_0 becomes macroscopic, that is, $N_0 \sim O(N)$. Eq. (3.38) then implies $\mu \leq 0$ and $-\beta\mu \sim O(1/N)$. We have set $\mu = 0$ in Eq. (3.39). Therefore, N_1 in Eq. (3.39) gives the maximum of the contribution from the excited state at low temperature.

We replace the summations in Eq. (3.39) by an integral over the single-particle energy ϵ with the density of states $D(\epsilon)$,

$$D(\epsilon)d\epsilon = \frac{\epsilon^2}{2(\hbar\bar{\omega})^3}d\epsilon. \quad (3.40)$$

The formula (3.40) can be derived as follows. We estimate the number of the states, $N(\epsilon)$, whose energies are smaller than ϵ , which is equivalent to the number of positive integer sets $\{n_x, n_y, n_z\}$ satisfying $0 < (n_x\hbar\omega_x + n_y\hbar\omega_y + n_z\hbar\omega_z) \leq \epsilon$. Geometrically, this corresponds to a volume, $(\epsilon/\hbar\omega_x)(\epsilon/\hbar\omega_y)(\epsilon/\hbar\omega_z)/6$. Therefore, we obtain $N(\epsilon) = \frac{1}{6}\epsilon^3/(\hbar\bar{\omega})^3$, Where $\bar{\omega}^3 = \omega_x\omega_y\omega_z$. A relation $D(\epsilon) = dN(\epsilon)/d\epsilon$ gives Eq. (3.40).

Using Eq. (3.40) to rewrite the summations in Eq. (3.39), we obtain

$$\begin{aligned} N_1 &= \int_0^\infty \frac{D(\epsilon)d\epsilon}{\exp(\beta\epsilon) - 1} \\ &= \left(\frac{k_B T}{\hbar\bar{\omega}}\right)^3 \zeta(3), \quad T \leq T_c \end{aligned} \quad (3.41)$$

where

$$\zeta(3) = \int_0^\infty \frac{x^2 dx}{e^x - 1} = 1.202... \quad (3.42)$$

The transition temperature is defined by

$$N = \zeta(3) \left(\frac{k_B T_c}{\hbar\bar{\omega}}\right)^3. \quad (3.43)$$

For $T \leq T_c$, we have

$$N = N_0 + \zeta(3) \left(\frac{k_B T}{\hbar\bar{\omega}}\right)^3, \quad (3.44)$$

and therefore

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3, \quad T \leq T_c. \quad (3.45)$$

The exponent is changed from 3/2 (for gas confined in box) to 3 (for gas confined in harmonic potentials).

The total energy E in Eq. (3.36) is calculated in the thermodynamic limit; $N \rightarrow \infty$, $\bar{\omega} \rightarrow 0$, $N\bar{\omega}^3 = \text{finite}$. The result is

$$\begin{aligned} E &= 3Nk_B T \frac{g_4(z)}{g_3(z)}, & T > T_c \\ &= 3 \frac{(k_B T)^4}{(\hbar\bar{\omega})^3} \zeta(4), & T \leq T_c \end{aligned} \quad (3.46)$$

where with $z = \exp(\beta\mu)$

$$g_n(z) \equiv \sum_{i=1}^{\infty} \frac{z^i}{i^n}, \quad (3.47)$$

and $\zeta(4) = \pi^4/90 = 1.082\dots$

To summarize, Bose-Einstein condensation of a free Bose gas is the approximation which is valid when the number of atoms in the condensate is very small, hence its ground state energy is the lower limit of a ground state energy of other cases of the Bose-Einstein condensation.

3.4 Ground State Energy from the Thomas-Fermi Approximation

This section is devoted to the calculation of the ground state energy of the Bose-Einstein condensate under the three-dimensional Thomas-Fermi approximations.

We start from the three-dimensional Ginzburg-Pitaevskii-Gross equation with a harmonic potential term,

$$\frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \Psi + g |\Psi|^2 \Psi = \mu \Psi. \quad (3.48)$$

Here, $g > 0$, means the strength of the inter-atomic interaction, and μ is the chemical potential. In the Thomas-Fermi approximation, the first term (the kinetic term) on the left hand side of Eq. (3.48) is neglected, which gives the number density of the condensate, $|\Psi|^2$, as

$$|\Psi|^2 = \frac{1}{g} \left(\mu - \frac{1}{2} m \omega_x^2 x^2 - \frac{1}{2} m \omega_y^2 y^2 - \frac{1}{2} m \omega_z^2 z^2 \right). \quad (3.49)$$

Hence, the number of particles N is given by

$$N = \int_{-x_0}^{x_0} dx \int_{-y_0}^{y_0} dy \int_{-z_0}^{z_0} dz |\Psi|^2, \quad (3.50)$$

where x_0 , y_0 and z_0 are defined as

$$\begin{aligned} x_0 &\equiv \left(\frac{2\mu}{m\omega_x^2} \right)^{1/2}, \quad y_0 \equiv \left(\frac{2}{m\omega_y^2} \right)^{1/2} \left(\mu - \frac{1}{2} m \omega_x^2 x^2 \right)^{1/2}, \\ z_0 &\equiv \left(\frac{2}{m\omega_z^2} \right)^{1/2} \left(\mu - \frac{1}{2} m \omega_x^2 x^2 - \frac{1}{2} m \omega_y^2 y^2 \right)^{1/2}. \end{aligned} \quad (3.51)$$

Substituting (3.49) and (3.51) into (3.50), we obtain

$$N = \frac{8\pi}{15g} \left(\frac{2}{m\omega_x^2} \right)^{1/2} \left(\frac{2}{m\omega_y^2} \right)^{1/2} \left(\frac{2}{m\omega_z^2} \right)^{1/2} \mu^{5/2} \quad (3.52)$$

which gives

$$\mu = \left(\frac{15g}{8\pi} \right)^{2/5} \left(\frac{m\omega_x^2}{2} \right)^{1/5} \left(\frac{m\omega_y^2}{2} \right)^{1/5} \left(\frac{m\omega_z^2}{2} \right)^{1/5} N^{2/5}. \quad (3.53)$$

From the thermodynamic identity,

$$\mu = \frac{\partial E}{\partial N}, \quad (3.54)$$

and from Eq. (3.53), we have the energy in the three-dimensional case, denoted by E_{3D} ,

$$E_{3D} = \frac{5}{7} \left(\frac{15g}{8\pi} \right)^{2/5} \left(\frac{m\omega_x^2}{2} \right)^{1/5} \left(\frac{m\omega_y^2}{2} \right)^{1/5} \left(\frac{m\omega_z^2}{2} \right)^{1/5} N^{7/5}. \quad (3.55)$$

To summarize, because we neglected the kinetic energy term in the Ginzburg-Pitaevskii-Gross equation, the Thomas-Fermi approximation is valid when the

number of atoms in the condensate is very large, and its ground state energy is the upper limit of a ground state energy of other cases of Bose-Einstein condensation.

3.5 Ground State Energy of Neutral Bosons: Short-Range Interaction Case

In this section, by following the work of Gordon Baym and C.J. Pethick[26] the ground state energy of Bose-Einstein condensation for neutral bosonic atoms is presented.

It is known that Bose-Einstein condensation in experiments with cooled and trapped atoms can be described within the framework of the Ginzburg-Pitaevskii-Gross Theory. Validity of such a description has been analysed by Stenholm [41]. In a situation where the trap can be modeled by an anisotropic harmonic oscillator potential and the inter-atomic interactions can be replaced by the effective pseudo-potential involving s-wave scattering length, the ground state energy for condensed bosons of mass m is given by the Ginzburg-Pitaevskii-Gross functional,

$$E[\Psi] = \int d\vec{r} \left[\frac{\hbar^2}{2m} |\nabla \Psi(\vec{r})|^2 + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) |\Psi(\vec{r})|^2 + \frac{2\pi \hbar^2 a}{m} |\Psi(\vec{r})|^4 \right]. \quad (3.56)$$

Here $\Psi(\vec{r})$ is the condensate wavefunction, ω_x , ω_y , and ω_z are angular frequencies characterizing the external potential of the anisotropic trap and a is the s-wave scattering length. The wavefunction satisfies the normalization condition,

$$\int d(\vec{r}) |\Psi(\vec{r})|^2 = N. \quad (3.57)$$

For a system of weakly interacting gas at $T = 0$, N is essentially the total number of atoms in the trap. The exact form of the wavefunction can be determined

by minimizing the energy functional in Eq. (3.56) with the normalization constraint Eq. (3.57). Such a minimization results in the Ginzburg-Pitaevskii-Gross equation,

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + \frac{4\pi\hbar^2 a}{m} |\Psi(\vec{r})|^2 \right] \Psi(\vec{r}) = \mu \Psi(\vec{r}). \quad (3.58)$$

For simplicity, we consider the case in which the magnetic trap is an axially symmetric. Then we have $\omega_x = \omega_y = \omega_\perp$, and it is convenient to express Eq. (3.56)- Eq. (3.58) in terms of the scaled variables defined as,

$$\begin{aligned} \vec{r}_1 &= \vec{r}/a_\perp, \\ \nabla_1 &= a_\perp \nabla, \\ E_1 &= E/\hbar\omega_\perp, \\ \Psi_1(\vec{r}_1) &= \sqrt{\frac{a_\perp^3}{N}} \Psi(\vec{r}), \\ \mu_1 &= \mu/\hbar\omega_\perp, \\ u_1 &= \frac{8\pi a N}{a_\perp}, \end{aligned} \quad (3.59)$$

where

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}. \quad (3.60)$$

We now have

$$\frac{E_1(\Psi)}{N} = \int d\vec{r}_1 \frac{1}{2} \left[|\nabla_1 \Psi_1(\vec{r}_1)|^2 + (x_1^2 + y_1^2 + \lambda_0^2 z_1^2) |\Psi_1(\vec{r}_1)|^2 + \frac{u_1}{2} |\Psi_1(\vec{r}_1)|^4 \right], \quad (3.61)$$

with

$$\lambda_0 = \frac{\omega_z}{\omega_\perp} \quad (3.62)$$

being the anisotropy parameter of the trap,

$$\int d\vec{r}_1 |\Psi_1(\vec{r}_1)|^2 = 1 \quad (3.63)$$

and

$$\left[-\nabla_1^2 + (x_1^2 + y_1^2 + \lambda_0^2 z_1^2) + u_1 |\Psi_1(\vec{r}_1)|^2 \right] \Psi_1(\vec{r}_1) = 2\mu_1 \Psi_1(\vec{r}_1). \quad (3.64)$$

Since it is not possible to find exact analytic solution to Eq. (3.64), various numerical techniques have therefore been developed to study the ground state property of such systems within the framework of the Ginzburg-Pitaevskii-Gross theory. These techniques involve either the direct numerical minimization of Eq. (3.53) subject to the constraint Eq. (3.63) [42] or numerical integration of Eq. (3.64) or its time dependent version, Gross-Pitaevskii equation [43]. Another approach is to use the variational method which has been extensively used in different branches of physics. The main advantage of this method is that with a suitable guess for the form of the wavefunction, it is possible to save a lot of computational effort and time. In addition, it may also provide physical insights which generally get obscured in the complicated computational procedures. The first study of this kind was done by Baym and Pethick in light of the experimental observation in ^{87}Rb . They took the trial wavefunction for the ground state as

$$\Psi(\vec{r}) = N^{1/2} \Omega_\perp^{1/2} \Omega_z^{1/2} \left(\frac{m}{\pi \hbar} \right)^{3/4} e^{-m(\Omega_\perp x^2 + \Omega_\perp y^2 + \Omega_z z^2)/2\hbar}, \quad (3.65)$$

with effective frequencies, ω_\perp and ω_z , treated as variational parameters. However, the wavefunction in Eq. (3.65) brings out only the qualitative features of the condensate, e.g., expansion of the condensate in different directions, shifts in the angular frequencies and the scaling behavior of energy with the number of atoms in the trap. Further, this form of the wavefunction is valid only for small number of atom in the trap.

