Quantum phases of atomic gases in optical lattices

Iori Tanabe

May, 2011
(Modified in June 2011)

Undergraduate Honors Thesis
2011

Department of Physics, Applied Physics and Astronomy, SUNY Binghamton,
Binghamton NY 13902
Research Advisor:
Dr. Theja De Silva, Assistant Professor, Department of Physics, Applied Physics and Astronomy

Members of the Committee:
Dr. Masatsugu Suzuki, Professor, Department of Physics, Applied Physics and Astronomy

Dr. Bruce White, Associate Professor, Department of Physics, Applied Physics and Astronomy
Acknowledgement

First of all, I would like to thank the Physics department of Binghamton University to give me the opportunity to study physics and take part in the individual research project with Dr. Theja De Silva. I would like to thank Dr. Masatsugu Suzuki and Dr. Bruce Whit for agreeing to be on this honors thesis committee.

I also would like to thank Andrew Snyder to give me a lot of help and insights on my project. Discussing problems with him not only deepened my understanding of the subject but also taught me the importance of the team work.

Most especially, I would like to express my gratitude to my supervisor Dr. Theja De Silva. This thesis could not have written without him. Not only he gave me the support throughout my research projects, but also he always encouraged me and believed my capability of achievement in study of physics more than anyone else. Without him, so many things would have been impossible to be achieved.
Abstract

The high degree of tunability in cold atom experimental systems offer a unique opportunity to explore fundamental physical phenomena associates with many body systems. One such direction is atomic gases subjected to a combined harmonic oscillator and optical lattice potentials. In this thesis, I study two optical lattice systems; one is ultra-cold fermions in one dimensional optical lattices and the other is hard-core bosons in optical superlattices. The Fermi-Hubbard model is used to describe the system of quantum fermionic gas, and I calculate the particle density, various compressibilities and double occupation of the particle. Then I use local density approximation to extract the thermodynamic quantities in trapped environment. The ultracold hardcore boson is described by the Bose-Hubbard Hamiltonian. To take the hardcore constrains into consideration, the bosonic Hamiltonian is mapped into a spin Hamiltonian. Then, I use variational approach to study the superfluid insulator transition. In particular, I calculate the ground state energy, superfluid density and particle density and examine the dimensional crossover. The effect of underlying trapping potential is taken into account by local density approximation.
Contents

1 Introduction ........................................... 1
   1.1 Ultracold bosons .................................. 2
   1.2 Ultracold fermions ................................ 2
   1.3 Superfluid and Mott-insulator transition .......... 3
   1.4 Experimental methods to achieve the ultracold temperature .......... 3
   1.5 Optical lattices ................................... 5

2 Repulsively interacting ultracold fermions in one dimensional optical lattices .......... 7
   2.1 Introduction ...................................... 7
   2.2 The model ........................................ 7
   2.3 Particle density .................................. 8
   2.4 Compressibility .................................. 10
   2.5 Double occupation ................................ 12
   2.6 The effect of the trapping potential ............... 15

3 Superfluid-Insulator transition of hardcore bosons in an optical superlattice .......... 18
   3.1 Introduction ...................................... 18
   3.2 The model ........................................ 18
   3.3 Superfluid density and particle density ............. 20
   3.4 Effect of trapping potential ......................... 23
   3.5 Dimensional cross over ............................ 24
   3.6 The effect of interaction ........................... 26

4 Conclusion ............................................ 28
1 Introduction

To study the ultracold atomic gases has kept attracting the attention of physicists. One of the important things to study quantum gases in optical lattices is that it allows us to explore the property of matters which is very difficult to examine with the real materials. The experimental technique for the ultracold atomic gases have been developed rapidly since the Bose-Einstein condensates first realized in 1995 at the University of Colorado at Boulder using Rubidium atoms [1] and at MIT with Sodium atoms [2]. This experimental development provides us with the very useful environment to study the solid state physics and condensed matter physics. One of the reasons for that is because ultracold atomic gases in an optical lattice are described by the Hubbard models, while a Hubbard model is also an approximate model used to describe the transition between conducting and insulating systems in solid state physics and condensed matter physics.

In this thesis I will study the ultracold fermions in one dimensional optical lattices and ultracold hardcore bosons in two dimensional optical superlattices. In order to study the two-component ultracold fermionic gas in an optical lattice, the Fermi-Hubbard model is used. Since the Fermi-Hubbard model is an important approximate model used in solid state physics, the experimental realization of a ultracold fermionic gas in an optical lattice opens up the possibility to directly address the unsolved problems of solid state physics. While the experimental development is achieved to realize this system, the external trapping potential and its effect of compressibility are theoretically studied. My study will focus on those properties of the one dimensional ultracold fermionic gases. Then I will study the hardcore bosons in two dimensional optical superlattices. Especially I will focus on superfluid to Mott insulator phase transition as functions of chemical potential and tunneling energy. In order to study the bosons in optical lattices, the Bose-Hubbard model is used. My study will focus on the hardcore bosons with the infinite on-site repulsion in superlattices. A phase transition is generated by the energy mismatch of the superlattices, and to understand the phase transition without the effect of thermal fluctuations is very interesting problems of condensed matter physics.

