Chapter I

Introduction

I.1 Bose Einstein Condensation: A review

Bose Einstein Condensation (BEC) is a very interesting and experimentally challenging topic in today's research field. The theoretical prediction of Bose Einstein condensation dates back about eighty years. In 1924, the eminent scientist Satyendra Nath Bose worked with the statistics of photons and explained the black body radiation by introducing the famous Bose distribution function [1]

\[ f(\epsilon_n) = \frac{1}{\exp[(\epsilon_n - \mu)/k_BT] - 1}, \]

where \( \epsilon_n \) is the energy of a single particle state \( (n) \), \( \mu \) is the chemical potential, \( k_B \) is the Boltzmann constant and \( T \) is the temperature in absolute scale. Subsequently Einstein extended Bose's idea to a gas of non-interacting, massive bosons (particles with integral spin), whose total number is fixed. For bosons there is no restriction on the number of particles per state \( i.e. \) any number of identical bosons can be accommodated in the same quantum state. Einstein noticed that, below a certain temperature, a macroscopic fraction of the total number of bosons would occupy the lowest-energy single-particle state [2]. In his words: "A separation is effected; one part condenses, the rest remains a saturated ideal gas". This phenomenon is known as Bose Einstein Condensation. BEC is discussed in detail in most text-books on statistical mechanics [3].
I.1.1 Historical development

Although BEC was predicted in 1924, its experimental realization in dilute gases of alkali atoms was fruitful just in the last decade – in 1995. Fourteen years after the prediction of BEC, London suggested that the superfluidity in liquid $^4$He might be a consequence of a transition to BEC [4]. But due to strong correlations induced by interatomic interactions, the occupation in the lowest quantum state reduced very much, even at absolute zero temperature. So attempts began with weakly interacting Bose gases which are expected to give a higher condensate fraction. But the main problem was, at such low temperature needed to achieve BEC, the gases either liquefy or solidify, thereby increasing interatomic interaction due to close proximity between atoms. In 1959, Hecht remarked that spin-polarized (electron spins parallel) hydrogen atoms might be a good candidate for a weakly interacting Bose gas [5]. Because the attraction between two such $H$-atoms is very weak, which does not allow molecule formation, and as needed in BEC, it remains in gaseous phase at low temperatures. However, at that time the cooling technology was not so advanced, so Hecht’s idea received little attention. But after two decades, when sufficient information about interatomic interactions between spin-aligned $H$-atoms were in hand, Hecht’s arguments were confirmed [6]. Ultimately in 1998 (three years after achieving BEC in other alkali gases) BEC was observed in atomic hydrogen [7].

Since the eighties, attempts were made to search for BEC in extremely dilute Bose gases, so that average inter-particle separation, $n^{-1/3} \sim 10^2$ nm ($n$ being the number density), is much larger than the range of inter-particle interactions $\sim 10^{-1}$ nm. This reduces the probability of molecule formation to practically zero. Any molecule may act as a nucleus of ordinary condensation. To preserve the bosonic atoms in gaseous phase, one has to practically eliminate three and higher body collisions leading to formation of molecules, thereby causing depletion of BEC. Molecule formation is possible only through such collisions, so that two atoms collide to form a molecule, while the third takes up the released binding energy as its kinetic energy. BEC occurs when the mean inter-particle separation is comparable to the thermal de Broglie wavelength $\lambda_T$. Hence
to get an idea of the critical temperature ($T_{cr}$) required to achieve BEC of bosonic alkali atoms, we can compare the thermal de Broglie wavelength

$$\lambda_T = \sqrt{2\pi\hbar^2/mk_BT_{cr}}$$

with the mean interatomic separation, $n^{-\frac{1}{3}}$ ($m$ being the mass of the atom). Since $n$ is in the range of $10^{13} - 10^{15}$ cm$^{-3}$, $T_{cr}$ turns out to be in the range from 100 nK to a few μK. Two important experimental difficulties were: (1) to attain this extremely low temperature and (2) to find a container for the gas. Any material container will involve collisions with the walls of the container, which leads to loss (due to absorption by the wall) and heating. So the gases were trapped magneto optically. The required temperature was achieved by laser cooling [8] followed by evaporative cooling [9].