To find the ground state energy from the trial wavefunction of Baym and Pethick, we substituting Eq. (3.65) into Eq. (3.56). We thus obtain

$$E_0(\Omega_\perp, \Omega_z) = N\hbar \left(\frac{\Omega_\perp}{2} + \frac{\omega_\perp^2}{2\Omega_\perp} + \frac{\Omega_z}{4} + \frac{\omega_z^2}{4\Omega_z} + \frac{Nam^{1/2}}{(2\pi\hbar)^{1/2}} \Omega_\perp \Omega_z^{1/2} \right). \quad (3.66)$$

For an isotropic case in which $\Omega_{\perp} = \Omega_z$, $\omega_{\perp} = \omega_z$, we find

$$E_0(\Omega) = N\hbar\left(\frac{3\Omega}{4} + \frac{3\omega_{\perp}^2}{4\Omega} + \frac{Nam^{1/2}}{(2\pi\hbar)^{1/2}}\Omega^{3/2}\right). \quad (3.67)$$

3.6 Ground State Energy of Charged Bosons: Long-Range Interaction Case

This section is devoted to the review of the work of Takeya Tsurumi, Hirofumi Moris and Miki Wadati [33] in which the authors evaluated the ground state energy of charged bosons confined in an isotropic trap. The problem is rather academic, but turns out to be quite interesting because of the expectation that the Bose-Einstein condensation for charges boson under magnetic traps will be observed in future. In previous section, the interaction between neutral atoms which deal with short-range interaction is well approximated by the delta function, $V(\vec{r}) = g\delta(\vec{r}_i - \vec{r}_j)$ [26]. Hence for the charges boson case, the interaction which accounts for long-range interaction was approximated by the Coulomb potential, $V(\vec{r}) = g/|\vec{r}_i - \vec{r}_j|$ [33]. Hence, the Ginzburg-Petaevskii-Gross energy functional becomes

$$\begin{aligned} E[\Psi] &= \int d\vec{r} \left[\frac{\hbar^2}{2m} |\nabla\Psi|^2 + \frac{1}{2}m\omega^2 r^2 |\Psi|^2 \right] \\ &+ \frac{1}{2} \int d\vec{r} \int d\vec{r}' U(\vec{r} - \vec{r}') |\Psi(\vec{r})|^2 |\Psi(\vec{r}')|^2, \end{aligned} \quad (3.68)$$

where the trap is assumed to be an isotropic harmonic potential, and

$$U(\vec{r}) = g/|\vec{r}|. \quad (3.69)$$

The coupling constant g can be positive or negative in this section.

From the assumption that the ground state wavefunction $\Psi(\vec{r})$ depends only on $r = |\vec{r}|$, using the integral formula for fixed \vec{r} ,

$$\int_0^{\pi} d\theta \sin\theta (r^2 + r'^2 - 2rr'\cos\theta)^{-1/2} = \begin{cases} 2/r & (\text{for } r' < r) \\ 2/r' & (\text{for } r' > r) \end{cases}, \quad (3.70)$$

the last term in Eq. (3.70)

$$\frac{g}{2} \int d\vec{r} d\vec{r}' \frac{1}{|\vec{r} - \vec{r}'|} |\Psi(\vec{r})|^2 |\Psi(\vec{r}')|^2 = 16\pi^2 g \int_0^\infty dr r^2 |\Psi(\vec{r})|^2 \int_r^\infty dr' r'^2 |\Psi(\vec{r}')|^2. \quad (3.71)$$

The ground state energy can be calculated by the variational method. Choose a trial wavefunction,

$$\Psi(\vec{r}) = C \exp\left(\frac{-r^2}{2d^2}\right), \quad (3.72)$$

where C and d are real constants to be determined. The particle number N and the ground state energy are found to be

$$N = C^2 \pi^{3/2} d^3, \quad (3.73)$$

$$E = \frac{3\pi^{3/2} \hbar^2 C^2 d}{4m} + \frac{3\pi^{3/2} m\omega^2 C^2 d^5}{4} + \frac{\sqrt{2}}{2} \pi^{5/2} g C^4 d^5. \quad (3.74)$$

By use of Eq. (3.73), we eliminate the normalization constant C in Eq. (3.74).

The result is

$$E(d) = \frac{3\hbar^2 N}{4md^2} + \frac{3m\omega^2 N d^2}{4} + \frac{N^2 g}{(2\pi)^{1/2} d}. \quad (3.75)$$

It is convenient to introduce a dimensionless parameter λ ,

$$\lambda \equiv d/d_0 \quad (3.76)$$

where $d_0 \equiv [\hbar/(m\omega)]^{1/2}$. Then Eq. (3.75) is rewritten as

$$E(\lambda) = \frac{1}{2} N \hbar \omega \left[\frac{3}{2} (\lambda^{-2} + \lambda^2) + \sigma \lambda^{-1} \right], \quad (3.77)$$

where

$$\sigma \equiv \sqrt{\frac{2}{\pi}} \frac{N g}{\hbar \omega} \left(\frac{m\omega}{\hbar} \right)^{1/2}. \quad (3.78)$$

One can show that $E(\lambda)$ has an absolute minimum irrespective of the sign of σ , that is, the condensate of long-range interacting bosons under harmonic traps is stable both for repulsive and attractive interactions.

Next, consider the Bose-Einstein condensate of charged bosons confined in magnetic traps. Based on the result obtained in Eq. (3.77), the ground state energy can be found. Setting $g = e^2$, e being the electric charge, Eq. (3.77) becomes

$$E(\lambda) = \frac{1}{2}N\hbar\omega \left[\frac{3}{2}(\lambda^{-2} + \lambda^2) + \sigma_e\lambda^{-1} \right], \quad (3.79)$$

where

$$\sigma_e \equiv \sqrt{\frac{2}{\pi}} \frac{Ne^2}{\hbar\omega} \left(\frac{m\omega}{\hbar} \right)^{1/2}. \quad (3.80)$$

Note that, σ_e is positive. We then minimize $E(\lambda)$ with respect to λ . The condition. $\partial E/\partial\lambda = 0$ gives

$$3\lambda^4 - 3 - \sigma_e\lambda = 0. \quad (3.81)$$

For a weak interaction case where σ_e is small, the approximate solution of Eq. (3.81) is $\lambda \approx 1 + (\sigma/12)$. Using this in Eq. (3.79), we obtain

$$E = \frac{3}{2}N\hbar\omega \left(1 + \frac{\sigma_e}{3} \right). \quad (3.82)$$

In the non-interaction limit $\sigma_e \rightarrow 0$, the exact result $E = 3N\hbar\omega/2$ for harmonic oscillators is recovered.

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Chapter 4

Results

This chapter is devoted to present the result of applying the path integral to calculate the ground state energy of charge bosons confined in an isotropic traps including the approximated density matrix and the wavefunction. We will show the detail of the calculation for the cases in which the inter-atomic interaction is approximated by Coulomb potential (long-range interaction) in Section 4.1 and screened Coulomb potential (intermediate-range interaction) in Section 4.2.

4.1 Ground State Energy with Coulomb Potential

This section is devote to the detail of using variational Feynman path integral to obtain the ground state energy of charged bosons confined in an isotropic trap. It is known that this trap can be approximated by a harmonic oscillator potential, and the inter-atomic interaction is approximated by Coulomb potential. Hence, the Lagrangian of such a system is

$$L = -\frac{m}{2} \sum_{i=1}^N [\dot{\vec{r}}_i^2(\tau) + \omega_x^2 x_i^2(\tau) + \omega_y^2 y_i^2(\tau) + \omega_z^2 z_i^2(\tau)] + \frac{1}{2} \sum_{i \neq j}^N \frac{U_0}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \quad (4.1)$$

where m is the atomic mass of the alkali gas, ω_x , ω_y and ω_z are the frequencies in the x , y and z direction respectively, U_0 is a real constant and

$$|\vec{r}_i(\tau) - \vec{r}_j(\tau)|^{-1} = [(x_i(\tau) - x_j(\tau))^2 + (y_i(\tau) - y_j(\tau))^2 + (z_i(\tau) - z_j(\tau))^2]^{-1/2}.$$

For an isotropic magnetic trap, we know that $\omega_x = \omega_y = \omega_z$. Then the Lagrangian

in Eq. (4.1) becomes

$$L = -\frac{m}{2} \sum_{i=1}^N [\dot{\vec{r}}_i^2(\tau) + \omega^2 r_i^2(\tau)] + \frac{1}{2} \sum_{i \neq j}^N \frac{U_0}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|}. \quad (4.2)$$

