# Chapter 1

# Introduction

### **1.1** Bose Einstein condensation: An overview

Bose-Einstein condensation (BEC) is a fundamental quantum statistical effect with no classical analogue. The Bose statistics was first put forward by Satyendra Nath Bose in the year 1924, in connection with the black body radiation from hot gas of photons [1]. Later, Einstein pointed out that the same statistics could be obeyed by other particles with integral spins. In the year 1925, Einstein predicted that at very low temperature a large fraction of atoms of an ideal Bose gas (IBG) might be condensed in the lowest quantum state. This phenomenon is known as Bose-Einstein condensation [2]. The distribution of atoms over the quantized state is determined by the Bose-Einstein distribution function given as

$$f = \frac{1}{e^{\frac{(\epsilon-\mu)}{k_B T}} - 1} \tag{1.1}$$

where  $\mu$  is the chemical potential,  $\epsilon$  is the energy of a single particle state,  $k_B$  is the Boltzmann constant. Thus, BEC could be defined as the macroscopic occupation of bosons in the single particle ground state below a critical temperature  $T_c$ .

In 1995, BEC was observed in a remarkable series of experiments on vapors of rubidium and sodium in which the atoms are confined in magnetic traps and cooled down to an extremely low temperature of the order of  $\mu K$  [3, 4, 5]. The first evidence of condensation emerged from time-of-flight measurements. Though, the experiments of 1995 on the alkalis are considered as the milestone in the history of BEC, the experimental and theoretical research on this unique phenomenon is much older. In particular, superfluidity in helium was considered as a possible manifestation of BEC [6]. The strong interparticle interaction hindered an unambiguous signature of BEC in the system of helium [7, 8]. Efforts have been made to achieve BEC in hydrogen gas are also much older. In a series of experiments, hydrogen atoms were cooled and trapped by the magnetic field observing BEC was still limited due to the recombination of atoms to form molecules [9, 10, 11, 12, 13]. In 1980s, laser cooling techniques and magneto-optical trapping were developed to cool and trap neutral atoms [14, 15, 16]. Alkali atoms are especially wellsuited to laser-based cooling because their optical transition can be excited by available lasers. By combining laser and evaporative cooling, experimentalists eventually succeeded in reaching the temperature and density required to observe BEC [17, 18, 19]. The most relevant feature of these trapped Bose gases are that they are inhomogeneous and finite size. Thus, BEC shows up not only in momentum space as it happens in superfluid helium but also in coordinate space. This double possibility of investigating the condensation process is very interesting from experimental as well as from the theoretical point of view. As a consequence of the inhomogeneity of the system, the two-body interaction plays an important role. Despite the very dilute nature of these gases, the interatomic interaction has significant effect on important measurable quantities. The number of atoms is truly finite ranging typically from a few thousand to several million. The inhomogeneity of the system makes the problem nontrivial. However, the dilute nature of the gas allows one to describe the effect of interaction in a fundamental way. In practice, a single physical parameter the s-wave scattering length  $a_s$ , is sufficient to obtain an accurate description. The theory of weakly interacting bosons in the external trap is generally described by Gross Pitaevskii mean-field theory [20, 21]. We have witnessed extensive applications of GP mean-field theory to define the static, dynamic and thermodynamic behaviour of dilute Bose gas just after experimentally verifying BEC. Though most of the static, dynamic and thermodynamic properties of BEC are well reproduced by the GP mean-field theory, it has important limitations. It completely ignores any interatomic correlation between the particles. So, the many-body wave function for this method is just the simple product of single particle wave functions. The contact  $\delta$  potential

can not represent the true interatomic interaction, especially for a 3D attractive BEC. It leads to an essential singularity in the Hamiltonian. In the recent experiments, as the interatomic interaction can be smoothly tuned from strong repulsive to strong attractive by utilizing Feshbach resonance this is beyond the scope of any mean-field theory. For an accurate description of such strongly correlated Bose gas, one requires exact many-body calculation i.e., solution of many-body Schrödinger equation.