After decades of heroic attempts, Bose Einstein condensation was first realized experimentally in gases of alkali atom vapors in 1995 – rubidium ($^{87}$Rb) [10], sodium ($^{23}$Na) [11] and lithium ($^7$Li) [12]. The total number of protons, neutrons and electrons (all fermions) in these isotopes of alkali atoms is even. Hence such an atom behaves as a boson. Due to the successful creation of BEC for the first time in breakthrough experiments in trapped dilute atomic alkali gases E. A. Cornell, C. E. Wieman of Joint Institute for Laboratory Astrophysics (JILA) [10] and W. Ketterle, of Massachusetts Institute of Technology (MIT) [11] received the 2001 Nobel Prizes in physics.

I.1.2 BEC: A new state of matter

The atomic condensate extends over a few tenths of a millimeter. At this very low temperature, the de Broglie wave of one atom overlaps that of the nearby ones since $\lambda_T$ is comparable to the average interatomic separation. Hence the many-body system emerges as essentially a single quantum system, where all the atoms behave in a coherent manner. The transition from ordinary gaseous phase to BEC corresponds to a transition from a set of disordered atoms to coherent matter waves. Therefore the entire system can be described by a single macroscopic wavefunction - the "condensate wavefunction". So BEC gives a unique opportunity to explore quantum phenomena on
a macroscopic scale.

The most important features of trapped BEC are its inhomogeneity and finite size. The number of atoms undergoing BEC is $\sim 10^3 - 10^6$. The confining traps are well approximated by harmonic potentials. The trapping frequency $\omega_{ho}$ defines the oscillator length as $a_{ho} = (\hbar/m\omega_{ho})^{1/2}$, which is the characteristic length scale of these Bose Einstein condensed systems. In actual experiments $a_{ho}$ is $\sim$ a few microns.

### I.2 Review of various theoretical methods

#### I.2.1 Mean-field approach

The theoretical study of Bose Einstein Condensation develops its full richness only after realistic interatomic interactions are included. Although the density of the atomic cloud is extremely low, two-body collisions and two-body correlations play important roles in the detailed properties of the condensate [13]. It is a nontrivial many-body problem, but the very dilute nature of the trapped gases allows one to study the ground and low-lying states of the interacting bosons. Since the experimental observation of BEC in 1995 in dilute alkali gases, the theoretical study of these systems are mainly centered around the mean-field approximation like the Hartree-Fock (HF) theory for the many-body system [13, 14, 15, 16]. The mean-field single particle equation is given by

$$
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(r) \right] \psi(r) + \int d\mathbf{r}' |\psi(\mathbf{r}')|^2 V(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}) = E\psi(\mathbf{r}),
$$

(1.1)

where $V_{\text{trap}}(r)$ is the externally applied trapping potential and $V(\mathbf{r}-\mathbf{r}')$ is the two-body interaction ($\mathbf{r}$ and $\mathbf{r}'$ are the positions of the two interacting particles). In mean-field approach each atom moves in an average field produced by the motion of all the other atoms. In very dilute condition the interaction between atoms is so weak that each atom only feels the other atoms as an average background cloud in which they move. Due to the fact that the range of interatomic interaction is much smaller than the average interatomic separation, one can approximately replace the interatomic interaction by the shape-independent approximation, also called the pseudopotential approximation, which
uses a zero-range contact two-body interaction, $V(\vec{r} - \vec{r}') = g\delta(\vec{r} - \vec{r}')$, (where $g$ is the strength constant), as opposed to an extended potential with a well-defined shape. In case of cold and dilute gases, contact interaction is justified, because here only binary collisions at low energy are relevant, as most of the time the atoms are in the asymptotic region. These low-energy interactions between a pair of particles is characterized by a single parameter, the $s$-wave scattering length $a_s$ [17], which is related to $g$ ($g = 4\pi\hbar^2a_s/m$) and the effective interaction becomes [13, 14]

$$V(\vec{r} - \vec{r}') = \frac{4\pi\hbar^2a_s}{m}\delta(\vec{r} - \vec{r}') . \quad (I.2)$$