From Chapter 2, we have known that ground state energy can be evaluated from variational Feynman path integration technique as (c.f. Eq. (2.53))

$$E_0 \leq E'_0 - \frac{1}{\beta} \langle S - S' \rangle_{S'}$$

where S' is the trial action which we can find its ground state energy exactly. Then choosing the trial action to be the form of harmonic oscillator with the frequency Ω being the variational parameter,

$$S' = -\frac{m}{2} \sum_{i=1}^N \int_0^\beta [\dot{\vec{r}}_i^2(\tau) + \Omega^2 \vec{r}_i^2(\tau)] d\tau, \quad (4.3)$$

the density matrix can easily be evaluated by transforming the propagator of harmonic oscillator in real time to the negative imaginary time. The result which can be found in a standard textbook of Feynman path integration [44] takes the form

$$\rho'(\vec{r}, \beta, \vec{r}', 0) = \left(\frac{m\Omega}{2\pi\hbar \sinh(\Omega\beta)} \right)^{\frac{3N}{2}} \cdot \exp \left\{ \frac{-Nm\Omega}{2\hbar \sinh(\Omega\beta)} [(\vec{r}^2 + \vec{r}'^2) \cosh(\Omega\beta) - 2\vec{r}\vec{r}'] \right\}. \quad (4.4)$$

Next, consider the average term, $\langle S - S_0 \rangle_{S'}$ in Eq. (2.53). Since the Lagrangian in Eq. (4.2) has the same kinetic part as the trial action in Eq. (4.3), then we obtain

$$\langle S - S' \rangle_{S'} = -\frac{m}{2} \sum_{i=1}^N \int_0^\beta d\tau (\omega^2 - \Omega^2) \langle \dot{\vec{r}}_i^2(\tau) \rangle_{S'} + \frac{U_0}{2} \sum_{i \neq j}^N \int_0^\beta d\tau \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'}. \quad (4.5)$$

We see that Eq. (4.5) contains the average over quantities like $\langle \dot{\vec{r}}_j^2(\tau) \rangle_{S'}$ and $\langle 1/|\vec{r}_i(\tau) - \vec{r}_j(\tau)| \rangle_{S'}$. These quantities can be evaluated from the generating functional [44] defined as

$$\left\langle \exp \left(\int_0^\beta d\tau \vec{f}(\tau) \cdot \vec{r}(\tau) \right) \right\rangle_{S_0} = \frac{\int D[\vec{r}(\tau)] \exp \left[S_0 + \int_0^\beta d\tau \vec{f}(\tau) \cdot \vec{r}(\tau) \right]}{\int D[\vec{r}(\tau)] \exp[S_0]} \quad (4.6)$$

with end point conditions

$$\vec{r}(\beta) = r_2, \quad \vec{r}(0) = r_1$$

and $f(\tau)$ is an arbitrary function of imaginary time. By following the standard way of evaluation of path integral, we write

$$\vec{r}(\tau) = \vec{r}_{cl} + \vec{y}(\tau),$$

with $\vec{y}(\beta) = 0 = \vec{y}(0)$.

We have known from Feynman and Hibbs [44] that the term linear in $y(\tau)$ that appears together with $\vec{f}(\tau)$ will vanish from above condition. So the remaining terms containing $\vec{y}(\tau)$ the denominator and the numerator are the same and cancel out. We are thus left with is the exponential of the two classical actions, that is,

$$\left\langle \exp \left(\int_0^\beta d\tau \vec{f}(\tau) \cdot \vec{r}(\tau) \right) \right\rangle_{S_0} = \exp(S_f - S_0). \quad (4.7)$$

Hence, we can see that the quantities of interest can be extracted from the formula in Eq. (4.7) by performing the functional differentiation with respect to $\vec{f}(t)$ and setting it to be zero. For example,

$$\begin{aligned} \left\langle \vec{r}(\tau) \exp \left(\int_0^\beta d\tau \vec{f}(\tau) \cdot \vec{r}(\tau) \right) \right\rangle_{S_0} &= \frac{\delta}{\delta \vec{f}(\tau)} [\exp(S_f - S_0)] \\ &= \frac{\delta S_f}{\delta \vec{f}(\tau)} [\exp(S_f - S_0)]. \end{aligned} \quad (4.8)$$

Therefore, by evaluating both sides when $\vec{f}(\tau) \equiv 0$, we obtain

$$\langle \vec{r}(\tau) \rangle_{S_0} = \frac{\delta S_f}{\delta \vec{f}(\tau)} \quad (4.9)$$

We can continue this process to get the second derivatives as

$$\begin{aligned} \left\langle \vec{r}(\tau) \cdot \vec{r}(s) \right\rangle_{S_0} &= \frac{\delta^2}{\delta \vec{f}(\tau) \delta \vec{f}(s)} \exp(S_f - S_0) |_{f \equiv 0} \\ &= \left[\frac{\delta^2 S_f}{\delta \vec{f}(\tau) \delta \vec{f}(s)} + \frac{\delta S_f}{\delta \vec{f}(\tau)} \frac{\delta S_f}{\delta \vec{f}(s)} \right]_{f \equiv 0}. \end{aligned} \quad (4.10)$$

Actually, since S_f is quadratic in $\vec{f}(\tau)$, the quantities $\langle \vec{r}(\tau) \rangle_{S_0}$ and $\langle \vec{r}(\tau) \cdot \vec{r}(s) \rangle_{S_0}$ can be directly evaluated in terms of $\delta S_f / \delta \vec{f}(\tau)$ and $\delta^2 S_f / \delta \vec{f}(\tau) \delta \vec{f}(s)$, which is independent of $\vec{f}(\tau)$

Next, by applying the generating functional technique, we can evaluate the quantities $\langle \vec{r}_j(\tau) \rangle_{S'}$ and $\left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'}$ in Eq. (4.5). First, we will evaluate the quantities $\langle \vec{r}_i(\tau) \rangle_{S'}$ by introducing the Lagrangian of forced harmonic oscillator in three dimensions as

$$L_f = \sum_{i=1}^N \left[\frac{m}{2} \dot{\vec{r}}_i^2(\tau) + \frac{m\Omega^2}{2} \vec{r}_i^2(\tau) - \vec{f}_i(\tau) \cdot \vec{r}_i(\tau) \right] \quad (4.11)$$

and the classical action S' can be evaluated easily. From Feynman and Hibb we have

$$\begin{aligned} S_f &= \sum_{i=1}^N \left\{ \frac{m\Omega}{2 \sinh(\Omega\beta)} \left[(\vec{r}_i^{\prime 2} + \vec{r}_i^{\prime\prime 2}) \cosh(\Omega\beta) - 2 \vec{r}_i^{\prime} \cdot \vec{r}_i^{\prime\prime} \right. \right. \\ &\quad - \frac{2 \vec{r}_i^{\prime\prime}}{m\Omega} \int_0^\beta \vec{f}_i(\tau) \sinh \Omega(\beta - \tau) d\tau - \frac{2 \vec{r}_i^{\prime\prime}}{m\Omega} \int_0^\beta \vec{f}_i(\tau) \sinh \Omega\tau \\ &\quad \left. \left. - \frac{2}{(m\Omega)^2} \int_0^\beta \int_0^\beta \vec{f}_i(\tau) \cdot \vec{f}_i(s) \sinh \Omega(\beta - \tau) \sinh(\Omega s) d\tau ds \right] \right\}. \quad (4.12) \end{aligned}$$

where \vec{r}_i^{\prime} and $\vec{r}_i^{\prime\prime}$ are initial and final points in the configuration space, $\beta = 1/kT$, T is absolute temperature, and k is Boltzmann's constant.

Next, substituting S_f in Eq. (4.12) into Eq. (4.10) we obtain

$$\begin{aligned} \left\langle \vec{r}_i(\tau) \cdot \vec{r}_i(s) \right\rangle_{S_0} &= \left[\frac{\delta^2 S_f}{\delta \vec{f}(\tau) \delta \vec{f}(s)} + \frac{\delta S_f}{\delta \vec{f}(\tau)} \frac{\delta S_f}{\delta \vec{f}(s)} \right]_{f \equiv 0} \\ &= \frac{3}{m\Omega} \frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} + \left[\frac{\vec{r}_i^{\prime} \sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + \frac{\vec{r}_i^{\prime\prime} \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right]^2 \\ &= \langle \vec{r}_i^2(\tau) \rangle_{S'}. \quad (4.13) \end{aligned}$$

Then, we consider that quantity $\langle 1/|\vec{r}_i(\tau) - \vec{r}_j(\tau)| \rangle_{S'}$ in Eq. (4.5). By the definition of Dirac delta function,

$$\int d^3 r f(\vec{r}) \delta^3(\vec{r} - \vec{r}') = f(\vec{r}'), \quad (4.14)$$

we can express the quantity $\langle 1/|\vec{r}_i(\tau) - \vec{r}_j(\tau)| \rangle_{S'}$ through this definition as

$$\left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \left\langle \int d^3 r \delta(\vec{r}(\tau) - (\vec{r}_i(\tau) - \vec{r}_j(\tau))) \cdot \frac{1}{|\vec{r}(\tau)|} \right\rangle. \quad (4.15)$$

Next, using the integral form of the Dirac delta function in Eq. (4.15) we obtain

$$\left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \left\langle \int \frac{d^3 r}{r(\tau)} \int_{-\infty}^{\infty} \frac{d^3 k}{(2\pi)^3} \exp \left[i\vec{k} \cdot (\vec{r}(\tau) - (\vec{r}_i(\tau) - \vec{r}_j(\tau))) \right] \right\rangle_{S'} \quad (4.16)$$

$$= \int_{-\infty}^{\infty} \frac{d^3 r}{r(\tau)} \int \frac{d^3 k}{(2\pi)^3} \exp \left[i\vec{k} \cdot \vec{r}(\tau) \right] \left\langle \exp \left[-i\vec{k} \cdot (\vec{r}_i(\tau) - \vec{r}_j(\tau)) \right] \right\rangle_{S'}. \quad (4.17)$$

The exponential term on the right hand side of Eq. (4.17) factorizes so that

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} &= \int \frac{d^3 r}{r(\tau)} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \exp(ik_x x) \langle \exp[-ik_x(x_i - x_j)] \rangle_{S'_x} \\ &\quad \times \int \frac{dk_y}{2\pi} \exp(ik_y y) \langle \exp[-ik_y(y_i - y_j)] \rangle_{S'_y} \\ &\quad \times \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \exp(ik_z z) \langle \exp[-ik_z(z_i - z_j)] \rangle_{S'_z}. \end{aligned} \quad (4.18)$$

Our next task is to evaluate the exponential term for coordinate. Consider the x -coordinate, we can write it as

$$\langle \exp(-ik_x(x_i - x_j)) \rangle_{S'_x} = \frac{\int D[x(\tau)] [\exp(-S'_x) \cdot \exp(-ik_x(x_i - x_j))]}{\int D[x(\tau)] \exp(-S'_x)}. \quad (4.19)$$

