Chapter 1

Introduction

1.1 Motivation

The observation of Bose Einstein Condensation (BEC) in the year 1995 [1, 2, 3] and subsequent achievement of Fermi degeneracy [4, 5, 6] in the ultracold, dilute gases opened a new chapter in the atomic and molecular physics where the particle statistics and their interactions started to play the central role rather than the study of single atoms or photons. These development yielded many theoretical [7, 8, 9, 10, 11] and experimental investigations [1, 2, 3, 12, 13, 14] in the field of ultra cold atoms. Bose-Einstein condensation was predicted in 1924 by Albert Einstein and Satyendra Nath Bose [15, 16]. According to which when bosonic atoms are cooled to a very low temperature they all occupy single ground state. Laser cooling combined with evaporation cooling techniques allowed in 1995 for experimental observation for Bose-Einstein Condensation (BEC) [1, 2, 3]. E. A. Cornell, C. E. Wieman [17]
and W. Ketterle [18] received the Nobel prize in 2001, for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms and for early fundamental studies of the properties of the condensates.

In the past several years, two major new developments have considerably enlarged the range of physics which is accessible with ultracold gases. They are associated with (i) the ability to tune the interaction strength in cold gases by Feshbach resonances [19, 20] and (ii) the possibility to change the dimensionality with optical potentials and, in particular, to generate strong periodic potentials for cold atoms through optical lattices [21]. Both developments, either individually or in combination, allow to enter a regime, in which the interactions even in extremely dilute gases can no longer be described by a picture based on non-interacting quasi-particles. The appearance of such phenomena is characteristic for the physics of strongly correlated systems. For a long time, this area of research was confined to the dense and strongly interacting quantum liquids of condensed matter or nuclear physics. By contrast, gases - almost by definition - were never thought to exhibit strong correlations.

The best example where the physics of ultra cold atoms entered the areas of strongly correlated systems is the seminal 1998 paper of Jaksh et.al [22] on the prediction of superfluid-Mott insulator quantum phase transition in cold atoms in an optical lattice which was subsequently observed by Greiner
et al. [21] in 3-Dimensions, Spielman et al. [23] in 2-Dimensions and Stöferle et al. [24] in 1-Dimension. These were a breakthrough moments in which atomic physics and quantum optics have met the condensed matter physics.

A physical system that crosses the boundary between two phases changes its properties in a fundamental way. For example it may melt or freeze. This macroscopic change is driven by microscopic fluctuations. The phase transitions which occur at zero temperature are called as Quantum Phase Transitions. These phase transitions are one of the unsolved problems in the condensed matter physics and it has been the subject of considerable attention recently [25]. For a system of a temperature of absolute zero, all thermal fluctuations are frozen out, while quantum fluctuations prevail. These microscopic quantum fluctuations can induce a macroscopic phase transition in the ground state of a many-body system when the relative strength of two competing energy terms is varied across a critical value. A prominent example of such a quantum phase transition is the change from superfluid phase to the Mott insulator phase in a system of ultra cold bosonic atoms with repulsive interactions hopping through a lattice potential [26, 27]. This system was first studied theoretically in the context of superfluid to Mott insulator transition in liquid helium [26]. In the superfluid phase, each atom is spread out over the entire lattice, with long range phase coherence. But in insulating phase, exact numbers of atoms are localized at individual lattice
site, with no phase coherence across the lattice.

The study of quantum phase-transitions in systems of interacting bosons is an exciting area with a fruitful interplay between theory [26, 27, 28, 29, 30, 31, 32, 33, 34, 35], numerical simulations [36, 37, 38, 39], and experiments. A variety of experimental systems have been studied: liquid $^4$He in porous media like vycor or aerogel [40]; microfabricated Josephson-junction arrays [41, 42]; the disorder-driven superconductor-insulator transition in thin films of superconducting materials like bismuth [43]; flux lines in type-II superconductors pinned by columnar defects aligned with an external magnetic field [44]. The best example from the point of view of comparing theory with experiments, is the atoms trapped in optical-lattice potentials. In a system where the number of atoms per site is an integer, Greiner et al. [21] have observed a superfluid-Mott insulator transition for $^{87}$Rb atoms, trapped in a three-dimensional optical-lattice potential, by changing the strength of the onsite potential. Subsequently superfluid to Mott insulator transition has been observed in two-dimensional [23] and one-dimensional optical lattices [24].