Depending on the sign of $a_s$ (+ve or -ve) the effective interaction becomes repulsive or attractive in nature respectively. Using this interaction the mean-field equation reduces to the well-known Gross-Pitaevskii (GP) equation [18, 19] in the zero-temperature limit:

$$\left[ -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\vec{r}) + \frac{4\pi\hbar^2(A-1)a_s}{m}\left| \Phi(\vec{r}) \right|^2 \right]\Phi(\vec{r}) = \mu\Phi(\vec{r}) , \quad (I.3)$$

where $A$ is the number of atoms, $\Phi(\vec{r})$ is the condensate wavefunction and $\left| \Phi(\vec{r}) \right|^2 = n(\vec{r})$ is the condensate density. The chemical potential $\mu$ is related to the energy by $\frac{\partial E}{\partial A}$. The factor $(A-1)$ follows from number-conserving Schrödinger quantum mechanics. The above equation is similar to the time-independent Schrödinger equation except for the term $g\Phi^3(\vec{r})$ which is responsible for the non-linear nature of GP equation. This term represents the mean-field produced by other particles. The stationary GP equation can be solved analytically only in two limiting cases: namely perturbative regime and Thomas-Fermi (TF) regime. In the (ideal gas) perturbative regime, which occurs for condensates with a very small number of atoms, the interaction energy can be treated as a weak perturbation, and GP equation reduces to a simple algebraic equation [20]. By contrast, when $A$ is large enough, the kinetic energy of the atoms can be neglected in comparison with the interaction energy and one enters the TF regime. Then also explicit analytical expressions for the condensate ground state properties can be obtained from the reduced algebraic equation [15]. Except for the above two limiting cases, GP equation has to be solved numerically [21, 22, 23; 24, 25, 26] which becomes computationally very difficult for highly asymmetric traps. Very recently Mateo and Delgado [20] derived approximate
analytical expressions for the static properties of the condensate by incorporating the zero-point energy contribution. They have shown that the expression reduces to the correct analytical formulas in both the limiting cases (TF and perturbative regimes), and it remains valid in between these two extreme cases also. However their treatment is valid in the mean-field regime only.

In a mean-field approach the many-body wavefunction is written as a product of single particle wavefunctions, which are obtained variationally.

\[ \Phi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A) = \Pi_{i=1}^A \psi_i(\vec{r}_i) \]

The many-body wavefunction does not have any dependence on the relative separations of two or more particles and thus it lacks two and higher body correlations. Since the GP equation is based on mean-field theories, it also lacks any correlations between particles. But the importance of two-body correlations in BEC has been stressed in the literature [27, 28, 29]. Leggett [14] has pointed out that the GP equation method does not correspond to any well-defined ansatz for the many-body wavefunction. Cherny and Brand further showed [30] that the replacement of an actual interaction by a contact pseudopotential, which leads to an ultraviolate divergence, gives an incorrect treatment of short-range correlations, whose contribution is found to be substantial. Only gross and average properties can be described by the mean-field approximation. Moreover, due to non-linear nature (presence of \( \Phi^3(\vec{r}) \) term) of the GP equation standard quantum mechanics is not applicable without concession. The contact \( \delta \)-function interaction does not represent the real interatomic force. Esry and Greene [31] have shown that \( \delta \)-function is not suitable as a replacement of the realistic two-body interaction in exact theories in more than one dimension, as the Hamiltonian then becomes unbound from below and the ground state energy diverges for an attractive zero range potential. In a hyperspherical calculation done by Bohn et al. [32], in which they considered only the lowest harmonic (called \( K \)-harmonic approximation), it has been shown that for such attractive \( \delta \)-function interaction, solutions are usually obtained in the metastable region disregarding the singularity at the origin and the condensate is stable below a critical number of particles. When this critical number
exceeds the system collapses altogether due to the disappearance of local minimum. This is discussed in detail in Chapter VI. The mean-field theory is valid only when the system is extremely dilute, mathematically expressed by the condition \( n|a_s|^3 < 1 \), \( n|a_s|^3 \) is called the gas parameter. In most experiments on BEC the values of the gas parameter are in the range of \( 10^{-8} - 10^{-4} \), so in this limit mean-field GP theory works very well. In an experiment performed by Stamper-Kurn et al. [33], they have achieved a condensate containing \( 10^6 - 10^7 \) atoms and the corresponding value of \( n|a_s|^3 \) is \( 10^{-3} \). In 2000, in another experiment, performed by Cornish et al. at JILA [34] \( n|a_s|^3 \) is tuned to a value of \( 10^{-2} \) containing only ten thousand \( ^{85}\text{Rb} \) atoms in the condensate. They have employed Feshbach resonance technique [17] to control \( a_s \) by the external magnetic field. This is reflected in changing the effective two-body interaction in the atomic condensate by tuning the scattering length to any desired value including the change in sign from negative to very large positive. At this large values of \( n|a_s|^3 \), the question of validity of the GP theory naturally arises. Therefore as the system becomes more dense, the particles come close to each other and we cannot neglect the effect of correlations. So at higher densities the mean-field approximation breaks down. Although a lot of work has already been carried out to study the static (ground state), dynamic (collective excitations) and thermodynamic properties of the condensate by GP equation method, but due to the above drawbacks one has to go beyond the mean-field theory.