We can see that the numerator is

$$\int D[x(\tau)] \exp[-S'_x - ik_x(x_i - x_j)] = \int D[x(\tau)] \exp[-(S'_{x_i} + ik_x x_i)] \cdot \exp[-(S'_{x_j} - ik_x x_j)] \quad (4.20)$$

Substitute Eq. (4.20) into Eq. (4.19), we obtain

$$\begin{aligned} \langle \exp(-ik_x(x_i - x_j)) \rangle_{S'_x} &= \left(\frac{\int D[x_i(\tau)] \exp[-(S'_{x_i} + ik_x x_i)]}{\int D[x_i(\tau)] \exp(-S'_{x_i})} \right) \\ &\quad \times \left(\frac{\int D[x_j(\tau)] \exp[-(S'_{x_j} - ik_x x_j)]}{\int D[x_j(\tau)] \exp(-S'_{x_j})} \right). \end{aligned} \quad (4.21)$$

It is convenience to write

$$\frac{\int D[x_i(\tau)] \exp[-(S'_{x_i} + ik_x x_i)]}{\int D[x_{x_i}(\tau)] \exp(-S'_{x_i})} = K_{x_i}^+ \quad (4.22)$$

and

$$\frac{\int D[x_j(\tau)] \exp[-(S'_{x_j} - ik_x x_j)]}{\int D[x_{x_j}(\tau)] \exp(-S'_{x_j})} = K_{x_i}^-. \quad (4.23)$$

Next, we define

$$f^\pm(\tau) = \pm ik_x \delta(\tau - s), \quad (4.24)$$

then the exponential term on the left hand side of Eqs. (4.22) and (4.23) can be written as,

$$\begin{aligned} S'_{x_i} + ik_x x_i(\tau) &= \int_0^\beta \frac{m}{2} (\dot{x}_i^2(\tau) + \Omega^2 x_i^2(\tau)) + \int_0^\beta ds ik_x \delta(\tau - s) x_i(s) \\ &= \int_0^\beta \frac{m}{2} (\dot{x}_i^2(\tau) + \Omega^2 x_i^2(\tau)) + \int_0^\beta d\tau f^+(\tau) x_i(\tau) \end{aligned} \quad (4.25)$$

and

$$\begin{aligned} S'_{x_j} - ik_x x_j(\tau) &= \int_0^\beta \frac{m}{2} (\dot{x}_j^2(\tau) + \Omega^2 x_j^2(\tau)) + \int_0^\beta ds (-ik_x) \delta(\tau - s) x_j(s) \\ &= \int_0^\beta \frac{m}{2} (\dot{x}_j^2(\tau) + \Omega^2 x_j^2(\tau)) + \int_0^\beta d\tau f^-(\tau) x_j(\tau). \end{aligned} \quad (4.26)$$

Substitute Eq. (4.25) into Eq. (4.22) and Eq. (4.26) into Eq. (4.23) we find that $K_{x_i}^+$ and $K_{x_i}^-$ can be evaluated easily by using the solution of the force harmonic oscillator (c.f. Eq. (4.12)), and we can see that the force-independent terms are canceled out by the denominator. Then Eq. (4.22) and (4.23) become

$$\begin{aligned} K_{x_i}^\pm &= \exp \left[\frac{x'_i}{\sinh(\Omega\beta)} \int_0^\beta f^\pm(\tau) \sinh \Omega(\beta - \tau) d\tau + \frac{x''_i}{\sinh(\Omega\beta)} \int_0^\beta f^\pm(\tau) \sinh(\Omega\tau) d\tau \right. \\ &\quad \left. + \frac{1}{2m\Omega \sinh(\Omega\beta)} \int_0^\beta \int_0^\beta f^\pm(\tau) f^\pm(s) \sinh \Omega(\beta - \tau) \sinh(\Omega s) d\tau ds \right]. \end{aligned} \quad (4.27)$$

Then using Eq. (4.24) we obtain

$$K_{x_i}^\pm = \exp \left[\pm ik_x x'_i \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} \pm ik_x x''_i \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} - \frac{k_x^2}{2m\Omega} \frac{\sinh \Omega(\beta - \tau) i \sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} \right]. \quad (4.28)$$

Using the above result, Eq. (4.21) can be expressed as,

$$\begin{aligned} \langle \exp(-ik_x(x_i - x_j)) \rangle_{S'_x} &= K_{x_i}^+ K_{x_j}^- \\ &= \exp \left[ik_x(x'_i - x'_j) \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + ik_x(x''_i - x''_j) \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} - \frac{k_x^2}{m\Omega} \frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right]. \end{aligned} \quad (4.29)$$

Similarly y and z terms can be evaluated in the same way, Thus Eq. (4.18) can be express as,

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle &= \int \frac{d^3r}{r} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \exp(ik_x x) K_{x_i}^+ K_{x_j}^- \\ &\quad \times \int_{-\infty}^{\infty} \frac{dk_y}{2\pi} \exp(ik_y y) K_{y_i}^+ K_{y_j}^- \cdot \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \exp(ik_z z) K_{z_i}^+ K_{z_j}^- \end{aligned} \quad (4.30)$$

Again we will interest only the x -coordinate on the right hand side of Eq.

(4.30), from Eq. (4.28) and Eq. (4.29), we can write

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \exp(ik_x x) K_{x_i}^+ K_{x_j}^- &= \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \cdot \exp(ik_x x) \times \\ \exp \left[ik_x(x'_i - x'_j) \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + ik_x(x''_i - x''_j) \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} - \frac{k_x^2}{m\Omega} \frac{\sinh \Omega(\beta - \tau) \sinh \Omega\tau}{\sinh(\Omega\beta)} \right]. \end{aligned} \quad (4.31)$$

Hence, the k -integral can be evaluated by using the relation

$$\int_{-\infty}^{\infty} dx \exp(-ax^2 + bx) = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}\right), \quad (4.32)$$

and Eq. (4.31) becomes

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \exp(ik_x x) K_{x_i}^+ K_{x_j}^- &= \frac{1}{2\pi} \left[\frac{\pi m\Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2} \times \\ \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \cdot \left(x + (x'_i - x'_j) \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + (x''_i - x''_j) \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right)^2 \right] \\ &= \frac{1}{2\pi} \left[\frac{\pi m\Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2} \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right] \end{aligned}$$

$$\begin{aligned} & \times \left(x^2 + 2x(x'_i - x'_j) \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + (x''_i - x''_j) \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right) \\ & + \left((x'_i - x'_j) \frac{\sinh \Omega(\beta - \tau)}{\sinh(\Omega\beta)} + (x''_i - x''_j) \frac{\sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right)^2 \Big]. \end{aligned} \quad (4.33)$$

Apparently, the y and z term take the similar form as in Eq. (4.33).

At this point we can make a discussion. If we consider the system of Bose-Einstein condensation that is composed of identical particles. At finite temperature (β is finite), we must take into account the permutation symmetry in the density matrix. That is the permutation must be included in the partition function

$$Z = \int \frac{1}{N!} \sum_P \xi^P \rho_D(P\vec{r}, \beta; \vec{r}, 0) d\vec{r} \quad (4.34)$$

where

$\xi \equiv \pm 1$ for boson/fermion respectively

$\rho_D \equiv$ density matrix for distinguishable system

$P \equiv$ permutation operator

Then the full density matrix of the many-body Bose-Einstein condensation particle, at finite temperature, can be found by collecting all terms in

$$\rho_D(\vec{r}', \beta; \vec{r}'', 0) = \sum_i \Psi_i(\vec{r}') \Psi_i^*(\vec{r}'') e^{-\beta E_i}. \quad (4.35)$$

It is a very tough task to evaluate the density matrix in Eq. (4.35) because we must take the symmetry into account. However, finding the ground state energy is an easier task since at zero temperature (in the limit $\beta \rightarrow \infty$) the higher order terms in the summation decay more rapidly than the first leading term or the term involving the ground state energy. That is, in the limit $\beta \rightarrow \infty$, the zeroth order term dominates,

$$\lim_{\beta \rightarrow \infty} \rho_D(\vec{r}', \beta; \vec{r}'', 0) = \Psi_0(\vec{r}') \Psi_0^*(\vec{r}'') e^{-\beta E_0}. \quad (4.36)$$

Hence, the ground state energy can be found from the coordinate-independent term in the exponent so that the permutation between end-point needs not to be performed.

Consider Eqs. (4.13) and (4.33). If we neglect the end-point dependent terms, Eq. (4.13) becomes

$$\langle \vec{r}_i^2(\tau) \rangle_{S'} = \frac{3}{m\Omega} \frac{\pi m \Omega i \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \quad (4.37)$$

and Eq. (4.33) becomes

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} \exp(ik_x x) K_{xi}^+ K_{xj}^- &= \frac{1}{2\pi} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2} \\ &\times \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} x^2 \right] \end{aligned} \quad (4.38)$$

Similarly, y and z terms, we get

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dk_y}{2\pi} \exp(ik_y y) K_{yi}^+ K_{yj}^- &= \frac{1}{2\pi} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2} \\ &\times \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} y^2 \right] \end{aligned} \quad (4.39)$$

and

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \exp(ik_z z) K_{zi}^+ K_{zj}^- &= \frac{1}{2\pi} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2} \\ &\times \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} z^2 \right] \end{aligned} \quad (4.40)$$

Substituting Eqs. (4.38), (4.39) and (4.40) into Eq. (4.30), we obtain

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} &= \int \frac{d^3 r}{r} \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{3/2} \\ &\times \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} (x^2 + y^2 + z^2) \right]. \end{aligned} \quad (4.41)$$

Since $x^2 + y^2 + z^2 = r^2$, then

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} &= \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \\ &\times \int \frac{d^3 r}{r} \cdot \exp \left[\frac{-m \Omega \sinh(\Omega \beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} r^2 \right] \end{aligned} \quad (4.42)$$

We next transform the integral from cartesian coordinates to spherical coordinates, by using the relation

$$\int d^3 r = \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} r^2 \sin \theta dr d\theta d\phi, \quad (4.43)$$

then Eq. (4.42) becomes

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} &= \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \\ &\times \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \exp \left[\frac{-m \Omega \sinh(\Omega \beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} r^2 \right] \\ &\times r \sin \theta dr d\theta d\phi \end{aligned} \quad (4.44)$$

$$\begin{aligned} &= \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \\ &\times 4\pi \int_0^{\infty} \exp \left[\frac{-m \Omega \sinh(\Omega \beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} r^2 \right] r dr. \end{aligned} \quad (4.45)$$

The r -integral can be evaluated by using the relation

$$\int_0^{\infty} e^{-ax^2} x dx = \frac{1}{2a}, \quad (4.46)$$

so that Eq. (4.45) becomes

$$\begin{aligned} \left\langle \frac{1}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} &= \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \\ &\times 2\pi \left[\frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)}{m \Omega \sinh(\Omega \beta)} \right]. \end{aligned} \quad (4.47)$$

At this point, we have evaluated the important quantities, $\langle \vec{r}_i^2(\tau) \rangle_{S'}$ and $\langle 1/|\vec{r}_i(\tau) - \vec{r}_j(\tau)| \rangle_{S'}$. The next task is to use such quantities to evaluate the

quantity $\langle S - S' \rangle_{S'}$, and finally to evaluate the ground state energy of charged bosons.