Experiments in such optical lattices have several advantages over their condensed-matter counterparts [45]. The underlying microscopic model are known precisely, for example bosons in the optical lattice are best described by Bose-Hubbard model, [22]. The model parameters as well as the op-
tical lattice dimension can be controlled. And finally the optical lattice can be made either disorder free or introduce it in a controlled manner. There are several proposals in this direction; they include the use of a laser speckle [46, 47, 48, 49, 50, 51, 52], the use of heavy atoms, which provide a quasi-static potential for lighter atoms [53, 54], and finally the addition of a superlattice potential with a wave length incommensurate with that of the lattice potential [55, 56, 57, 58].

Disordered in the system allow localization of waves (particles), both in quantum and classical systems, and increasing disorder induces a insulating phase [59, 60] and the transition is known as Anderson localization. The occurrence of this Anderson transition strongly depends on the dimensionality of the system: in one-dimension, a localized phase is expected as soon as disorder is present [61]. The interplay of interaction and disorder in the strongly correlated system is still a key question which lack clear solution and still attract lot of attention. In the one-dimensional bosonic systems the competition between interaction and disorder have been studied using variety of methods [62, 63, 64, 65, 66, 67]. These studies support a general phase diagram which consist of superfluid (SF), Mott insulator (MI) and Bose glass (BG).
1.2 Objectives

Recent experiments in ultracold atomic gases showing superfluid to Mott insulator quantum phase transitions [21, 23, 24] by fine tuning the parameters of the Hamiltonian offer possibility of studying disorder induced transitions in controlled manner. Especially when the disorder is introduced by addition of superlattice potential with a wave length incommensurate with that of the lattice potential [55, 56, 57, 58]. Motivated by the possibility of studying Bose glass phase within the ultracold atoms in the optical lattice, we devote this work in the study the one dimensional Bose-Hubbard model in the presence of different types of inhomogeneous local potentials.

Our main objectives in this work are:

1. to develop a suitable finite size density matrix renormalization group method which can handle all type of inhomogeneity in the local potential,

2. to develop a method for identifying different phases like superfluid, Mott insulator and Bose glass,

3. and study the Bose-Hubbard model in the presence of inhomogeneous potential and obtain its phase diagram.

Bose Hubbard model is not solvable even in one dimension. One of the
best numerical method available to study the one dimensional quantum system is the density matrix renormalization group method developed by White in 1992 [68, 69]. This method have been applied to a variety of problems and couple of good reviews which deal with DMRG and its applications are by Schollwöck [70] and by Hallberg [71]. There are problems in extending this method directly to the systems with inhomogeneous potentials [72]. There are several approach to circumvent these difficulties. One way is to prepare all the blocks so that they provide the proper environment for each other at each step of DMRG and let these blocks grow in parallel keeping the boundary conditions for each block almost unchanged during the course of the calculation [72]. Another implementation when the system have incommensurate potential is based on a matrix-product state variational formulation [73] which enables them to start sweeping from any state. In practice, they have started from either a random or a classical state contrary to the usual warm-up method. In this work we propose a simple method of dealing with systems with any kind of local inhomogeneity.

The Bose Hubbard model in the presence of inhomogeneous local potential is given by

\[ \mathcal{H} = -t \sum_{<i,j>} (a_i^\dagger a_j + H.c) + \frac{U}{2} \sum_i n_i (n_i - 1) + \sum_i \mu_i n_i. \]  

(1.1)

The first term in Eq. (1.1) represents the kinetic energy associated with
the hopping of bosons from site \( i \) to its nearest-neighbor site \( j \) with amplitude \( t \). \( a_i^\dagger (a_i) \) is the boson creation (annihilation) operator at site \( i \) and they obey commutation relation \( [a_i^\dagger, a_j] = \delta_{ij} \) and associated number operator is \( n_i = a_i^\dagger a_i \). The second term is associated with onsite repulsion with the interaction strength equal to \( U \). The Bose-Hubbard model consist of just first two terms in the model (1.1). The inhomogeneity due to local potential is introduced through the third term where we consider in this work

- \( \mu_i = \lambda \cos(Qi) \), with \( Q \) either commensurate to the underlying lattice, for example \( Q = \pi \) or incommensurate, for example \( Q = \frac{1+\sqrt{5}}{2} \), the golden mean.