# 1.2 Theoretical description of quantum many boson system in the external trap

The many-body Hamiltonian describing N interacting bosons confined in an external trap is given by

$$\hat{H} = \int dr \hat{\psi}^{\dagger}(\vec{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\vec{r}) \right] \hat{\psi}(\vec{r}) + \frac{1}{2} \int d\vec{r} d\vec{r'} \hat{\psi}^{\dagger}(\vec{r}) \hat{\psi}^{\dagger}(\vec{r'}) V(\vec{r'} - \vec{r}) \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r'})$$
(1.2)

where  $\hat{\psi}^{\dagger}(r)$ ,  $\hat{\psi}(r)$  are bosonic creation and annihilation operators respectively.  $V(\vec{r} - \vec{r'})$  is the two-body interaction potential. Thus, the many-body problem is nontrivial and practically impossible to solve for systems with a large number of particles. Different techniques have been adopted for reproducing the experimental findings. We discuss some of the prospective theoretical methods below.

#### 1.2.1 Mean-field method

The mean-field description of dilute Bose gas was developed by Bogoliubov [22], the key point is to separate the condensate contribution to the bosonic field operator

$$\hat{\psi}(\vec{r},t) = \phi(\vec{r},t) + \hat{\psi}'(\vec{r},t),$$
(1.3)

where  $\phi(r, t)$  is the expectation value of the field operator equivalent to order parameter and  $\psi'$  is the depletion in the wave function. Using Heisenberg's equation with the many-body Hamiltonian [Eq. 1.2] the time evolution of the many-body

field operator is given by

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{r},t) = [\hat{\psi},H] = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + \int d\vec{r}'\hat{\psi}^{\dagger}(\vec{r}',t)V(\vec{r}'-\vec{r})\hat{\psi}(\vec{r}',t)\right]\hat{\psi}(\vec{r},t).$$
(1.4)

Bogoliubov approach is valid if the depletion is small, so we can replace  $\hat{\psi}(\vec{r},t)$  by field operator  $\phi(r,t)$ . Since, the temperature of the trapped system is very low, so the interatomic separation is longer than the range of the interatomic interaction potential. The collisions between the atoms are of binary type and contact  $\delta$  interaction can be considered as the effective interaction with the *s*-wave scattering length  $(a_s)$  as the strength of the potential. So,  $V(r - r') = g\delta(r - r')$ , where  $g = \frac{4\pi\hbar^2 a_s}{m}$  is the strength of the interaction and *m* is the mass of each boson. By substituting the contact delta interaction and considering the wave function as  $\phi(\vec{r},t) = \phi(\vec{r})e^{\frac{-i\mu t}{\hbar}}$  where  $\mu$  is the chemical potential and  $\phi(r)$  is real and normalized to unity, the above equation can be reduced to

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 + g|\phi(\vec{r})|^2\right]\phi(\vec{r}) = \mu\phi(\vec{r}).$$
(1.5)

This equation, called the Gross-Pitaevskii equation (GPE), was derived independently and simultaneously by Gross and Pitaevskii [20, 21]. For this reason, this equation is called the Gross-Pitaevskii (GP) equation. The limitations of the mean-field GP theory and the necessity of exact many-body calculation for the description of the strongly interacting bosons in reduced dimension are already described before.

#### 1.2.2 Many-body methods

Quantum Monte Carlo method is an *ab initio* process that keeps all interatomic correlations. By utilizing diffusion Monte Carlo [23, 24, 25] and variational Monte Carlo [26] method one can solve the full N-body Schrödinger equation but the method is not capable of handling the systems with particle number exceeding hundred. Regular experiments on BEC performed at different laboratories like MIT, JILA and RICE University contain huge amount of particles varrying from few hundreds to several thousands,  $N \sim 10^4$ . So, the DMC method is not applicable for such a large particle system though, it is an exact many-body method. At the same time, the mean-field approach is applicable for such a large particle system but it cannot extract any many-body physics since it disregards all correlations between the particles. The inclusion of correlations between the particles is a very important issue for the interacting bosons. So, the direct study of the experimental findings of static, dynamic and thermodynamic properties is still an open challenging area of research. In experiments, one has full control to tune the number of particles in the trap, interaction strength and the external trap geometry. So, one has to look for an *ab initio* but approximate many-body method to go beyond the uncorrelated mean-field theory and exact many-body method like DMC method with particle number constraint. Hyperspherical harmonic expansion method (HHEM) is a popular many-body method which has vast and successful application in atomic and nuclear physics [27, 28, 29, 31, 32]. HHEM includes all types of correlations between the particles and can handle realistic interatomic interaction between the particles in the trap.