We now evaluate the quantities $\langle S - S' \rangle_{S'}$ in Eq.(4.5), To do so, we substituting Eqs.(4.37) and (4.47) into Eq.(4.5). Then Eq.(4.5) can be rewritten as

$$\begin{aligned} \langle S - S' \rangle_{S'} &= -\frac{m}{2} \sum_{i=1}^N \int_0^\beta d\tau (\omega^2 - \Omega^2) \frac{3}{2m\Omega} \left(\frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right) \\ &\quad - \frac{U_0}{2} \sum_{i \neq j}^N \int_0^\beta d\tau \frac{1}{(2\pi)^2} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{3/2} \left[\frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} \right]. \end{aligned} \quad (4.48)$$

We may write the summation as,

$$\sum_{i=1}^N \equiv N \quad \text{and} \quad \sum_{i \neq j}^N \equiv N(N-1) \approx N^2,$$

where N is a number of atoms in the system. So, Eq. (4.48) becomes

$$\begin{aligned} \langle S - S' \rangle_{S'} &= -\frac{3N}{2} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \int_0^\beta d\tau \left(\frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right) \\ &\quad - \frac{N^2}{2} U_0 \left(\frac{m\Omega}{\pi} \right)^{1/2} \int_0^\beta d\tau \left[\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{3/2} \left[\frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} \right] \\ &= -\frac{3N}{2} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \int_0^\beta d\tau \left(\frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right) \\ &\quad - \frac{N^2}{2} U_0 \left(\frac{m\Omega}{\pi} \right)^{1/2} \int_0^\beta d\tau \left[\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{1/2}. \end{aligned} \quad (4.49)$$

It is difficult to integrate this equation. However we can use the approximation in the integrand. Let us start from the definition

$$\sinh x = \frac{e^x - e^{-x}}{2}. \quad (4.50)$$

Then the integrand of second term on the right hand side of Eq. (4.49) becomes

$$\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} = \frac{2(1 - e^{-2\Omega\beta})}{(1 - e^{-2\Omega(\beta-\tau)})(1 - e^{-2\Omega\tau})}. \quad (4.51)$$

In the limit $\beta \rightarrow \infty$ we find that

$$\beta - \tau \approx \beta, \quad (4.52)$$

so that

$$\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} = \frac{2}{1 - e^{-2\Omega\tau}}. \quad (4.53)$$

Using geometric series

$$\frac{1}{1 - x} = 1 + x + x^2 + \dots \quad \text{for } -1 < x < 1, \quad (4.54)$$

we can write

$$\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \approx 2(1 + e^{-2\Omega\tau} + e^{-4\Omega\tau} + \dots). \quad (4.55)$$

As $\beta \rightarrow \infty$, the zeroth order term dominates the rest of the series. Thus

$$\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \approx 2, \quad (4.56)$$

so that

$$\frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} = \frac{1}{\frac{\sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}} \approx 1/2. \quad (4.57)$$

Finally substitute Eqs. (4.56) and (4.57) into Eq. (4.49), we get

$$\begin{aligned} \langle S - S' \rangle_{S'} &= -\frac{3N}{2} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \frac{1}{2} \int_0^\beta d\tau - \frac{N^2}{2} U_0 \left(\frac{m\Omega}{\pi} \right)^{1/2} 2^{1/2} \int_0^\beta d\tau \\ &= -\frac{3N}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \beta - \frac{U_0}{2} \left(\frac{2m\Omega}{\pi} \right)^{1/2} N^2 \beta, \end{aligned} \quad (4.58)$$

By checking the dimension, we can restore \hbar into Eq. (4.58)

$$\langle S - S' \rangle_{S'} = -\frac{3N\hbar}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \beta - \frac{U_0}{2} \left(\frac{2m\Omega}{\pi\hbar} \right)^{1/2} N^2 \beta. \quad (4.59)$$

Now it is easy to evaluate the ground state energy by recalling Eq. (2.53)

$$E_0 \leq E'_0 - \frac{1}{\beta} \langle S - S' \rangle_{S'}.$$

Hence, the upper bound of the ground state energy is

$$E_0 = E'_0 - \frac{1}{\beta} \langle S - S' \rangle_{S'} \quad (4.60)$$

and E'_0 in Eq. (4.60) can easily be evaluated; it is the ground state of trial action S' in Eq. (4.3) which is the action of harmonic oscillator. E'_0 is the ground state energy of harmonic oscillator which can be found in any standard textbook of quantum mechanics [44],

$$E'_0 = \frac{3N\hbar\Omega}{2}. \quad (4.61)$$

Substituting Eqs. (4.59) and (4.61) into Eq. (4.60), we find that the ground state energy is

$$\begin{aligned} E_0 &= \frac{3N\hbar\Omega}{2} + \frac{3N\hbar}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} \Omega^{1/2} N^2 \\ &= \frac{3}{4} N \hbar \Omega + \frac{3}{4} N \hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2. \end{aligned} \quad (4.62)$$

Next, we will approximate the density matrix, and the ground state wave function. We begin with Eq. (2.50) as

$$\rho(\vec{r}', \beta; \vec{r}, 0) = \rho'(\vec{r}', \beta; \vec{r}, 0) \cdot \exp \langle S - S' \rangle_{S'}.$$

Then substituting $\rho'(\vec{r}', \beta; \vec{r}, 0)$ from Eq. (4.4) and the quantity $\langle S - S' \rangle_{S'}$ from Eq. (4.59) and setting \hbar equal the unity, we find that

$$\begin{aligned} \rho(\vec{r}', \beta; \vec{r}, 0) &= \left[\frac{m\Omega}{2\pi \sinh(\Omega\beta)} \right]^{3N/2} \exp \left(\frac{-m\Omega N}{2 \sinh(\Omega\beta)} [(\vec{r}^2 + \vec{r}'^2) \cosh(\Omega\beta) - 2\vec{r}\vec{r}'] \right) \\ &\quad \times \exp \left(-\frac{3N}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \beta - \frac{U_0}{2} \left(\frac{2m\Omega}{\pi} \right)^{1/2} \beta N^2 \right), \end{aligned} \quad (4.63)$$

Next we approximate the prefactor by using Eq. (4.50),

$$\begin{aligned} \left[\frac{m\Omega}{2\pi \sinh(\Omega\beta)} \right]^{3N/2} &= \left(\frac{m\Omega}{\pi} \right)^{3N/2} \left(\frac{1}{e^{\Omega\beta} - e^{-\Omega\beta}} \right)^{3N/2} \\ &= \left(\frac{m\Omega}{\pi} \right)^{3N/2} \left(\frac{e^{-\Omega\beta}}{1 - e^{-2\Omega\beta}} \right)^{3N/2}. \end{aligned} \quad (4.64)$$

Again by using the geometric series, we find that

$$\left[\frac{m\Omega}{2\pi \sinh(\Omega\beta)} \right]^{3N/2} = \left(\frac{m\Omega}{\pi} \right)^{3N/2} e^{-\frac{3}{2}N\Omega\beta} (1 + e^{-2\Omega\beta} + e^{-4\Omega\beta} + \dots)^{3N/2}. \quad (4.65)$$

For the ground state energy, we take the limit β approaches infinity, so we keep only the zeroth order term. Then Eq. (4.65) become

$$\left[\frac{m\Omega}{2\pi \sinh(\Omega\beta)} \right]^{3N/2} = \left(\frac{m\Omega}{\pi} \right)^{3N/2} \exp\left(\frac{-3N\Omega\beta}{2}\right), \quad (4.66)$$

Then we substitute Eq. (4.66) into Eq. (4.63), we find that

$$\begin{aligned} \rho(\vec{r}', \beta; \vec{r}, 0) &= \left(\frac{m\Omega}{\pi} \right)^{3N/2} \exp\left(\frac{-m\Omega N}{2 \sinh(\Omega\beta)} [(\vec{r}'^2 + \vec{r}^2) \cosh(\Omega\beta) - 2\vec{r}'\vec{r}]\right) \\ &\times \exp\left(-\frac{3}{4}N\Omega\beta - \frac{3N\beta\omega^2}{4\Omega} - \frac{U_0}{2} \left(\frac{2m\Omega}{\pi}\right)^{1/2} \beta N^2\right), \end{aligned} \quad (4.67)$$

In the limit $\beta \rightarrow \infty$ we can approximate

$$\frac{1}{\sinh(\Omega\beta)} = 0, \quad \text{and} \quad \frac{\cosh(\Omega\beta)}{\sinh(\Omega\beta)} \approx 1. \quad (4.68)$$

Restoring \hbar into Eq. (4.67) by checking the dimension and using Eq. (4.68), Eq. (4.67) becomes

$$\begin{aligned} \rho(\vec{r}', \beta; \vec{r}, 0) &= \left(\frac{m\Omega}{\pi\hbar} \right)^{3N/2} \exp\left(\frac{-m\Omega N}{2\hbar} (\vec{r}'^2 + \vec{r}^2)\right) \\ &\times \exp\left[-\left(\frac{3}{4}N\hbar\Omega + \frac{3}{4}N\hbar\frac{\omega^2}{\Omega} + \frac{U_0}{2} \left(\frac{2m\Omega}{\pi\hbar}\right)^{1/2} N^2\right) \beta\right] \end{aligned} \quad (4.69)$$

Comparing Eq. (4.69) with Eq. (4.36) we obtain

$$E_0 = \frac{3}{4}N\hbar\Omega + \frac{3}{4}N\hbar\frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar}\right)^{1/2} N^2, \quad (4.70)$$

and

$$\psi_0(\vec{r}') = \prod_{i=1}^N \psi_i(\vec{r}'_i) = \left(\frac{m\Omega}{\pi\hbar} \right)^{3N/4} \exp\left[\frac{-m\Omega N}{2\hbar} \vec{r}'^2\right]. \quad (4.71)$$

Hence $\psi_0(\vec{r})$ is the ground state wavefunction of charged bosons which is of a Gaussian form and it is the product of N single-particle state wavefunctions $\psi_i(\vec{r}_i)$;

$$\psi_i(\vec{r}_i) = \left(\frac{m\Omega}{\pi\hbar}\right)^{3/4} \cdot \exp\left(-\frac{m\Omega}{2\hbar}\vec{r}_i^2\right). \quad (4.72)$$

Moreover, E_0 in Eq. (4.70) is the ground state energy which is the same as Eq. (4.62).