- \( \mu_i \) is a random number distributed uniformly between \( \lambda \) and \( -\lambda \)

- \( \mu_i \) is defined by quasi-periodic potential, for example Fibonacci chain.

In each of these cases, we address the basic phase diagram. In this work all the energy scale have been set by taking \( t = 1 \).

The Bose-Hubbard model in the absence of inhomogeneity has been studied by many methods [26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39] and these investigations have yielded basic phase diagrams which basically consist of superfluid and Mott insulator phases. The ground state of Bose Hubbard model depends on the value of density of bosons \( \rho \) and the ratio of
$U/t$. For $\rho \neq n$, where $n$ is an integer, the ground state is always a superfluid. However, a quantum phase transition from superfluid to Mott insulator is possible when $\rho = n$ with some critical interaction $U_C/t$ which depends on the dimensionality and $\rho$. For example one dimensional Bose Hubbard has $U_C/t \sim 3.4$ for $\rho = 1$. The study of Bose Hubbard model has been extended to the presence of long range interactions [34, 35, 36, 74, 75, 76]. The extended Bose-Hubbard model has additional phases, a charge density wave especially when the density $\rho$ is half-integer. Recently new exotic phases like supersolid [76, 77, 78, 79, 80, 81, 82], solitonic phases [76, 82, 83] and hidden order [84] have been predicted.

Disorder Bose Hubbard model has also been attracted lots of interest in the last two decades [26, 27]. The study has been mainly motivated by its application to liquid $^4$He in porous media like vycor or aerogel [40]. Disorder introduces a new phase called Bose glass phase and the basic phase diagram of disordered Bose Hubbard model is known. Recently, the study has been extended to the quasi-periodic Bose-Hubbard model and localization in one-dimensional cold atomic gases [85].

The phase diagram of the one dimensional Bose Hubbard models, which consist of superfluid, Mott insulator, density wave, and Bose glass phases have been obtained by studying the global properties of the ground state wave function. For example, superfluid phase can be characterized by power law
decay of superfluid correlation function, zero gap in the single particle energy
spectrum, finite compressibility. The Mott insulator phase has finite gap and
zero compressibility where as the Bose glass phase has zero gap but is com-
pressible and the superfluid correlation function decay exponentially. These
characteristic are very useful in understanding the phase diagram model (1.1).
However, in the context of understanding these phases in the optical lattice
experiments, additional complications arises due to the presence of overall
harmonic trap potential. Bose Hubbard model in the presence of trap poten-
tial has been studied recently [86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97]. In
the presence of these trap potential, the system does not have a global phase
and superfluid and Mott insulator co-exist. These results have been veri-
fied by many experiments [98, 99]. To study the co-existence of superfluid,
Mott insulator and Bose glass, it is essential to develop a method based on
local properties rather than the global properties. In this work we develop a
method based on local compressibility to understand different phases within
the finite size density matrix renormalization group.

1.3 Overview

This report is planed in the following manner. In this chapter we discussed
the general motivations and objectives of this work. We briefly review the
density matrix renormalization group method and its basic principles in the
Chapter (2). In this chapter, we also present in detail the method of our calculation of obtaining the phase diagram of pure Bose Hubbard model using the finite size density matrix renormalization group method and obtain its phase diagram. The limitation of applying the DMRG method in the case of inhomogeneous system is discussed in the Chapter (3). We proceed this chapter with a simple solution to these problems by suitably choosing a superblock configuration when the system size is increased. Our results based on this method are given in the Chapter (4) to (6). The results of model (1.1) in the limit of hardcore bosons in the presence of periodic commensurate and incommensurate potentials are discussed in the Chapter (4) and we obtain its phase diagram. The results of the model (1.1) with commensurate and incommensurate potential is given in Chapter (5). The results with random and Fibonacci potentials are discussed in the Chapter (6). We conclude all our results in the Chapter (7) and present the future prospectives of this study.

The most suitable title of this thesis could have been *Quantum Phase Transitions in inhomogeneous lattices*. However, for some technical reasons the present title is retained.