I.2.2 Local-density approximation and Correlated basis function approach

Many theoretical groups around the world have been studying the effects of atom-atom interaction beyond mean-field. The most commonly used approach adopted by the physicists to calculate the leading corrections beyond mean-field theory is to expand the ground state energy per particle \( E/A \) of the homogeneous Bose gas (for repulsive interaction) in terms of \( \sqrt{n|a_s|^3} \) [35, 36]:

\[
\frac{E}{A} = \frac{2\pi \hbar^2 n}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (na_s^3)^{1/2} + \frac{8(4\pi - 3\sqrt{3})}{3} (na_s^2)\ln(na_s^2) + O(na_s^3) \right]. \tag{1.5}
\]
The first term in the above equation was calculated by Bogoliubov [37]. It represents the energy of the homogeneous Bose gas and is equivalent to the mean-field term in the GP equation. The term proportional to $(na_s^3)^{3/2}$ is named as LHY term after Lee, Huang and Yang [38] who derived it first. The logarithmic term was first calculated by Wu [39]. Including the correction term over the mean-field term into the energy functional leads to the modified Gross-Pitaevskii (MGP) equation:

$$
\begin{align*}
&\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\vec{r}) + \frac{4\pi\hbar^2(A-1)a_s}{m} \mid \Phi(\vec{r}) \mid^2 \right] \Phi(\vec{r}) \\
&+ \frac{4\pi\hbar^2(A-1)a_s}{m} \mid \Phi(\vec{r}) \mid^2 \times \left[\frac{32}{3\sqrt{\pi}}a_s^{3/2}(A-1)^{1/2} \right] \Phi(\vec{r}) = \mu \Phi(\vec{r}) ,
\end{align*}
$$

where the logarithmic term has not been included. In Ref. [35] the authors have studied and compared the static properties of the condensate by two methods: local-density approximation (LDA), based on the above expansion and ultimately leading to MGP equation and correlated basis function (CBF) approach, which includes correlation effects induced by the repulsive $(a_s > 0)$ interatomic potential. Their results show that both higher order terms in the low-density expansion, beyond GP theory and explicit dynamical correlations have effects of the order of percent for $A \sim 10^7$ hard sphere bosons in the condensate. A variational approach was adopted by A. Banerjee and M. P. Singh [40] to investigate the effect of interatomic correlations on the ground state properties for the trapped Bose gas in LDA. Their results are in agreement with the analytic estimates of the corrections due to the higher order terms in the expansion. But the presence of logarithmic term in the expansion brings a qualitative change in the density profile of the condensate for large $A$. A later publication [41] however shows that the higher order terms introduce significant corrections to the frequencies of collective oscillations of the condensate in the large-gas-parameter regime. The proper choice for the variational form of density is the most crucial, on which the accuracy of the results depends. In all the above literatures no realistic interatomic interaction is chosen, only model potential is used. Moreover, the treatments are mostly applicable for purely repulsive interactions $(a_s > 0)$. The need for a more realistic potential has become more important with the cases of stronger attraction or larger densities, where critical phenomena like collapse of a condensate [42] and conversion into molecular BEC [43] occur.
I.2.3 Quantum Monte Carlo method