4.2 Ground State Energy with Screened Coulomb Potential

In Section 4.1 we have evaluated the ground state energy of charged bosons confined in an isotropic trap, whose the inter-atomic interaction is described by long-range interaction which is approximated by Coulomb potential. In this section we will consider the intermediate-range interaction approximated by Screened Coulomb potential, because we expect that the ground state energy of charged bosons with intermediate-range interaction may be different from long-range interaction case.

By using the variational Feynman path integration mentioned in Sections 2.3 and 4.1, we will evaluate the ground state energy of charged bosons confined in an isotropic trap with a screened Coulomb potential. Thus, the Lagrangian of such a system is

$$L = -\frac{m}{2} \sum_{i=1}^N [\dot{\vec{r}}_i^2(\tau) + \omega^2 \vec{r}_i^2(\tau)] + \frac{1}{2} \sum_{i \neq j}^N \frac{U_0 \exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|}. \quad (4.73)$$

Following Eq. (4.5) we can write

$$\langle S - S' \rangle_{S'} = -\frac{m}{2} \sum_{i=1}^N \int_0^\beta d\tau (\omega^2 - \Omega^2) \langle \dot{\vec{r}}_i^2(\tau) \rangle_{S'} + \frac{U_0}{2} \sum_{i \neq j}^N \int_0^\beta d\tau \left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} \quad (4.74)$$

where S' is the trial action which same as Eq. (4.3) and the quantity $\langle \dot{\vec{r}}_i^2(\tau) \rangle_{S'}$ is also same as Eq. (4.37).

Next consider the integrand in the second term on the right hand side of Eq. (4.74), by following the definition of the delta function in Eq. (4.14), we can write

$$\left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \left\langle \int_{-\infty}^{\infty} d^3r \delta(\vec{r} - (\vec{r}_i(\tau) - \vec{r}_j(\tau))) \frac{\exp[-\mu|\vec{r}|]}{|\vec{r}|} \right\rangle_{S'}. \quad (4.75)$$

Using the integral form of the delta function in Eq. (4.75), we obtain

$$\left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \left\langle \int_{-\infty}^{\infty} d^3r \frac{e^{-\mu r}}{r} \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} \exp[i\vec{k}(\vec{r} - (\vec{r}_i(\tau) - \vec{r}_j(\tau)))] \right\rangle_{S'}. \quad (4.76)$$

So we can write

$$\left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \int_{-\infty}^{\infty} d^3r \frac{e^{-\mu r}}{r} \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} \exp(i\vec{k} \cdot \vec{r}) \left\langle \exp[i\vec{k}(\vec{r}_i(\tau) - \vec{r}_j(\tau))] \right\rangle_{S'}. \quad (4.77)$$

Evaluating the k -integral by using the process from Eq. (4.18) to Eq. (4.41), we obtain

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} \exp(i\vec{k} \cdot \vec{r}) \left\langle \exp[i\vec{k}(\vec{r}_i(\tau) - \vec{r}_j(\tau))] \right\rangle_{S'} = \\ & \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \cdot \exp \left[\frac{-m \Omega \sinh(\Omega \beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} r^2 \right]. \end{aligned} \quad (4.78)$$

Substituting Eq. (4.78) into Eq. (4.77) we obtain

$$\begin{aligned} & \left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \\ & \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega \beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} \right]^{3/2} \int \frac{d^3r}{r} \exp \left[\frac{-m \Omega \sinh(\Omega \beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega \tau)} r^2 - \mu r \right]. \end{aligned} \quad (4.79)$$

Transforming the integral to the spherical coordinates by using Eq. (4.43), and integrating over θ and ϕ variables. Then, Eq. (4.79) becomes

$$\left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = \frac{(4\pi)}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega\beta)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{3/2} \int_0^\infty dr r \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} r^2 - \mu r \right]. \quad (4.80)$$

Next we evaluate the r -integral in Eq. (4.80),

$$\int_0^\infty dr r \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} r^2 - \mu r \right] \equiv \int_0^\infty dx x e^{-ax^2 - bx}. \quad (4.81)$$

Let

$$u = ax^2 + bx,$$

then

$$du = 2ax dx + b dx,$$

The integral in Eq. (4.81) becomes

$$\begin{aligned} \int_0^\infty dx x e^{-ax^2 - bx} &= \frac{1}{2a} \int_0^\infty dx [(2ax + b) - b] e^{-ax^2 - bx} \\ &= \frac{1}{2a} \left[\int_0^\infty dx (2ax + b) e^{-ax^2 - bx} - b \int_0^\infty dx e^{-ax^2 - bx} \right]. \end{aligned} \quad (4.82)$$

We can see that the first term on the right hand side of Eq. (4.82) can be integrated easily. Thus

$$\int_0^\infty dx (2ax + b) e^{-ax^2 - bx} = \int_0^\infty du e^{-u} = 1, \quad (4.83)$$

We next evaluate the second term on the right hand side of Eq. (4.82). It is convenient to write

$$I = \int_0^\infty dx e^{-ax^2 - bx} = \exp\left(\frac{b^2}{4a}\right) \int_0^\infty dx \exp\left[-a\left(x + \frac{b}{2a}\right)^2\right]. \quad (4.84)$$

Let $w = x + b/2a$, then $dw = dx$ and the lower limit of the integral in Eq. (4.84) becomes $b/2a$. Then the integral in Eq. (4.84) can be written as

$$I_1 = \int_{b/2a}^{\infty} dw \exp(-aw^2) \quad (4.85)$$

Using another dummy variable v , and denoting the lower limit of the integral as

$$b/2a = w_0 = v_0, \quad (4.86)$$

we can write

$$I_1^2 = \int_{w_0}^{\infty} \int_{v_0}^{\infty} dw dv \exp[-a(w^2 + v^2)]. \quad (4.87)$$

For $w_0 = v_0 = 0$, I_1^2 can be evaluated easily by transforming it to polar coordinates, so we obtain

$$I_0^2 = \int_0^{\pi/2} \int_0^{\infty} r dr d\theta \exp(-ar^2) = \frac{\pi}{4a} \quad (4.88)$$

We note that I_0^2 is the integral for the case that the lower limits of the integral I_1^2 are zero ($w_0 = v_0 = 0$).

For the case that $w_0 = v_0 = b/2a$, it is easy to evaluate the integral I_1^2 Eq. (4.87) by writing it as,

$$\begin{aligned} & \int_{b/2a}^{\infty} \int_{b/2a}^{\infty} dw dv \exp[-a(w^2 + v^2)] \\ &= \int_0^{\infty} \int_0^{\infty} dw dv \exp[-a(w^2 + v^2)] - \int_0^{b/2a} \int_0^{b/2a} dw dv \exp[-a(w^2 + v^2)], \end{aligned} \quad (4.89)$$

We have known from the table of integral [45] that

$$\int_0^{b/2a} \exp[-a^2x] dx = \frac{1}{2} \sqrt{\pi} \operatorname{Erf} \left[\frac{b}{2a} \right], \quad (4.90)$$

where $\operatorname{Erf}[x]$ is the error function, and its lowest term is given by

$$\operatorname{Erf} [x] \simeq \frac{2x}{\sqrt{\pi}}, \quad (4.91)$$

so Eq. (4.90) becomes

$$\int_0^{b/2a} \exp[-x^2] dx = \frac{b}{2a} \quad (4.92)$$

from Eq. (4.90) and Eq. (4.91) we find that Eq. (4.92) is valid when $\frac{b}{a} \ll 1$, in otherwise case this gives zero, so that the second term on the right hand side of Eq. (4.89) becomes

$$\int_0^{b/2a} \int_0^{b/2a} dw dv \exp[-a(w^2 + v^2)] = \frac{b^2}{4a^2}. \quad (4.93)$$

Then substituting Eq. (4.88), and Eq. (4.93) into Eq. (4.89), we obtain

$$I_1^2 = \int_{b/2a}^{\infty} \int_{b/2a}^{\infty} dw dv \exp[-a(w^2 + v^2)] = \frac{\pi}{4a} - \frac{b^2}{4a^2} \quad (4.94)$$

thus

$$I_1 = \left[\frac{\pi}{4a} - \frac{b^2}{4a^2} \right]^{1/2} \quad (4.95)$$

and hence Eq. (4.84) becomes

$$\int_0^{\infty} dx e^{-ax^2 - bx} = \exp\left(\frac{b^2}{4a}\right) \left[\frac{\pi}{4a} - \frac{b^2}{4a^2} \right]^{1/2}. \quad (4.96)$$

Next substituting Eq. (4.83) and Eq. (4.96) into Eq. (4.82) we find that

$$\int_0^{\infty} dx x e^{-ax^2 - bx} = \frac{1}{2a} - \frac{1}{4a} \left[\frac{\pi}{a} - \frac{b^2}{a^2} \right]^{1/2} \exp\left(\frac{b^2}{4a}\right) \quad (4.97)$$

Recalling Eq. (4.81), we can see that

$$a = \frac{m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \quad \text{and} \quad b = \mu.$$

This expression is applicable even when $\mu \ll 1$, so we can write

$$\begin{aligned} & \int_0^{\infty} dr r \exp \left[\frac{-m\Omega \sinh(\Omega\beta)}{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} r^2 - \mu r \right] \\ &= \frac{1}{2} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} - \left(\frac{\mu}{4} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} \right. \\ & \left. \left[\pi \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} - \mu^2 \left(\frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} \right)^2 \right]^{1/2} \right. \\ & \left. \exp \left[\frac{\mu^2}{4} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m\Omega \sinh(\Omega\beta)} \right] \right). \end{aligned} \quad (4.98)$$