In hyperspherical harmonic expansion formalism, the Schrödinger equation is separated in relative coordinate and centre of mass coordinate. The relative equation of motion is solved by transforming the coordinates into Jacobi coordinates. The total wave function can be written in terms of hyperspherical coordinates. The hyperspherical coordinates are constituted by the hyperradius r and (3N-4) = (3A-1) hyperangles. Out of these (3A-1) hyperangles, 2A hyperangles  $(\varphi_j, \vartheta_j, j = 1, 2, ..., A)$  are related with the A Jacobi vectors  $(\vec{\zeta_1}, ..., \vec{\zeta_A})$  and (A-1) angles  $(\phi_2, \phi_3, ..., \phi_A)$  give the relative length of the Jacobi vectors. By taking projection on a particular HH basis total Schrödinger equation can be reduced to a set of coupled differential equations (CDE). These CDEs are solved numerically to get the eigenvalues. However, serious difficulties arise if we increase the particle number beyond three. The appropriate conservation of quantum numbers and proper symmetrization of the HH basis are difficult task. Due to the inclusion of first-, second-, and all higher-order correlations the degeneracy of the HH basis increases with particle number. This in turn increases the number of CDEs, the dimension of the two-body interatomic potential matrix. The degeneracy of HH basis reduces the rate of convergence. To handle such situation numerically is very difficult. For these reasons, the application of the HHEM is mainly limited only for the three particle system. Thus, the direct application of HHEM to describe the experimental findings of BEC is not possible, since the number of particles in the system are quite large.

As most of the experimentally prepared condensates are dilute in nature so the range of the interatomic interaction is smaller than the particle separation. The contributions of three- and higher-body correlations are negligible and can be omitted without hesitation as relevant contribution comes only from two-body correlations. Choosing a subset of full HH basis exactly manifests the idea presented here. This truncated subset will basically include only two-body correlations and ignore all higher-body correlations. Based on this idea, Das and Chakrabarti have developed correlated potential harmonic expansion method (CPHEM) by utilizing the truncated HH basis. This new basis set is called the correlated potential harmonic (CPH) basis. In the past decade, CPHEM successfully explained all the static, thermodynamic and statistical properties of BEC observed in JILA and RICE trap [34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44]. My present research work basically focuses on the calculation of several statistical fluctuations and thermodynamic properties of trapped dilute interacting BEC by utilizing CPHEM method. A detailed description of the applied methodology is given in Chapter 2.1. As PHEM keeps the effect of all possible two-body correlations, by construction it is able to go beyond the uncorrelated GP mean-field theory. Uses of van der Waal's interaction provides the realistic experimental scenario. Especially, PHEM is extremely successful to describe the correlated attractive bosons which collapse beyond a critical number. PHEM is also able to take care of the finite size effect and goes beyond mean-field theory to describe the condensation process.

Recent experimental observations suggest that the interaction strength, lattice depth and geometry of the considered trap have a strong influence on the nature of the interacting Bose-Einstein condensate. The situation becomes more interesting in reduced dimension where the effect of quantum fluctuation is more prominent [45, 46, 47, 48]. For the bulk condensate, especially described by the GP mean-field theory, only the lowest orbital is 100% populated. However, the strongly interacting bosons in the external trap exhibit smooth transition from condensation to fragmentation when several natural orbitals have significant population. The study of fragmented condensate (means that the particles macroscopically occupy several single particle states and is built up by taking a symmetrized product of several single particle states) is beyond the scope of any many-body methodology described so far [20, 21, 49, 50, 51, 52]. In recent literature, we find that multiconfigurational time-dependent Hartree method for boson (MCTDHB) [53, 54, 55, 56, 57, 58] is the most efficient exact many-body calculation to describe strongly correlated BEC in reduced dimension [54, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68]. MCTDHB is formulated in multiconfigurational ansatz i.e., a sum of all possible different configurations of N particles in M orbitals weighted by complex time-dependent coefficients and time-dependent orbitals [69, 70, 71, 72] [see Chapter 2.2]. By utilizing MCTDHB we can very precisely identify different states like condensation and fragmentation of a ultracold Bose gas in a harmonic trap and also in optical lattices.

Out of different recent experiments to extract rich many-body physics, the strongly interacting bosons in optical lattice is the most challenging area of research [45, 46, 73, 74, 75, 76, 77, 78, 79, 80]. The optical lattice offers the perfect isolation of the system from the environment which facilities to study whether thermalization is ubiquitous in nature. Optical lattice also offers a new kind of transition which is a continuous phase transition from coherent superfluid (SF) to incoherent Mott insulating phase. Unlike the thermal phase transition which is most commonly studied area in BEC,  $SF \rightarrow MI$  transition is purely quantum phase transition. The effect of quantum fluctuations in 1D plays the most important role. Thus, quantum fluctuation in an optical lattice and consequent study of atom number fluctuation is still an open problem in the context of many-body physics.