The correlation effects beyond mean-field can be investigated through numerical calculations based on quantum Monte Carlo methods [44, 45, 46, 47, 48, 49, 50]. An essentially exact solution of the many-body Schrödinger equation can be obtained by diffusion Monte Carlo (DMC) [44, 46, 48] and variational Monte Carlo (VMC) [45]. methods, among them DMC is the most promising one. Giorgini et al. [47] have used a DMC method for calculating ground state energy of bosons interacting through different model potentials with $a_s > 0$. They have found that the expansion [Eq. (I.5)] remains valid for $n|a_s|^3 < 10^{-3}$, consistent with most experiments. In Ref. [51] the authors have shown that the mean-field term (first term) in Eq. (I.5) is the lower bound for the exact ground state energy of a uniform gas of bosons interacting through non-negative, finite-range, spherical, two-body potential. Ref. [47] shows that the expansion [Eq. (I.5)] continues to be a good approximation, if only the LHY term is included over the Bogoliubov mean-field term and provided the logarithmic term is dropped, for values of gas-parameter $n|a_s|^3 > 10^{-3}$. For $n|a_s|^3 > 1.385 \times 10^{-3}$ the logarithmic term being negative becomes larger than the LHY term, hence violating the lower bound for energy.

DuBois and Glyde [45] have used VMC method to study the properties of trapped hard sphere interacting bosons beyond the dilute limit. They have achieved a gas parameter value of $n|a_s|^3 \simeq 0.21$, corresponding to liquid $^4$He at saturated vapor pressure. They have shown that as the density increases the effect of interaction depends separately on the particle number and the scattering length, but not only on $A|a_s|/a_{ho}$, as predicted by GP theory. In a later publication [46] the authors have adopted a definition of BEC using one-body density matrix (OBDM). They have adopted DMC procedure to calculate OBDM. In DMC formulation the choice of an initial trial wavefunction is the most crucial to get reliable results. The authors have reported an interesting finding in their results: for $n|a_s|^3 < 10^{-5}$ the condensate is well localized at the center of the trap, but as this parameter value increases, increased interaction depletes the condensate at the center and the condensate appears at the edges of the trap. The very same behavior is observed for liquid $^4$He also. Their results again verify the validity region for the GP
theory to be $n|a_s|^3 < 10^{-2}$.

Blume and Greene [48] also performed a DMC calculation to study the effect of correlations. These results confirm that the condensates are well described by the $s$-wave scattering length only, and the ground state energies do not depend on the details of the two-body potential for $n|a_s|^3 \leq 2 \times 10^{-3}$. For higher densities (large $a_s$ value), the MGP equation gives better results compared to GP. However, their calculation presents results up to fifty particles.

More recently Purwanto and Zhang [49] have investigated the many-body correlation effects by auxiliary-field quantum Monte Carlo method. They have found that in the Feshbach resonance regime, there is significant deviation in the energetics from the GP theory, with variation of scattering length.

### 1.2.4 Perturbative approach

McKinney et al. [52] developed a semianalytic many-body dimensional perturbation theory to compute the ground state energy and breathing-mode frequency of trapped bosons as a function of scattering length. Their results show a significant deviation from the mean-field results as the condensate becomes strongly interacting (for $a_s = 0.433$ o.u.).

### 1.2.5 Hyperspherical method

Another potentially useful treatment beyond mean-field, is an ab initio solution of the many-body linear Schrödinger equation by hyperspherical harmonic expansion method (HHEM) [53]. The Schrödinger equation for a system of $A$ identical bosons, each of mass $m$, confined by the harmonic trapping field $V_{\text{trap}}$ (acting on each individual boson) and interacting via two-body interaction $V$, is given by

$$\left[ -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_i^2 + \sum_{i=1}^{A} V_{\text{trap}}(\vec{x}_i) + \sum_{i<j=2}^{A} V(\vec{x}_i - \vec{x}_j) \right] \Psi(\vec{x}) = E \Psi(\vec{x}), \quad (1.7)$$

$\vec{x}$ being a short-hand notation for the set of position coordinates $\{\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A\}$ of $A$ bosons, $E$ is the total energy. In HHEM hyperspherical variables are defined in terms
of the Jacobi vectors, the \( i \)-th Jacobi coordinate being proportional to the separation vector of the \((i + 1)\)-th particle from the center of mass of the first \( i \) particles. In this way the center of mass motion is automatically separated and the relative motion of \( A \) particles is described in terms of \( N = (A - 1) \) Jacobi vectors. The wavefunction is expanded in the complete set of hyperspherical harmonics (HH), which are the eigenfunction of the grand orbital operator, spanning the hyperangular space. The relative Schrödinger equation then reduces to a system of coupled differential equations (CDE).

The method involves a total of \( 3A - 3 \) variables for the relative motion. With increase in particle number \( (A > 3) \), the calculation of coupling matrix elements [involving \((3A - 4)\) dimensional integrals] of all pairwise two-body potential and solving a large number of coupled differential equations become very difficult. Moreover, due to large degeneracy of HH basis and slow convergence rate of this expansion, the wavefunction is not represented sufficiently accurately with a small number of harmonics. Another difficult thing is the incorporation of the symmetry under exchange of any pair, required for the system of identical bosons. For these reasons the hyperspherical method in atomic and nuclear cases has been used fully for the three body system only \([54, 55, 56, 57]\). The exact hyperspherical calculation has so far been performed up to only \( A = 3 \) trapped bosons \([31, 58]\).

Since in the condensed state, the average interatomic separation is comparable to the de Broglie wavelength, the wavefunction of adjacent atoms overlap and the condensate can be described broadly as a single lump of quantum stuff \([13]\). So it is justified to assume that the basic properties of the condensate in the lowest approximation can be described by a single collective coordinate. The hyperradius can play this role. In the \( K \)-harmonic approximation \([32]\), the hyperspherical harmonic expansion (HHE) is restricted effectively to the first term only. However, the choice of zero range interaction in Ref. \([32]\) basically precludes any correlation. With one collective variable, only the gross features of the condensate can be described, leaving aside the finer details. Moreover for a contact interaction, this \( K \)-harmonic treatment (indeed any theoretical treatment) does not give rigorous result for an attractive \( \delta \)-function interaction \([32]\). Since it will lead to an essential attractive singularity, when all the particles converge to a point. The hyperspherical harmonics method was also used by Sørensen \textit{et al.} \([27, 28, 29]\) to include
the two-body correlation. They proposed a many-body equation involving two-body correlations, but faced the same type of difficulty in their calculation, namely, having to handle too many hyperangular variables simultaneously. So, instead of treating the full \( A \)-body Schrödinger equation exactly, they separate the full Hamiltonian into hyperradial and hyperangular parts and solve the latter adiabatically to study the hyperangular eigenvalue and wavefunction. The approximations made by them are highly restricted to very short range interaction. Faddeev [59] and Yakubovsky [60] equation methods are other standard few body methods which are also practicable only for a few particles.

### 1.2.6 Potential harmonic method: Our motivation

From the above discussion it is clear, that an \textit{ab initio} exact solution of the \( A \)-body Schrödinger equation for \( A > 3 \) is extremely difficult. So its direct application for trapped bosons in the condensate, which contains at least a few thousand bosons, is an impossible task. For an \textit{ab initio} but computationally simpler treatment for the Bose Einstein condensate, we have utilized the potential harmonic expansion method (PHEM) [61], which was originally proposed by Fabre de la Ripelle [62] for nuclear systems consisting of fermions. PHEM is an approximate form of HHEM where the principal assumption is the absence of higher-than-two-body correlations in the many-body wavefunction. Typical BEC, where the atomic cloud is required to be extremely dilute to avoid three and higher body collisions leading to recombination and consequent depletion of the condensate, is thus an ideal system for which this assumption is manifestly valid. Instead of the full hyperspherical harmonic basis, we use a restricted basis, called “potential harmonics” (PH) basis [63], which is a subset of the full HH basis. The name \textit{potential harmonic} basis is adopted as it is the subset of HH basis needed to expand the potential of the interacting pair. In PH basis, we assume that the contributions to the orbital and grand orbital (in \( 3N \)-dimensional space of the relative motion) quantum numbers come only from the interacting pair. Hence the relative separation vector (\( \vec{r}_{ij} = \vec{x}_i - \vec{x}_j \)) of the interacting pair \((ij)\) appears as an argument of the many-body wavefunction. Thus two-body correlations are included. However the wavefunction will have no
dependence on the relative separation of three or more particles. This implies inclusion of two-body correlations only and exclusion of more than two-body correlations. The single quantum nature of the entire condensate suggests that out of many degrees of freedom of the individual particles in the condensate, only a few are physically relevant, because the condensate is possible only at extremely low temperatures (low energy of the individual particles) and extremely low densities. Under this condition only binary collisions are relevant. Any pair out of $A$ atoms in the condensate can interact, while the rest of the particles in the condensate do not take part in any motion other than a collective one and are simply inert spectators. This suggests that most of the degrees of freedom of these spectators can be frozen while a single pair interacts. This reduces the physically relevant degrees of freedom of the condensate to just four—a global length (hyperradius) of the entire condensate and the three degrees of freedom (e.g., length and polar angles) of $\vec{r}_{ij}$. Mathematically, it is equivalent to choosing the PH subset of the full HH basis. Thus in potential harmonic expansion method, the expansion basis is greatly reduced in comparison to HHEM. The HHEM uses hyperspherical harmonics as the expansion basis of the many-body wavefunction [53], which includes two-body as well as higher body correlations (i.e. all correlations), thus causing great computational difficulty even when $A$ is just greater than three. Since any pair of particles can interact, the total wavefunction can be decomposed in Faddeev like components ($\phi_{ij}$), which depends on the corresponding relative vector and a global length. Using Faddeev like decomposition, and expanding each such component in the complete set of PH, the number of resulting coupled differential equations as well as the complexity of the calculation of the potential matrix elements are reduced drastically. Making the Faddeev component for the $(ij)$ interacting pair to be symmetric under $(ij)$-pair exchange, the total wavefunction becomes automatically totally symmetric. Freezing the irrelevant degrees of freedom of the spectators, all intermediate orbital and hyper-orbital angular momenta take zero eigenvalues and the wavefunction becomes totally independent of these variables and hence totally symmetric under any pair exchange among the spectators. Theoretically this method is applicable to any number of particles.
I.3 Thesis outline

After giving a brief introduction of Bose Einstein condensation and its experimental achievement in dilute alkali gases we have reviewed in this chapter the different theoretical tools that have been adopted to study the static, dynamic and thermodynamic properties of the condensate. We have explained briefly the hyperspherical harmonic expansion method and the practical difficulties for its application to more than three particles. Also presented is the reason for adopting potential harmonic expansion method assuming inclusion of two-body correlation only and justification of its application to dilute condensates.

In the subsequent chapters we present the following:

In Chapter II we first develop the theoretical method and the necessary calculations based on HHEM for a general case of \( A \) number of interacting particles starting from the \( A \)-body Schrödinger equation. Then we discuss the specific case for three \( (A = 3) \) trapped bosons. Next we present the theoretical framework for PHEM for a finite number of trapped interacting bosons forming the condensate. Finally we arrive at a system of coupled differential equation.

Chapter III contains the numerical method for solving the resulting CDE for the trapped bosonic atoms interacting via repulsive Gaussian potential. We apply PHEM to \(^{87}\text{Rb} \) and \(^{23}\text{Na} \) condensates containing upto fifty trapped bosons. Numerical difficulty prohibits the application of PHEM initially to larger number of particles.

In Chapter IV we first resolve the numerical difficulty. Then we show that the application of improved algorithm in the calculation of potential matrix element and the incorporation of a short range correlation function in the PH expansion basis allow us to handle condensates containing upto 14000 bosons.

Numerical results for \(^{87}\text{Rb} \) and \(^{23}\text{Na} \) condensates using a semi-realistic interatomic potential, whose parameters correspond to the experimental value of scattering length, are presented in Chapter V.

In Chapter VI we extend the application of PHEM to an attractive condensate where we have considered a realistic atom-atom potential, \textit{viz.}, van der Waals
interaction. We have considered the experimental scenario for $^7$Li and $^{85}$Rb condensates. Calculated critical numbers are in very good agreement with the experimental ones.

Chapter VII contains an interesting finding of our approach. For the attractive van der Waals potential one may wonder at the question: how can this attractive potential produce effective repulsion in the condensate for positive values of scattering length? Chapter VII presents a clear answer to this question providing a graphic demonstration of the situation.

In the last Chapter (Chapter VIII) on BEC we calculate temperature dependence of thermodynamic quantities like average energy and specific heat of the $^{23}$Na condensate containing a small number of interacting bosons.

In order to study the applicability of PHEM to a denser system than the BEC, we adopt this method, in Chapter IX, to small Helium clusters containing upto ten atoms.

Finally in the last Chapter (Chapter X) we draw our conclusions followed by a detailed discussion.