Next we substitute Eq. (4.98) into Eq. (4.80), we find

$$\begin{aligned}
& \left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} \\
&= \frac{1}{(2\pi)^3} \left[\frac{\pi m \Omega \sinh(\Omega\tau)}{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)} \right]^{3/2} \times \\
& \left\{ \frac{1}{2} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m \Omega \sinh(\Omega\beta)} - \left(\frac{\mu}{4} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m \Omega \sinh(\Omega\beta)} \right) \right. \\
& \left[\pi \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m \Omega \sinh(\Omega\beta)} - \mu^2 \left(\frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m \Omega \sinh(\Omega\beta)} \right)^2 \right]^{1/2} \\
& \left. \exp \left[\frac{\mu^2}{4} \frac{4 \sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{m \Omega \sinh(\Omega\beta)} \right] \right\} \quad (4.99)
\end{aligned}$$

By using the approximation in Eq. (4.56) and Eq. (4.57), we obtain

$$\left\langle \frac{\exp[-\mu|\vec{r}_i(\tau) - \vec{r}_j(\tau)|]}{|\vec{r}_i(\tau) - \vec{r}_j(\tau)|} \right\rangle_{S'} = (2\pi)^{-\frac{3}{2}} (m\Omega)^{\frac{1}{2}} - (2\pi)^{-\frac{3}{2}} \mu \left[\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right]^{\frac{1}{2}} \exp\left(\frac{\mu^2}{2m\Omega}\right). \quad (4.100)$$

Then we evaluate the quantity $\langle S - S' \rangle_{S'}$ by substituting Eq. (4.100) into Eq. (4.74) and using the quantity $\langle \vec{r}_i(\tau) \rangle_{S'}$ in Eq. (4.37), we find that

$$\begin{aligned}
\langle S - S' \rangle_{S'} &= -\frac{3N}{2} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \int_0^\beta d\tau \left(\frac{\sinh \Omega(\beta - \tau) \sinh(\Omega\tau)}{\sinh(\Omega\beta)} \right) \\
& - \frac{4\pi N^2 U_0}{2} \left[(2\pi)^{-\frac{3}{2}} (m\Omega)^{\frac{1}{2}} - (2\pi)^{-\frac{3}{2}} \mu \left[\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right]^{\frac{1}{2}} \exp\left(\frac{\mu^2}{2m\Omega}\right) \right] \int_0^\beta d\tau. \quad (4.101)
\end{aligned}$$

Again, by using the approximation in Eq. (4.57), Eq. (4.101) becomes

$$\begin{aligned}
\langle S - S' \rangle_{S'} &= -\frac{3N}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \int_0^\beta d\tau - \frac{4\pi N^2 U_0}{2} (2\pi)^{-\frac{3}{2}} (m\Omega)^{\frac{1}{2}} \int_0^\beta d\tau \\
& - \frac{4\pi N^2 U_0}{2} (2\pi)^{-3/2} \mu \left[\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right]^{\frac{1}{2}} \exp\left(\frac{\mu^2}{2m\Omega}\right) \int_0^\beta d\tau. \quad (4.102)
\end{aligned}$$

Next integrating over the time τ , we obtain

$$\begin{aligned}
\langle S - S' \rangle_{S'} &= -\frac{3N}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) \beta - N^2 U_0 \left(\frac{m\Omega}{2\pi} \right)^{\frac{1}{2}} \beta \\
& - \frac{N^2 U_0}{(2\pi)^{1/2}} \mu \left[\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right]^{\frac{1}{2}} \exp\left(\frac{\mu^2}{2m\Omega}\right) \beta. \quad (4.103)
\end{aligned}$$

Then, to evaluate the ground state energy we begin with Eq. (4.60) in which the upper bound of the ground state energy can be written as

$$E_0 = E'_0 - \frac{1}{\beta} \langle S - S' \rangle_{S'} ,$$

where E'_0 is the ground state energy of harmonic oscillator which corresponds to the trial action S' in Eq. (4.3). So

$$E'_0 = \frac{3N\hbar\Omega}{2} .$$

Thus by using such E'_0 and the quantity $\langle S - S' \rangle_{S'}$ from Eq. (4.103) (after restoring \hbar by checking dimension), the upper bound of the ground state energy is

$$\begin{aligned} E_0 &= \frac{3}{2}N\hbar\Omega + \frac{3}{4}N\hbar \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2 \\ &\quad + \frac{U_0\mu}{(2\pi)^{1/2}} \left[\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right]^{\frac{1}{2}} \exp\left(\frac{\mu^2}{2m\Omega}\right) \hbar^{\frac{1}{2}} N^2 \\ &= \frac{3}{4}N\hbar\Omega + \frac{3}{4}N\hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2 \\ &\quad + \frac{U_0\mu}{(2\pi)^{1/2}} \left(\frac{\pi}{2} - \frac{\mu^2\hbar}{m\Omega} \right)^{1/2} \exp\left(\frac{\mu^2\hbar}{2m\Omega}\right) N^2, \end{aligned} \quad (4.104)$$

where this expression is applicable even when $\mu \ll 1$.

Then, from Eq. (2.48), Eq. (4.4) and Eq. (4.104), the approximated density matrix with \hbar set equal the unity is

$$\begin{aligned} \rho(\vec{r}', \beta; \vec{r}, 0) &= \rho'(\vec{r}', \beta; \vec{r}, 0) \cdot \exp\langle S - S' \rangle_{S'} \\ &= \left[\frac{m\Omega}{2\pi \sinh(\Omega\beta)} \right]^{3N/2} \exp \left[\frac{-m\Omega N}{2 \sinh(\Omega\beta)} [(\vec{r}^2 + \vec{r}'^2) \cosh(\Omega\beta) - 2\vec{r}\vec{r}'] \right] \\ &\quad \times \exp \left\{ -\beta \left[\frac{3N}{4} \left(\frac{\omega^2 - \Omega^2}{\Omega} \right) - N^2 U_0 \left(\frac{m\Omega}{2\pi} \right)^{1/2} \right. \right. \\ &\quad \left. \left. + \frac{N^2 U_0 \mu}{(2\pi)^{1/2}} \left(\frac{\pi}{2} - \frac{\mu^2}{m\Omega} \right)^{1/2} \exp\left(\frac{\mu^2}{2m\Omega}\right) \right] \right\}. \end{aligned} \quad (4.105)$$

Next using the approximation from Eq. (4.66), Eq. (4.68) and restoring \hbar , Eq. (4.105) becomes

$$\begin{aligned} \rho(\vec{r}', \beta; \vec{r}, 0) &= \left(\frac{m\Omega}{\pi\hbar} \right)^{3N/2} \exp \left[-\frac{m\Omega N}{2\hbar} (r'^2 + r^2) \right] \\ &\times \exp \left\{ -\beta \left[\frac{3}{4} N \hbar \Omega + \frac{3}{4} N \hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2 \right. \right. \\ &\left. \left. + \frac{U_0 \mu}{(2\pi)^{1/2}} \left(\frac{\pi}{2} - \frac{\mu^2 \hbar}{m\Omega} \right)^{1/2} \exp \left(\frac{\mu^2 \hbar}{2m\Omega} \right) N^2 \right] \right\}. \end{aligned} \quad (4.106)$$

Comparing Eq. (4.106) with Eq. (4.36), we obtain

$$\begin{aligned} E_0 &= \frac{3}{4} N \hbar \Omega + \frac{3}{4} N \hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2 \\ &+ \frac{U_0 \mu}{(2\pi)^{1/2}} \left(\frac{\pi}{2} - \frac{\mu^2 \hbar}{m\Omega} \right)^{1/2} \exp \left(\frac{\mu^2 \hbar}{2m\Omega} \right) N^2 \end{aligned} \quad (4.107)$$

and

$$\Psi_0(\vec{r}') = \left(\frac{m\Omega}{\pi\hbar} \right)^{\frac{3N}{4}} \cdot \exp \left(\frac{-m\Omega N}{2\pi\hbar} r'^2 \right), \quad (4.108)$$

where Eq. (4.107) is valid even when $\mu \ll 1$.

Chapter 5

Discussion and Conclusion

This work is based on the observation of the Bose-Einstein condensation phenomena arisen by trapping alkali atoms in magnetic field. These alkali atoms are composite bosons and neutral atoms of which the inter-atomic interaction is short-range and well approximated by the delta function. We extended the investigation beyond the short-range interaction, i.e. long-range and intermediate-range interaction, by using Feynman path integration. For the long-range interaction, it is approximated by using the Coulomb potential. For intermediate-range interaction, it is approximated by the Screened Coulomb potential.

Since the problem of charged bosons in an isotropic trap can be formulated in the form of Feynman path integral, we have constructed the basic ideas of the Feynman path integral in Chapter II. We have reviewed also how the variation Feynman path integral can be used to evaluate the ground state energy of the charged bosons.

In Chapter III, we have presented the basic equation which describes the Bose-Einstein condensation. For the time-independent case, we use Ginzburg-Pitaevskii-Gross equation which is equivalent to the time-independent nonlinear Schrödinger equation. We have reviewed some recent researches which evaluate the ground state energy of the neutral bosons and the charged bosons. For the charged bosons case, we have reviewed the works of Takeya Tsurumi, Hirofumi Moris, and Miki Wadati. They began by choosing a trial wavefunction in the form of Gaussian as

$$\Psi(\vec{r}) = C \exp\left(\frac{-r^2}{2d^2}\right). \quad (5.1)$$

Then by using the Ginzburg-Pitaevskii-Gross energy functional, which the interatomic interaction term was approximated by Coulomb potential, they have evaluated the ground state energy of the charged bosons confined in an isotropic trap as

$$E_0(d) = \frac{3\hbar^2 N}{4md^2} + \frac{3m\omega^2 Nd^2}{4} + \frac{N^2 g}{(2\pi)^{1/2} d}. \quad (5.2)$$

In chapter IV, we have calculated the upper bound of the ground state energy of the charged bosons confined in an isotropic trap by using the variational path integration method. In this method, we have used the Feynman-Jensen inequality, i.e.

$$\langle e^F \rangle \geq \exp\langle F \rangle, \quad (5.3)$$

to evaluate the upper bound of the ground state energy. Then we have used the approximation that the temperature approach zero. Hence the upper bound of ground state energy is obtained [44] as

$$E_0 = E' - \frac{1}{\beta} \langle S - S' \rangle_{s'}. \quad (5.4)$$

Finally, the upper bound of the ground state energy for the coulomb potential case is

$$E_0 = \frac{3}{4} N \hbar \Omega + \frac{3}{4} N \hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2, \quad (5.5)$$

and for the Screened Coulomb potential case is

$$E_0 = \frac{3}{4} N \hbar \Omega + \frac{3}{4} N \hbar \frac{\omega^2}{\Omega} + U_0 \left(\frac{m\Omega}{2\pi\hbar} \right)^{1/2} N^2 + \frac{U_0 \mu}{(2\pi)^{1/2}} \left(\frac{\pi}{2} - \frac{\mu^2 \hbar}{m\Omega} \right)^{1/2} \exp \left(\frac{\mu^2 \hbar}{m\Omega} \right) N^2, \quad (5.6)$$

where this expression, Eq. (5.6), is applicable even when $\mu \ll 1$, and we have evaluated the wavefunction for a single-particle state as

$$\Psi(\vec{r}') = \left(\frac{m\Omega}{\pi\hbar} \right)^{3/4} \exp \left[-\frac{m\Omega}{2\hbar} \vec{r}'^2 \right]. \quad (5.7)$$