## **1.3** Research Motivation

My thesis addresses two different avenues of fluctuation properties of ultracold atoms in the external trap. The first part considers, bulk condensate in the harmonic as well as in anharmonic trap, solved by CPHEM. The main focus is to study the nature of quasi phase transition at the transition point and how the phase transition is affected by the nature of interaction (attractive and repulsive interaction) as well as by the external trap geometry (harmonic and anharmonic trap). The results are supported by the detailed study of several statistical and thermodynamic properties like ground state probability distribution, condensate fraction, fluctuation in the ground state occupation, several orders of central moment and specific heat. Several characteristic temperatures corresponding to the peak point or inflexion point (transition point) of the thermodynamic quantities are discussed. The origin of this quasi phase transition is thermal.

The many-body time-independent Schrödinger equation has been solved for a large number of bosons trapped in a harmonic as well as in an anharmonic trap. We have included all two-body correlations and realistic interatomic interaction like van der Waal's interaction. By these choices we can go beyond the mean-field regime and finite size effect has also been considered. Several statistical fluctuations and thermodynamics properties as mentioned above have been studied for attractive interacting  $^{7}Li$  atoms in a harmonic trap. The choice of the parameters mimic the experimental situation of RICE university. Probably the first theoretical study of thermal evolution of the root-mean-square fluctuation or standard deviation, several orders of central moment of the fluctuation has been presented. All of them show a sharp peak around the transition temperature. As there is no sharp discontinuity in these statistical and thermodynamic properties so no signature of true phase transition is evident. The study of the above-mentioned statistical properties for the repulsively interacting BEC of  ${}^{87}Rb$  in a harmonic trap as well as in anharmonic trap have been presented. The system parameters for  ${}^{87}Rb$  in harmonic trap mimic the JILA trap experiment. Although, it can be concluded that the anharmonic trapping favours BEC process, the true phase transition is not possible for such mesoscopic BEC. The energy fluctuation for both repulsive and attractive interacting BEC of  $^{7}Li$  and  $^{87}Rb$  have been studied. The effect of interaction on the average energy, energy fluctuation and relative energy fluctuation have been observed. We define three characteristic temperature from the inflexion point of the fluctuation curves. They will be close to critical transition temperature for truly thermodynamic limit.

The second part of my thesis considers few strongly interacting bosons in the external harmonic trap and also in an optical lattice. The few-body time-dependent Schrödinger equation is solved by MCTDHB. From the time-dependent manybody wave function we calculate many-body information entropy, one- and twobody correlation function which are further utilized to describe the  $SF \rightarrow MI$ transition in 1D optical lattice. The  $SF \rightarrow MI$  is a continuous phase transition for a truly few-body bosonic system and the transition is associated with the effect of quantum fluctuation. At the transition point, the global correlation of SFphase is lost and each boson occupies a single site entering in MI phase. This quantum phase diffusion process is related to the atom number fluctuation [81, 82]. This atom number fluctuation process has been experimentally observed in optical lattices via quantum collapse and revival dynamics [83]. Unlike the different measures of the thermal fluctuations described earlier, the  $SF \rightarrow MI$  transition is associated with the atom number fluctuation. In this part of my work, we study in detail the  $SF \rightarrow MI$  transition both for shallow-to-deep lattice and weak-to-strong interaction strength which are beyond the scope of the study of Bose-Hubbard (BH) theory. We consider  $SF \to MI$  transition for both the shortrange (contact) and long-range (dipolar) interactions and make a link between the several order of coherence and entropy production at the transition point.

## 1.4 Thesis outline

The structure of this thesis follows:

#### Chapter 2: Methodology

This chapter provides the formalism of two many-body methods CPHEM and MCTDHB. In the first section, we describe the potential harmonic (PH) basis calculation and inclusion of a short-range correlation function in the PH basis to calculate the correlated potential harmonic (CPH) basis. The choice of the system parameters has been done in such a way to mimic the realistic experimental scenario of JILA and RICE trap. By utilizing these parameters, we have calculated the full energy spectrum for the <sup>87</sup>Rb and <sup>7</sup>Li in harmonic trap also for the <sup>87</sup>Rb in anharmonic trap. In the section, we describe the MCTDHB method. Utilizing this methodology we solve the time-dependent Schrödinger equation to get the many-body wave function for few stronggly interacting bosons. The process of

fragmentation from the condensation and phase transition from  $SF \rightarrow MI$  can be studied by utilising MCTDHB method.

#### Chapter 3: Statistical fluctuation and thermodynamic properties

Statistical fluctuation for the ideal Bose gas in the grand canonical ensemble shows the grand canonical catastrophe. To explain experimental findings, the whole focus moved on to the description of fluctuation in the canonical and microcanonical ensemble. Again, the experimental observation of statistical fluctuation is more relevant with the interacting Bose gas. So, the fluctuation properties of the interacting Bose gas has been discussed in detail. The recursion relation for the calculation of partition function is given and also the formulas to calculate the ground state probability distribution, several orders of central moment and specific heat are provided.

Chapter 4: Statistical fluctuation of attractive BEC in harmonic trap The statistical properties of the attractive interacting condensate of  $^{7}Li$  in harmonic trap are discussed. The temperature variation of ground state probability distribution, condensate fraction, fluctuation in the ground state occupation, several orders of central moment are presented. The quasi phase transition is observed for the mesoscopic condensate. This work has been published in Physica A 481, 79, (2017).

Chapter 5: Statistical fluctuation of repulsive BEC in anharmonic trap The statistical properties of the repulsive interacting condensate of  ${}^{87}Rb$  in anharmonic trap are discussed. The temperature variation of ground state probability distribution, condensate fraction, fluctuation in the ground state occupation, several orders of central moment and specific heat are presented. The quasi phase transition is observed for the mesoscopic condensate. The characteristic temperatures corresponding to the inflexion point of the specific heat versus temperature curve are obtained and their dependence on the anharmonicity parameter are discussed. This work has been published in **Physica A 526, 121053, (2019)**.

## Chapter 6: Effect of interaction on energy fluctuation of BEC in harmonic trap

Average energy for repulsive interacting  ${}^{87}Rb$  atoms in JILA trap and attractive interacting  ${}^{7}Li$  atoms in RICE trap are calculated. Energy fluctuation and rel-

ative energy fluctuation for the two interacting systems are calculated to know the effect of interaction on these properties. For comparison, results for bosons in noninteracting limit and the ideal Bose gas in the thermodynamic limit are presented. This work is currently under review in **Physica A**.

#### Chapter 7: Fragmentation of BEC in harmonic trap

The mean-field approach can describe the fully condensed state since only one natural orbital is populated. Multi-orbital mean-field theory can probe the fragmented state. However, the pathway from condensation to fragmentation can be totally understood by an exact many-body method MCTDHB. By utilizing this methodology, fragmentation of strongly interacting BEC in harmonic oscillator trap is investigated. Variation of the one-body density and two-body density profile of the system show the fragmentation scenario. The occupation in the higher natural orbitals increases with the increase in the effective interaction. By following the evolution of natural orbitals the fragmentation process can be understood. The effect of contact interaction and dipolar interaction on the above-mentioned quantities are the key feature of this chapter. This work is currently under review in Scientific Reports 9, 17873 (2019).

#### Chapter 8: Statistical relaxation of BEC in optical lattice

Probing of the continuous phase transition from coherent superfluid phase to fragmented Mott insulating phase in a 1D optical lattice is the main focus of the present chapter. We observe the behaviour of the one-, two-body density and Shannon information entropy for the interaction quench and lattice depth quench. How the system relaxes to a maximum entropy state when we suddenly change the interaction strength has been observed. The system does not relax for the optical lattice depth quench. The entropy shows oscillatory behaviour. The onebody density and two-body density also show the relaxation and collapse-revival scenario respectively for the interaction and lattice depth quench. This work has already been accepted in **J. Phys. B 52, 215303, (2019).** 

## Chapter 9 : Atom number fluctuation calculation through the collapse - revival phenomena of correlation functions and Shannon information entropy

The effect of dipolar interaction on the relaxation process during the lattice depth

quench is the key feature to be discussed. The time evolution of the first-, secondorder correlation function and Shannon information entropy are observed. The effect of long-range repulsive tail of the dipolar interaction on these quantities is discussed in great detail. The timescale of the system to lose the initial coherence and entering in the incoherent Mott state also the timescale to revive the initial coherent phase are discussed. How the atom number fluctuation scenario for the few-bosonic system is measured by this collapse-revival phenomenon is discussed. This work has been published in **Symmetry 11, 909, (2019)**.

#### Chapter 10: Summary and conclusion

This chapter concludes the thesis with a summary of key results and an outlook for future work.