This thesis is organized as follows: in Chapter 1 I introduce the concept and the behavior of ultracold bosons and fermions, the superfluid and Mott-insulator transition, the experimental methods to achieve the ultracold temperature, and optical lattices. In chapter 2, the study of local thermodynamic quantities of ultracold fermions in one dimensional optical lattices is discussed. Finally in chapter 3, I discuss the phase transition between superfluid and Mott-insulator state of ultracold hardcore bosons in two dimensional optical lattices.
1.1 Ultracold bosons

As mentioned previously, I will study the ultracold hardcore bosons in optical lattices, and in order to know how cold the temperature is for the ultracold bosons, we need to think about the de Broglie wavelength. When the temperature $T$ is high, the de Broglie wavelength $\lambda_{dB} = \frac{\hbar}{(2Mk_B T)^{1/2}}$, where $M$ is the Boson Mass, is smaller than the interatomic distances, and we can describe the behavior of a dilute gas of atoms classically $[?]$. Quantum-degenerate gases are created when the temperature is cooled so that the de Broglie wave length becomes comparable to the spacing between atoms. The critical temperature $T_c$ for the quantum degeneracies occur is

$$T_c = \frac{2\pi \hbar^2}{Mk_B T_c \left[ \frac{n}{\zeta(3/2)} \right]^{2/3}},$$

where $n$ is the particle density and $\zeta(3/2) \approx 2.61$. At the temperature very close to absolute zero, whether the atoms are fermions or bosons changes the behavior of the dilute gas tremendously. Due to the Pauli exclusion principle, more than two fermions cannot occupy the same quantum state. Therefore, when fermionic quantum gas is cooled to the critical temperature, atoms of the gas start to occupy the lowest available energy state one by one. One the other hand, if the atoms of the dilute gas are boson, the atomic wave packets overlap together and start to occupy the same quantum ground state when the de Broglie wavelength becomes comparable to their interatomic distances. Due to the Heisenberg uncertainty principle, these atoms are no longer distinct particles but become a collective quantum object. This process is called as Bose-Einstein condensation. If we could gain high critical temperature by increasing the particle density $n$ in Equation (1), the realization of the BEC in experiments would be much easier. However, if we increase the particle density, the atoms in the optical lattices solidify or liquify before the BEC transition temperature is reached. Therefore, to have BEC we need to treat the dilute atomic gases of the density $n \approx 10^{14} \text{ cm}^{-3}$, and it forces the critical temperature to be below some hundred nano Kelvin.

1.2 Ultracold fermions

Another problem to address in this thesis is the one dimensional fermionic gases. Since Fermi-Dirac statistics is applied to the statistical distribution of fermions which obey the Pauli Exclusion Principle, noninteracting fermions can not condense into the same lowest quantum states when they are cooled below the critical temperature as bosons do. Nonetheless, Fermi gas can have a superfluid phase due to the interactions, and the study of Fermi gases has been one of the most interesting areas of
cold atoms. The quantum degeneracy in trapped Fermi gases was first realized by the group at JILA in 1999 with two spin components of $^{40}\text{K}$ atoms [3]. According to BCS theory, fermionic gases exhibit superfluidity as a result of ”condensation” of Cooper pairs formed at sufficiently low temperature. In the experiment conducted by JILA in 1999, the critical temperature to achieve the superfluid phase was too low to experimentally realize because the gas was so dilute. However, the effects of the quantum degeneracy were observed with $^{6}\text{K}$ fermionic gases in 2001 [4]. It was soon noticed that the Feshbach resonance is the crucial key to achieve superfluidity of Fermi gases [5].

1.3 Superfluid and Mott-insulator transition

At the temperature of absolute zero, although all thermal fluctuations disappear, phase transitions can still happen due to the fluctuations caused by Heisenberg’s uncertainty principle. In 1998 Peter Zoller of the University of Innsbruck in Austria and his co-workers published a paper claiming that a weakly interacting Bose gas in optical lattices should be able to change into Mott-insulator phase from superfluid phase [6]. In a superfluid phase, tunneling plays the big role to form coherent matter waves on the entire lattices sites. As we increase the lattice potential depth, the amount of tunneling decreases, which makes the transition from superfluid phase to Mott insulator phase where each lattice site is occupied by a single atom. In a Mott insulator phase the coherence between atoms on neighboring lattice sites are lost, and a matter wave interference pattern is no longer observed. Qualitatively, when an equal number of particles exists at each lattice site $i$ and $t \ll U$, where $t$ is a hopping term and $U$ is an interaction term, the strong repulsion interaction between the particles prevents them from moving freely from one site to another. In this case the system is incompressible, and the gas is in the Mott-insulator phase. On the contrary, when $t \gg U$, the particles can move freely from one site to another. The total wave function occupies the ground state of energy. This system is called as superfluid. (Figure 1)

1.4 Experimental methods to achieve the ultracold temperature

Various cooling methods have been developed to reach the ultracold temperature. In order to realize BEC in optical lattices, typically combinations of the laser cooling, magneto-optical trap and magnetic evaporating cooling are used. The laser cooling, or the doppler cooling, is the technique to reduce the momentum of the atoms by
applying the certain frequency of laser beams on them. This method can cool the
temperature of the atoms to a few micro Kelvin. To trap the atoms after cooling the
atoms, the method called the magneto-optical trap is usually used. This trapping is
created by adding the position dependent magnetic field to induce the position de-
pendent Zeeman effect. This trapping potential, however, destroys the homogeneity
of the system. In order to reduce the temperature even lower, the methods called
magnetic evaporation cooling is used. When the atoms are put inside the flask-
shaped magnetic trap, the energetic atoms escape from the trap and consequently
reduce the temperature of the remaining atoms inside the trap. Only about 10%
of the initial number of atoms remain when they reach the critical temperature for
BEC. Not only bosons but also bosonic Cooper pairs of fermions show interesting
properties when they are cooled to ultra-low temperature.

Figure 1: Superfluid-Mott insulator phase transition [7]
The left picture shows the matter wave interference pattern when the quantum gases
are in the superfluid phase. The right picture shows no matter wave interference
pattern when the gases are in the Mott-insulator phase.
1.5 Optical lattices

An Optical lattice is an artificial crystal of light and a crucial tool to study today’s atomic and condensed matter physics. The crystals of light trap atoms at very cold temperature and allows us to demonstrate how complex physical phenomena occurs such as high-temperature superconductivity with the experimentally accessible, simplified model. It is very difficult or even impossible to change the space between the atoms forming a real crystal lattice of a solid; however, an optical lattice makes such difficult task possible. An optical lattice is highly controllable by tuning the periodicity or intensity of the laser beams, and even one or two atoms can be isolated in each of the traps [8].

An optical lattice is the standing wave created by superimposing the counter-propagating lasers with the same wavelength and frequency. The atoms in the optical lattices experience the periodic potential due to the induced electric dipole moment. This oscillating dipole moment of the atoms by the oscillating electric light field creates a trapping potential $V_{\text{dip}}(\mathbf{r})$ described by

$$V_{\text{dip}}(\mathbf{r}) = -\mathbf{d} \cdot \mathbf{E}(\mathbf{r}) \propto \alpha(\omega_L)|\mathbf{E}(\mathbf{r})|^2,$$

where $\alpha(\omega_L)$ denotes the polarization of an atom, $\omega_L$ is the frequency of the laser light, and $\mathbf{E}(\mathbf{r})$ is the electric light field amplitude at position $\mathbf{r}$ [9]. The intensity of the laser light field $I(\mathbf{r})$ is proportional to $|\mathbf{E}(\mathbf{r})|^2$.

This periodic potential traps the ultracold gas of atoms inside the overlap region of the counter-propagating lasers. The periodic potential created by a single standing wave is described as

$$V_{\text{lat}}(x) = V_0 \sin^2(k_L x),$$

where $k_L = 2\pi/\lambda_L$ is the wave vector of the laser light, and $V_0$ denotes the potential depth of the optical lattice. For the case of three-dimensional optical lattices, a structure of the simple cubic lattice is created with the separation length between the lattice sites being $\lambda_i/2$, where $\lambda_i = \frac{2\pi}{k_i}, (i = x, y, z)$ is the wavelength of the laser beam. As discussed above, the properties of the lattices will be very difficult or impossible to change when we deal with the real solid matters. However, the artificial crystal of light allows us to experimentally control the parameters of the lattice such as geometry or potential. This high degree of controllability makes quantum gases in optical lattice become the remarkable model to test the fundamental condensed matter physics and quantum many body systems.

It is experimentally possible to make optical lattices having variety of geometrical shapes and dimensionality. One-dimensional optical lattice is a single standing wave
interference pattern formed by a pair of laser beams. Two-dimensional optical lattice is the two orthogonal standing waves. It is an array of one-dimensional potential tubes. Three-dimensional optical lattice is created by three orthogonal optical standing waves. This corresponds to a three-dimensional simple cubic lattice. (Figure 2)

The geometry of the optical lattices is under control by varying the angle for the laser beams to interfere, and the depth of the lattice can be changed by tuning the intensity of the laser beams.

![Figure 2: Optical lattices][10]

The picture (a) shows the two-dimensional optical lattice produced by the counter-propagating laser beam, and the picture (b) shows the three-dimensional optical lattice, which corresponds to a three-dimensional simple cubic lattice.
2 Repulsively interacting ultracold fermions in one dimensional optical lattices

2.1 Introduction

The Fermi-Hubbard model is used to study a two-component ultracold fermionic gas in an optical lattice. Since the Fermi-Hubbard model is also a very important concept in condensed matter physics to understand quantum many body system, the experimental realization of the Fermi-Hubbard model provides us with new insights to approach the unsolved problems with a highly controllable parameters. This was achieved recently by loading a fermionic quantum degenerate gas into a three-dimensional optical lattice [11], and the research of fermionic quantum gas started to directly connect to the research of condensed matter physics. While the significant experimental development of the fermionic quantum gas in optical lattices was achieved, theoretical study to understand the external trapping potential and its effect of compressibility has been addressed. The one-dimensional Hubbard model has the advantage to study those problems because it is considered as an exactly solvable model and is used as a model to explore various properties of the system. In order to study repulsively interacting ultracold fermionic gas in one dimensional optical lattices, the Bethe ansatz, which is a method for finding the solutions of the one-dimensional quantum many body models, is used to calculate the Fermi-Hubbard model [12]. There is always the underlying harmonic trapping potential exists in cold gas experiments, and the effect to vary the density across the optical lattice should be taken into considerations since this inhomogeneity induced by the trapping potential causes the spatial coexistence of metallic and insulating phases.

In the following sections, I calculate the local thermodynamic properties such as local density, number of double occupation sites, entropy and various compressibilities of ultracold Fermi gases in one dimensional optical lattices. The calculated local thermodynamic quantities are the parameters to detect the different phases of the ultracold gases.

2.2 The model

A two-component, ultracold fermionic atoms in one-dimensional optical lattices is described using the Fermi-Hubbard model with zero temperature limit.

\[ H = - \sum_{<ij>,\sigma} t_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}, \tag{4} \]
where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators for a Fermi atom in the spin state $\sigma = \uparrow, \downarrow$ at the lattice site $i$ and $j$, $U$ is the on-site interaction, and $\mu$ is the chemical potential. The density operator is $n_{ij,\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $<ij>$ denotes the nearest neighbor pair of sites. [14] Now I consider the optical lattices which having the harmonic confinement as a result of a trapping potential $V_i = \gamma R_i^2$ at site $i$. The local chemical potential $\mu$ can be written as $\mu - V_i$ assuming the local density approximation. Consequently, the chemical potential and particle number density monotonically change across the lattice. Also, this system has only the repulsive interaction, so $U$ can only have positive values. In experiments, the interaction $U$ can be tuned to negative or positive values by the technique called Feshbach resonance. The tunneling amplitude is empirically controlled by the intensity of the standing laser waves. Also, $U/t_\sigma$ can be controlled by the laser intensity since the tunneling amplitude $t_\sigma$ is exponentially sensitive to the laser intensity while the on-site interaction $U$ is weakly sensitive. Freezing the atomic motion in certain directions can reduce the dimensionality of the optical lattices. One-dimensional optical lattices can be experimentally formed by a strong confinement in the transverse direction combining two counter-propagating lasers, and this system so far have been realized with fermionic isotopes of potassium $^{40}$K and lithium $^6$Li, or fermionic ytterbium $^{173}$Yb. [14]

### 2.3 Particle density

For the case of spin independent tunneling $t_\uparrow = t_\downarrow = t$, the good approximation of the ground state energy per site $E(n, U, t) = t \times e(n, U/t = u)$ can be written based on the data obtained from the numerical solution of the Bethe-Ansatz method. In the region $0 \leq n = N/N_s \leq 1$, where $n$ is the filling factor, $N$ is the number of particles, and $N_s$ is the number of lattice sites, by Bethe-Ansatz I have

$$e(n, u) = -\frac{2f(u)}{\pi} \sin\left(\frac{\pi n}{f(u)}\right).$$

(5)

For the region $1 \leq n \leq 2$,

$$e(n, u) = (n - 1)u + \frac{2f(u)}{\pi} \sin\left(\frac{\pi(2 - n)}{f(u)}\right).$$

(6)

The function $f(u)$ is obtained from

$$-\frac{f}{\pi} \sin\left(\frac{\pi}{f}\right) = -2 \int_0^{\infty} J_0(x) J_1(x) \frac{x}{1 + e^{ux/2}} dx,$$

(7)
where $J_m$ is the $m$th order Bessel function. [15] The chemical potential is found by minimizing the grand canonical energy under the fixed total particle numbers, $\mu/t = \partial e/\partial n$,

$$\mu/t = \begin{cases} 
2 \cos \left( \frac{\pi n}{f(u)} \right), & 0 \leq n < 1 \\
 u + 2 \cos \left( \frac{\pi(2-n)}{f(u)} \right), & 1 < n \leq 2.
\end{cases} \tag{8}$$

The average particle densities are found by inverting this equation,

$$n = \begin{cases} 
0, & \mu/t < -2; \\
\frac{f(u)}{\pi} \arccos[-\mu/2t], & -2 \leq \mu/t \leq -2 \cos[\pi/f(u)] \\
1, & -2 \cos[\pi/f(u)] < \mu/t < u + 2 \cos[\pi/f(u)] \\
2 - \frac{f(u)}{\pi} \arccos[(\mu/t - u)/2], & u + 2 \cos[\pi/f(u)] \leq \mu/t \leq u + 2 \\
2, & \mu/t > u + 2.
\end{cases} \tag{9}$$

Figure 3 shows the particle density as a function of chemical potential $\mu/t$ for on-site interaction $U/t = 5$. For a representative value of on-site interaction $U/t = 5$, the zero temperature particle density as a function of chemical potential is shown in Figure 3. When $\mu/t$ is small, the $n$ is zero where the system is vacuum. As $\mu/t$, the first slope shows that the system is in the lower metallic state. The second flat region is the Mott-insulator phase where each lattice sites is occupied by one particle. Then, the second slope shows the upper metallic phase, and the highest flat region shows the bond insulator phase where each of all lattice sites is occupied with two particles having different spins.

![Figure 3](image.png)

**Figure 3.** Zero temperature particle density as a function of chemical potential $\mu$ at $U/t = 5$. 
2.4 Compressibility

Two compressibilities, $\kappa^*$ and $\kappa$ are described as

$$\kappa^* = \frac{\partial n}{\partial \mu}$$

(10)

and

$$\kappa = \frac{\kappa^*}{n}.$$  

(11)

They are calculated using the average particle density $n$ obtained in the previous section and become as follows:

$$\kappa^* = \left\{ \begin{array}{ll}
0, & \text{if } n=0,1,2; \\
\frac{f(u)}{2\pi} \frac{1}{\sqrt{1-\frac{\mu^2}{4}}}, & \text{if } \frac{f(u)}{\pi} \arccos\left[-\mu/2t\right] \\
\frac{f(u)}{2\pi} \frac{1}{\sqrt{1-(\frac{\mu}{2t})^2}}, & \text{if } 2 - \frac{f(u)}{\pi} \arccos\left[(\mu/t - u)/2\right] \\
\end{array} \right.$$  

(12)

$$\kappa = \left\{ \begin{array}{ll}
0, & \text{if } n=0,1,2; \\
\frac{f(u)}{2\pi} \frac{1}{\sqrt{1-\frac{\mu^2}{4}}} \frac{1}{\arccos\left[-\mu/2t\right]}, & \text{if } \frac{f(u)}{\pi} \arccos\left[-\mu/2t\right] \\
\frac{f(u)}{2\pi} \frac{1}{\sqrt{1-(\frac{\mu}{2t})^2}} \frac{1}{2-\frac{f(u)}{\pi} \arccos\left[(\mu/t - u)/2\right]}, & \text{if } 2 - \frac{f(u)}{\pi} \arccos\left[(\mu/t - u)/2\right]. \\
\end{array} \right.$$  

(13)

Figure 4 shows the compressibility $\kappa$ and Figure 5 shows the compressibility $\kappa^*$ as a function of chemical potential. The sharp peak of $\kappa$ at the edge of the trap is because of the low density. While this sharp peak is absent in $\kappa^*$, it shows two compressible regions corresponding to the lower metallic band and the upper metallic band. The three incompressible regions in these graphs correspond to a pinning of the density at $n=0$, 1, and 2 where they are in the insulator phases. These characteristic properties are directly related to the formation of gaps in the insulating phases.
Figure 4: Compressibility $\kappa = \kappa^*/n$ as a function of chemical potential $\mu$ at $U/t = 5$.

Figure 5: Compressibility $\kappa^* = \partial n/\partial \mu$ as a function of chemical potential $\mu$ at $U/t = 5$. 
2.5 Double occupation

The double occupation $d$ is described as

$$d = \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \quad (14)$$

$$= \frac{\partial e}{\partial U} \quad (15)$$

$$= (\frac{\partial e}{\partial f(u)}) \cdot (\frac{\partial f(u)}{\partial U}). \quad (16)$$

This becomes

$$d = \begin{cases} 
\frac{\pi}{f(u)} \int_0^{\infty} \frac{J_0(x)J_1(x)}{2(1+e^{u/2})^2} dx, & 0 \leq n \leq 1; \\
\frac{1}{f(u)} \int_0^{\infty} \frac{J_0(x)J_1(x)}{2(1+e^{u/2})^2} dx, & 1 \leq n \leq 2; \quad (17) 
\end{cases}$$

and the core compressibility $\kappa_c$ is expressed as

$$\kappa_c = \frac{\partial d}{\partial \mu} \quad (18)$$

which are shown in Figure 6 and Figure 7. Although I have fixed the on-site interaction $u$ to be 5, the qualitative behavior would be the same for all larger values of $u$. The three incompressible regions in Figure 7 corresponds to the density at $n = 0, 1, \text{ and } 2$. Since the core compressibility $\kappa_c$ measures only the core region, it is not sensitive to the edge of the cloud. In the insulating phases compressibilities are zero so they are discontinuous at densities $n = 0, 1, \text{ and } 2$. The peak corresponding to the lower band in Figure 4 and Figure 5 disappears in $\kappa_c$ shown in Figure 7. The core compressibility only reveals the double occupancy and the Mott insulator transition in the center of the trap. As we can see in Figure 7, when the chemical potential $\mu$ is large, the upper band is doubly occupied. For this case, $k_c$ and $k$ are identical to each other while $k_c$ is almost zero at the lower band. In Figure 8, two compressibilities $k$ and $k_c$ are compared for different values of on-site interactions $u$. When the chemical potential is large, the upper band is occupied so that the system has doubly occupied sites. For this case, $\kappa_c$ is identical to $\kappa^*$ at chemical potentials corresponding to the upper band, but it is almost zero at the lower band.
Figure 6: Double occupation $d$ as a function of chemical potential $\mu$ at $U/t = 5$.

Figure 7: Core compressibility $k_c$ as a function of chemical potential $\mu$ at $U/t = 5$. 
Figure 8: Compressibilities $k$ and $k_c$ as a function of particle density $n$. For three representative values of interactions. Black: $U/t = 1$, dark grey: $U/t = 5$, light grey: $U/t = 10$. 
2.6 The effect of the trapping potential

As mentioned before, the effect of the trapping potential \( V_{\text{trap},i} = \gamma R_i^2 \) at site \( i \) can be taken into account by replacing the chemical potential \( \mu \) with the local chemical potential \( \mu_{\text{local},i} = \mu - V_{\text{trap},i} \). The local density approximation assumes that the atomic system is locally homogenous with local chemical potentials \( \mu_{\text{local},i} \). Here \( \mu \) is the chemical potential at the center of the trap. Then combining this chemical potential with the experimentally measured column density profiles \( n(y,z) \) of the 1D lattice bundles, thermodynamic quantities can be extracted. The first step is to calculate the thermodynamic quantities with this trapping potential effect is to construct of the linear axial density \( n(z) = \int n(y,z) dy \).

Assuming the trapping potential is harmonic, we can describe \( V_{\text{trap}} \) as

\[
V_{\text{trap}} = \frac{1}{2} m \omega^2 z^2. \tag{19}
\]

and the local chemical potential \( \mu_{\text{local}} \) becomes

\[
\mu_{\text{local}} = \mu - \frac{1}{2} m \omega^2 z^2. \tag{20}
\]

The total number of the fermionic particles \( N \) is

\[
N = 2 \int_0^\infty dz \, n(z) \tag{21}
\]

Since \( dz = \frac{d\mu}{m \omega^2 \sqrt{2(\mu - \mu_{\text{local}})}} \), the total number of particle \( N \) and the total compressibility inside the trapping potential, \( \kappa_{\text{total}} = \int \kappa(t) \, dz \) become

\[
N = \sqrt{\frac{2}{m \omega^2}} \int_{-\infty}^{\mu} \frac{n(\mu)}{\sqrt{\mu - \mu_{\text{trap}}}} \, d\mu \tag{22}
\]

\[
\kappa_{\text{total}} = \sqrt{\frac{2}{m \omega^2}} \int_{-\infty}^{\mu} \frac{\kappa(\mu)}{\sqrt{\mu - \mu_{\text{trap}}}} \, d\mu. \tag{23}
\]

Let \( \bar{\mu} \) denotes \( \mu_{\text{local}}/t \), where \( t \) is the spin independent tunneling term. Then, I have

\[
N = \sqrt{\frac{2}{m \omega^2}} \int_{-\infty}^{\bar{\mu}} \frac{n(\bar{\mu})}{\sqrt{\bar{\mu} - \bar{\mu}_{\text{trap}}}} \, d\bar{\mu} \tag{24}
\]

\[
\kappa_{\text{total}} = \sqrt{\frac{2}{m \omega^2}} \int_{-\infty}^{\bar{\mu}} \frac{\kappa(\bar{\mu})}{\sqrt{\bar{\mu} - \bar{\mu}_{\text{trap}}}} \, d\bar{\mu}, \tag{25}
\]

and let me define \( \tilde{N} \) and \( \kappa_{\text{total}} \) as

\[
\tilde{N} = \int_{-\infty}^{\mu} \frac{n(\bar{\mu})}{\sqrt{\bar{\mu} - \bar{\mu}_{\text{trap}}}} \, d\bar{\mu} \tag{26}
\]
\[ \kappa_{\text{total}} = \int_{-\infty}^{\mu} \frac{\kappa(\tilde{\mu})}{\sqrt{\tilde{\mu} - \tilde{\mu}_{\text{trap}}}} \, d\tilde{\mu}. \] 

Similarly, for the double occupation \( d \), we can obtain \( \tilde{d} \) as

\[ \tilde{d} = \int_{-\infty}^{\mu} \frac{d(\tilde{\mu})}{\sqrt{\tilde{\mu} - \tilde{\mu}_{\text{trap}}}} \, d\tilde{\mu}. \] 

Figure 9 shows the compressibility as a function of the number of the particle particle \( \tilde{N} \) with the effect of trapping potential. In Figure 4 for the case without the trapping potential, the graph clearly shows where the system is in the insulating phase when \( \kappa = 0 \). However, Figure 9 does not have the region where \( \tilde{\kappa} = 0 \). This is because Figure 9 shows the compressibility of the entire lattice sites inside the trapping potential while Figure 4 shows the graph of the one lattice case. Since the trapping potential creates the inhomogeneity in the lattice, the metallic and insulating phases coexist in the optical lattice inside the trapping potential. The peaks in Figure 9 are the points where the phase transitions occur. The point for the peak appears shifts towards the bigger number of the particles \( \tilde{N} \) as the interaction \( U/t \) increases as expected. This is because particles repel each other when there is a strong interaction between particles. Figure 10 shows the double occupation \( \tilde{d} \) of the entire lattice sites sitting inside the trapping potential while Figure 6 shows the double occupation \( d \) of the one lattice site without the harmonic trapping potential. Therefore, Figure 10 shows the proportion of the double occupation sites in the entire lattice sites. For the small number of the particles \( \tilde{N} \), the double occupation \( \tilde{d} \) increases slowly because, for the small \( \tilde{N} \), there are a lot of empty sites for the particle to occupy, and the lattice sites do not need to be double occupied. After the point where \( \tilde{N} \) is around 4.5, the graph starts to increase monotonically. From this figure, it can be assumed that the each of all the lattice sites inside the trapping potential is occupied with one particle when \( \tilde{N} \) reaches around 4.5, and after this point, when more particles are added in the system, the doubly occupied sites are increased proportionally.
Figure 9: Compressibility with the effect of the harmonic trapping potential as a function of the number of the particle $\hat{N}$
Black: $U/t=1$, dark grey: $U/t=5$, light grey: $U/t=10$

Figure 10: Double Occupation with the effect of the harmonic trapping potential $U/t=5$
3 Superfluid-Insulator transition of hardcore bosons in an optical superlattice

3.1 Introduction

The old problem going back to the 1950’s to calculate the ground state energy of a dilute Bose gas keeps attracting the renowned attentions. If we think about the particles interacting only with a two-body potential enclosed in a cube box with the length L, the energy/particle in the thermodynamic limit is described as

\[ e(\rho) \equiv \lim_{N \to \infty} E_0(N, \rho^{-1/3}N^{1/3})/N \simeq 4\pi \mu \rho a, \]

where \( E_0(N, L) \) is the energy in three dimensions for a two-body potential, \( a \) is scattering length, \( \rho = N/V \) is fixed particle density, and \( \mu = \hbar^2/2m \) with the mass of a particle \( m \). To derive the equivalence for three-dimensional Bose gas were attempted in the 1950’s and 60’s for example by Bogoliubov. The ground state energy per particle in three-dimensions was derived as \( e(\rho) = 4\pi \mu \rho a \). For hard-core bosons the scattering length \( a \) is the diameter of the particles. However, this result was not able to apply for the two-dimensional Bose gases. The derivation of this problem was done by Shick in 1971 for a gas of hard discs, and the energy per particle is derived as \( e(\rho) = 4\pi \mu \rho \ln(\rho a^2)^{-1} \). In the meanwhile, the study of hardcore bosons on two dimensional lattices started to attract attentions, and the simulation algorithms have been attempted to construct. The mean-field and spin-wave calculations are developed to become the standard approach to solve the problems. In this chapter hardcore bosons on a two-dimensional square lattice is examined using Bose-Hubbard model. The ground state potential, the particle density and condensate density are calculated by variational method, and the transitions between compressible superfluid phase and incompressible Mott insulator are studied as functions of chemical potential and tunneling energy.

3.2 The model

The model I consider in this chapter is hardcore bosons in two-dimensional optical superlattices experiencing the anisotropic tunnelings. In laboratories, this system can be realized by superimposing the laser beams having different wavelengths and intensities. This is described by the Bose-Hubbard Hamiltonian:

\[ H = - \sum_{<ij>} t_{ij}(a_i^\dagger a_j + a_j^\dagger a_i) + U_0 \sum_i n_i(n_i - 1) - \mu \sum_i a_i^\dagger a_i, \]

(29)
where \(<ij>\) denotes the neighbors at lattice sites, \(t_{ij}\) is the hopping term, \(U\) is the on-site interaction, \(n_i\) is the number operator equals to \(a_i a_i^\dagger\), and \(\mu\) is the chemical potential. The hopping term \(t\) and the on-site interaction \(U_0\) are described as

\[
\begin{align*}
t &= \frac{\hbar^2}{2m} \left(\frac{2\pi}{\lambda}\right)^2 \frac{2}{\sqrt{\pi}} \frac{E_0}{E_R}^{1/4} \exp[-2(E_0/E_R)^{1/4}] \\
U_0 &= \frac{\hbar^2}{2m} \left(\frac{2\pi}{\lambda}\right)^2 a_s k \sqrt{\frac{8}{\pi}} [(E_0/E_R)^{1/4}]^3,
\end{align*}
\]

where \(E_0\) is the laser intensity and \(a_k\) is the scattering length. From Equation (30) and Equation (31), the tunneling energy \(t\) is exponentially sensitive to the laser intensity \(E_0\) while the interaction energy \(U_0\) is weakly sensitive to \(E_0\). Therefore, \(t/U_0\) can be controlled by tuning laser intensity. Now, because the on-site interaction term is hard to tackle theoretically and the interaction energy is proportional to the scattering length, let the interaction term vanish by setting the scattering length as infinity. In laboratories, this can be done by the technique called Feshbach resonance. The bosons I study in this chapter is the hardcore bosons. The hardcore constraint restricts the number of bosons to occupy a given site \(i\) to be only 0 or 1. It means that \(\hat{n}_i = a_i a_i^\dagger\) is only 0 or 1. Also, I think about the system with the anisotropic tunnelings, which means that hopping energies according to the direction for the nearest neighbors each along x and y-directions, and for the next nearest neighbors should be taken into account. Thus, the equation (29) becomes

\[
H = -\alpha t \sum_{<ij>} (a_i^\dagger a_j + a_j^\dagger a_i) - \beta t \sum_{<ij>} (a_i^\dagger a_j + a_j^\dagger a_i) - \gamma t \sum_{<ij>} (a_i a_j + a_j a_i) + \sum_i (-A)^i a_i^\dagger a_i - \mu \sum_i a_i^\dagger a_i,
\]

where \(\alpha\) and \(\beta\) denote the nearest neighbors along x-direction and y-directions, \(\gamma\) is the next nearest neighbors, and \(A\) is the energy mismatch of the tunneling amplitude of the superlattice. (Figure 11) Although this Hamiltonian allows any number of bosons to occupy the given lattice site, the number operator of hardcore bosons can only be 0 or 1, \(\hat{n}_i = 0\) or 1. To enforce this constraint, the two dimensional antiferromagnetic Heisenberg model is used by mapping \(a_i^\dagger \leftrightarrow S_i^\dagger\), \(a_i \leftrightarrow S_i\), and \(\hat{n}_i \leftrightarrow S_i^z + 1/2\). The acquired spin Hamiltonian is

\[
H = -\alpha t \sum_{<ij>} (S_i^\dagger S_j + S_j^\dagger S_i) - \beta t \sum_{<ij>} (S_i^\dagger S_j + S_j^\dagger S_i) - \gamma t \sum_{<ij>} (S_i^\dagger S_j + S_j^\dagger S_i) - \sum_i (\mu + (-A)^i) (S_i^z + 1/2).
\]
3.3 Superfluid density and particle density

The ground state energy $\Omega$ is calculated using the mean-field theory.

$$\Omega = \frac{\langle \psi | H | \psi \rangle}{N},$$

where $|\psi\rangle$ is the mean-field state vector, and $N$ is the total number of the lattice sites. The state vector is

$$|\psi\rangle = \Pi_i (u_i + v_i S_i^z) |0\rangle,$$

where $u_i = \sin(\frac{\theta_i}{2})$ is the amplitude of probability to be spin down, $v_i = \sin(\frac{\theta_i}{2})$ is the amplitude of probability to be spin up, and $\theta_i$ is the variational parameter. Up-spin corresponds to that there is one boson at a given site and down-spin corresponds to that there is no boson at a given site. The ground state energy $\Omega$ is obtained as

$$\Omega = -\frac{1}{2N} \{ \alpha t \sum_{<ij>} \sin \theta_1 \sin \theta_2 + \beta t \sum_{<ij>} \sin \theta_1 \sin \theta_2$$

$$+ \gamma t ( \sum_{<ij\text{-even}>} \sin^2 \theta_1 + \sum_{<ij\text{-odd}>} \sin^2 \theta_2)$$

$$+ \sum_{<ij\text{-odd}>} (\mu - A)(\cos \theta_1 + 1) + \sum_{<ij\text{-even}>} (\mu + A)(\cos \theta_2 + 1) \}.$$
The superfluid density $\rho_0$, the particle density $\rho$ are calculated by variational method, and they are obtained as

$$\rho_0 = \frac{1}{N} \langle \psi | a_i^\dagger a_i | \psi \rangle = \frac{1}{2} + \frac{1}{4} (\cos \theta_1 + \cos \theta_2)$$  \hspace{1cm} (36)$$

$$\rho = \frac{1}{N} \langle \psi | \tilde{a}^\dagger (k = 0) \tilde{a}(k = 0) | \psi \rangle = \frac{1}{16} (\sin \theta_1 + \sin \theta_2)^2.$$  \hspace{1cm} (37)$$

To determine the dependence of the chemical potential on the variational parameters $\theta_1$ and $\theta_2$, we minimize $\Omega$ with respect to each of $\theta_1$ and $\theta_2$. Then, Eqn (21) and Eqn (22) become

$$2(\alpha + \beta)t \cos \theta_1 \sin \theta_1 + 4\gamma t \cos \theta_1 \sin \theta_1 = (\mu - A) \sin \theta_1$$  \hspace{1cm} (38)$$

$$2(\alpha + \beta)t \cos \theta_2 \sin \theta_1 + 4\gamma t \cos \theta_2 \sin \theta_2 = (\mu + A) \sin \theta_2.$$  \hspace{1cm} (39)$$

Figure 12 below shows the superfluid density and particle density as a function of chemical potential $\mu$ and tunneling $t$ for an isotropic lattice $\alpha = \beta = 1$. These two graphs correspond each other. Three flat regions can be seen on each of the graph. In the graph below showing the particle density, there are no particle in the flat region on the bottom which is a vacuum. The second flat region in the middle is the half-filling region which is the bose-glass phase. The last flat region on the top is the Mott insulating phase.
Figure 12: Superfluid density and particle density  The picture above shows superfluid density and the picture below particle density as a function of chemical potential $\mu$ and tunneling $t$ for an isotropic lattice $\alpha = \beta = 1$
3.4 Effect of trapping potential

Now the local density approximation is added to the calculations done in the previous section. Optical lattices sit inside the trapping harmonic potential $V(r)$ described as

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

(40)

$$ = \frac{1}{2} m \omega^2 d^2 (i_x^2 + i_y^2), $$

(41)

where $d$ is the distance between the lattice sites. Therefore, we can study the inhomogeneity of the system by replacing the chemical potential $\mu$ with $\mu_0 - \frac{1}{2} m \omega^2 d^2 (i_x^2 + i_y^2)$. Figure 13 shows the particle density profile inside this trapping potential. We can see the Mott insulating phase, superfluid phase, bose glass phase and vacuum state coexist together inside the potential well. Around the center of the potential well, the particle density is 1 which is the Mott-insulator phase, and at the edge of the well, there are no particle which is a vacuum state.

Figure 13: Particle density inside the harmonic oscillator potential
For an isotropic lattice $\alpha = \beta = 1$. Three phases coexist together inside the potential well.
3.5 Dimensional cross over

Even though I work with two-dimensional superlattice in this thesis, changing the magnitude of tunneling energy along each of the direction can cause the change of dimensionality. Figure 14 shows how the superfluid density and particle density change by the effect of anisotropic tunneling. The hopping energy along x-direction is fixed by setting $\alpha = 1$ while the one along y-direction $\beta t$ varies. As the value $\beta$ is increased from 0 to 1, the dimensional crossover is observed. Although increasing the value of $\beta$, the particles does not start moving to the y-direction instantly, but rather the particle keeps moving only along x-direction. As Figure 15 shows, the dimensional cross over are observed by the change of the shape of the particle density distributions. The graph above in Figure 13 shows the particle density with $\beta = 0.05$, and the system is in the one-dimensional regime. The graph below shows the particle density with $\beta = 0.9$. Now we can see the shape of the graph has changed compared to the system in the one-dimensional regime, which means the system is in the two-dimensional regime.

![Figure 14: Superfluid density and particle density](image)

The figure above shows superfluid density and the figure below particle density for an anisotropic lattice $\alpha = 1$, $t/A = 0.5$
Figure 15: The dimensional cross over Particle density (a) \( \beta = 0.05 \) (b) \( \beta = 0.09 \)

For an anisotropic lattice \( \alpha = 1, \ t/A = 0.5 \) The figure above shows the particle density with \( \beta = 0.05 \), and the figure below shows the particle density with \( \beta = 0.09 \).
3.6 The effect of interaction

Next, the effect of interaction is added to our Hamiltonian described by the Eqn (2). The new Hamiltonian becomes

\[ H' = H + \sum_{<ij>} V_{ij}n_in_j, \]  

(42)

where \( V_{ij} \) is the interaction term. As before, mapping this Bose-Hubbard Hamiltonian into Spin Hamiltonian, we acquire

\[ H' = H + \sum_{<ij>} V_{ij}(S_i^z + \frac{1}{2})(S_j^z + \frac{1}{2}), \]  

(43)

where \( V_{ij} = V \) if \( i, j \) is the nearest neighbor, and \( V_{ij} = \delta V \) if \( i, j \) is the next nearest neighbor. Then, the ground state energy \( \Omega \) is derived by variational method and is minimized with respect to the variational parameters \( \theta_1 \) and \( \theta_2 \). We gain two equations below.

\[
\begin{align*}
2(\alpha+\beta)t\cos\theta_1 \sqrt{1 - \cos^2\theta_2} &= \sqrt{1 - \cos^2\theta_1}(-4\gamma t\cos\theta_1 - 2\gamma \delta V \cos\theta_1 + (\tilde{\mu} - A) - 2V \cos\theta_2) \\
2(\alpha+\beta)t\cos\theta_2 \sqrt{1 - \cos^2\theta_1} &= \sqrt{1 - \cos^2\theta_2}(-4\gamma t\cos\theta_2 - 2\gamma \delta V \cos\theta_2 + (\tilde{\mu} + A) - 2V \cos\theta_1)
\end{align*}
\]

(44)  

(45)

Figure 16 shows the superfluid density and particle density with the effect of interaction. When the chemical potential/energy mismatch of the lattice sites \( \mu/A \) is small, the particle density is very small where almost no particle exists as expected. As the interaction \( V/A \) is increased, at the region where \( \mu/A \) is between -0.5 and 0.5, the superfluid density suddenly becomes zero and the particle density becomes one, where the system is in the insulator state. It is because when the interaction energy is increased, particles start strongly repelling each other and eventually stop moving from one lattice site to another, but each of them stays in each of the lattice site to achieve the minimum energy.
Figure 16: Superfluid density (above) and particle density (below)
For an isotropic lattice $\alpha = \beta = 1$, $t/A = 0.24$
4 Conclusion

The recent experimental and theoretical developments of ultracold atomic gases started to address the unsolvable problems of solid state physics and condensed matter physics. I studied two systems in this thesis. One is the ultracold fermions in one dimensional optical lattices, and another is the ultracold hardcore bosons in two dimensional optical lattices.

The first system of a two-component ultracold Fermi gas in an optical lattice was described by the Fermi-Hubbard model. I calculated the particle density, compressibility, and double occupation for the system with zero temperature limit based on the Bethe-ansatz method and discussed the phase transitions between metallic and insulating phases with and without the effect of the harmonic trapping potential.

The second system of ultracold hardcore bosons in optical lattice Bose-Hubbard model was used to study the ultracold hardcore bosons in optical lattice. In order to enforce the hardcore constraints, the spin mapping was used. The ground state energy, superfluid density and particle density were calculated by the variational method. When the local density approximation was added to the system, I showed that insulating and superfluid phase coexisted together inside the trap. Also, the dimensional cross over and the effect of interaction were observed with the anisotropic tunneling energy.
References