If we compare our wavefunction, Eq. (5.7), with the wavefunction from the Ginzburg-Pitaevskii-Gross approach, Eq. (5.1), we conclude that

$$d^2 = \frac{\hbar}{m\Omega}. \quad (5.8)$$

Substituting this into Eq. (5.2) we get

$$E_0 = \frac{3}{4}N\hbar\Omega + \frac{3}{4}N\hbar\frac{\omega^2}{\Omega} + N^2g\left(\frac{m\Omega}{2\pi\hbar}\right)^{1/2}, \quad (5.9)$$

It is readily seen that our result, in the case of coulomb potential, Eq. (5.5) in good agreement with the result from the Ginzburg-Pitaevskii-Gross approach, Eq. (5.9), where $g = U_0 = e^2$

In conclusion, at small momentum, i.e. temperature approach zero, the system goes to a condense state. The bound state in the case of the coulomb potential can be described by the Ginzburg-Pitaevskii-Gross approach. In our study, the ground state energy are evaluated by the variational Feynman path integral and can be compared with the Ginzburg-Pitaevskii-Gross approach. Moreover, we find the agreement between the Ginzburg-Pitaevskii-Gross approach and the variational Feynman path integration. The Feynman-Jansen inequality implies the stability of the bound state because our ground state is stable.

From our result, the ground state energy of the Screened Coulomb case is stable and form a condense state. Finally, when the effect of the Screened Coulomb potential is neglected, the ground state is the same as of Coulomb potential as expected.

References

- [1] Bose, S. N. Planks Gestz and Lichtquantenhypothese. Zeitschrift fur Physik. 26(1924): 178-181.
- [2] Einstein, A. Quantum theory of the monoatomic ideal gas. Sitzber. Kgl. Preuss. Akad. Wiss. Ber. 22 (1924): 261.
- [3] Einstein, A. Quantum theory of the monoatomic ideal gas II. Sitzver. Kgl. Preuss. Akad. Wiss. Ber. 3 (1925): 3.
- [4] Griffin, A., Snoke, D. W. and Strigari, S., Eds. Bose-Einstein Condensation. Cambridge University Press, 1995.
- [5] Haug, K. Statistical Mechanics. New York: John Wiley & Sons, 1963.
- [6] London, F. The λ - phenomenon of liquid helium and the Bose - Einstein degeneracy. Nature. 141 (1938): 643.
- [7] Tisza, L. The λ - Transition Explained. Nature. 141 (1938): 913.
- [8] Bardeen, J., Cooper, L. N., and Schrieffer, J. R. Microscopic Theory of Superconductivity. Phys. Rev. 106 (1957): 162.
- [9] Safonov, A. I., Vasilyev, S. A., Yasnikov, I. S., Lukashevich, I. I., and Jakkola, S. Observation of quasicondensate in two - dimensional atomic hydrogen. Phys. Rev. Lett. 81 (November 1998): 4545.
- [10] Lin, J. L., and Wolfe, J. P. Bose - Einstein Condensation of paraexcitons in stressed Cu_2O . Phys. Rev. Lett. 71 (August 1993): 1222.
- [11] Chu, S., Hollberg, L., Bjorkholm, J. E., Cable, A., and Ashkin, A. Three - dimensional viscous confinement and cooling of atoms by resonance radiation pressure. Phys. Rev. Lett. 55 (July 1985): 48.
- [12] Anderson, M. H., Ensher, J. R., Matthews, M. R., Wieman, C. E., and Cornell, E. A. Observation of Bose - Einstein condensation in a dilute atomic vapor. Science. 269 (July 1995): 198-207.
- [13] Bradley, C. C., Sackett, C. A., Tollett, J. J., and Hulet, R. G. Evidence of Bose - Einstein condensation in an atomic gas with attractive interaction. Phys. Rev. Lett. 75 (August 1995): 1687-1690.
- [14] Bradley, C. C., Sackett, C. A., and Hulet, R. G. Bose - Einstein condensation of lithium: Observation of limited condensate number. Phys. Rev. Lett. 78 (February 1997): 985-989.

- [15] Davis, K. B., Mewes, M. O., Andrews, M. R., van Druten, N. J., Durfee, D. S., Kurn, D. M., and Ketterle, W. Bose – Einstein condensation in a gas of sodium atoms. Phys. Rev. Lett. 75 (November 1995): 3969-3973.
- [16] Dalfovo, F., Giorgini, S., Pitaevskii, L. P., and Stringari, S. Theory of Bose – Einstein condensation in trapped gases. Rev. Mod. Phys. 71 (April 1999): 463-512.
- [17] Cornell, E. A., Ensher, J. R., and Wieman, C. E. Experiment in dilute atomic Bose – Einstein condensation. Preprint, cond – mat: 9903109.
- [18] Ketterle, W., Durfee, D. S., and Stamper – Kurn, D. M. Making probing and understanding Bose – Einstein condensates. Preprint, cond – mat: 9904034.
- [19] Inguscio, M. Stringari, S., and Wieman, C., Eds., Bose – Einstein condensation in Atomic Gases. Proceeding of the international School of Physics “Enrico Fermi”. Amsterdam: IOS Press, 1999.
- [20] Fried, D. G., Killian, T. C., Willmann, L., Landhuis, D., Moss, S. C., Kleppner, D. and Greytak, T. J. Bose – Einstein condensation of atomic hydrogen, Phys. Rev. Lett. 81 (November 1998): 3811.
- [21] Han, D. J., Wynar, R. H., Courteille, Ph., and Heinzen, D. J. Bose – Einstein condensation of large number of atoms in a magnetic time – averaged orbiting potential trap. Phys. Rev. A. 57 (June 1998): R 4114.
- [22] Ernst, U., Marte, A., Schreck, F., Schuster, J., and Rempe, G. Bose – Einstein condensation in a pure Ioffe – Pritchard field configuration. Europhys. Lett. 41 (January 1998): 1.
- [23] Esslinger, T., Bloch, I., and Hansch, T. W. Bose – Einstein condensation in a quadrupole – Ioffe – configuration trap. Phys. Rev. A. 58 (October 1998): R 54.
- [24] Hau, L. V., Busch, B. D., Liu, C., Dutton, Z., Burns, M. M., and Golovchenko, J.
A. Near – resonant spatial images of confined Bose – Einstein condensation in a 4 – Dee magnetic bottle. Phys. Rev. A. 58 (July 1998): R 54.
- [25] Pitaevskii, L. P. Vortex lines in an imperfect Bose gas. Sov. Phys. JETP. 13 (August 1961): 451-454.

- [26] Baym, G., and Pethick, C. J. Ground – state properties of magnetically trapped Bose – Einstein condensated rubidium gas. Phys. Rev. Lett. 76 (January 1996): 6-9.
- [27] Edwards, M., and Burnett, K. Numerical solution of the nonlinear Schrodinger equation for small sample of trapped neutral atoms. Phys. Rev. A. 51 (February 1995): 1382-1386.
- [28] Alexandrov, A. S., and Mott, N. F. High Temperature Superconductors and Other Superfluids, Rep. Prog. Phys. 57 (1994): 1197.
- [29] Schafroth, M. R. Superconductivity of a Charged Ideal Bose Gas. Phys. Rev. 100 (1955): 463.
- [30] Foldy, L. L. Charged Boson Gas. Phys. Rev. 124 (1961): 649.
- [31] Bogoliubov, N. On the theory of superfluidity. J. Phys. USSR 11 (1947): 23-32.
- [32] Kim, Y. E., and Zubarev, A. L. Ground state of charged bosons confined in a harmonic trap. Phys. Rev. A. 64 (May 2001): 013603.
- [33] Tsurumi, T., Morse, H., and Wadati, M. Stability of Bose – Einstein Condensation Confined in Traps. preprint, cond – mat: 9912470 (December 1999).
- [34] Schramm, S., Laganke, K., and Koonin, S. E. Pycnonuclear triple – alpha fusion rates. Astrophys. J. 397 (1992): 579.
- [35] Feynman, R. P. Statistical Mechanics: A set of Lectures. Reading, Massachusetts: Benjamin, 1972.
- [36] Ginzburg, V. L., and Pitaevskii, L. P. On the Theory of Superfluidity. Sov. Phys. JETP 7 (1958): 858.
- [37] Gross, E. P. Hydrodynamics of a superfluid condensate. J. Math. Phys. (February 1963): 195-207.
- [38] Gross, E. P. Structure of a quantized vortex in boson systems. Nuovo Cimento 20 (1961): 454-477.
- [39] Huang, K., and Yang, C. N. Quantum-Mechanical Many-Body Problem with Hard-Sphere Interaction. Phys. Rev. 105 (1957): 767.
- [40] Parkins, A. S., and Walls, D. F. The physics of trapped dilute gas Bose-Einstein condensation. Phys. Rep. 303 (September 1998): 1.
- [41] Stenholm, S. Validity of the Gross-Pitaevskii equation describing bosons in a trap. Phys. Rev. A 57 (April 1998): 584.

- [42] Dalfovo, F., and Stringari, S. Bosons in anisotropic trap: Ground state and vortices. Phys. Rev. A 53 (April 1996): 2477-2485.
- [43] Dodd, R. J., Edwards, M., Williams, C. J., Clark, C. W., Holland, M. J., Ruprecht, P. A., and Burnett, K. Role of attractive interactions on Bose-Einstein condensation. Phys. Rev. A 54 (July 1996): 661-664.
- [44] Feynman, R. P., and Hibbs, A. R. Quantum Mechanics and Path Integrals. McGraw-Hill, 1965.
- [45] Spiegel, M. R. Schaum's Outline Series: Mathematical Handbook of Formulas and Tables. McGraw-Hill, 1990.



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

Vitae

Mr. Chakrit Nualchimplee was born on January 28, 1975 in Nakornratchasima. He received his B. Sc. degree in Physics from Ramkhamhaeng University in 1997.



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย