Ph.D. Thesis

Theory of Bose-Einstein Condensates in Optical Lattices

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Graduate School of Science and Engineering
Waseda University
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Shunji Tsuchiya
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Chapter 1

Introduction

In this chapter, we briefly review the history of Bose-Einstein condensation (BEC) and recent development of BEC experiments in trapped atomic gases. An emphasis is put on the recent progress of the study on Bose-Einstein condensates in optical lattices.

1.1 History of BEC

Bose-Einstein condensation (BEC) was first predicted by Einstein in 1925 [1] by applying the idea of Bose on a statistics of photons [2] to particles using de Broglie’s idea on matter wave. Einstein discussed an ideal gas of particles obeying Bose-Einstein statistics, which gives the mean occupation number of atoms in quantum state $i$ with the energy $\epsilon_i$ in equilibrium at temperature $T$ as

$$n_i = \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1}, \quad (1.1)$$

where $\mu$ is a chemical potential, $\beta = 1/k_B T$ and $k_B$ is Boltzmann’s constant. Equation (1.1) is called the Bose distribution function. Einstein predicted that macroscopic number of particles begins to condense in the lowest energy state and a phase transition occurs at a certain temperature. This phase transition is unique in the sense that it occurs without interaction between atoms. It is a pure consequence of Bose-Einstein statistics, namely bosons statistically tend to be in the same quantum state. This property is called the Bose stimulation which is derived quantum mechanically from the fact that the wave function for identical bosons have to be symmetric [3]. It can be understood if one considers a collision of two bosons in the presence of a weak interaction. When two particles in the states 1 and 2 are scattered into the states 3 and 4, assuming that the energy is conserved
in the process, i.e., $\epsilon_1 + \epsilon_2 = \epsilon_3 + \epsilon_4$, one can easily confirm the following identity for the Bose distribution function,

$$n_1n_2(1 + n_3)(1 + n_4) = (1 + n_1)(1 + n_2)n_3n_4.$$  \hfill (1.2)

Equation (1.2) shows that the rate of the process $(1, 2) \rightarrow (3, 4)$ and the opposite process is equal in equilibrium. The factor $1 + n_i$ means that the rate for a particle scattered into the state $i$ is enhanced by the factor $n_i$, when there are already $n_i$ particles in the state $i$. The formation and stabilization of Bose-Einstein condensates is entirely due to this property of Bose statistics.

After the prediction of Einstein, BEC was considered to be unrealistic by the assumption of ideal gas, and had not attracted much interest until the discovery of superfluidity. Superfluidity of liquid $^4$He was discovered by Kapitza [4] and, independently Allen and Miesner [5] in 1938. They found that the fluid flowed without any apparent viscosity below the transition temperature $T_\lambda$. Soon after the discovery of superfluidity, London proposed that superfluidity in liquid $^4$He is a manifestation of BEC [6]. Tisza phenomenologically introduced the two-fluid model which describes the character of liquid helium by two interpenetrating fluids, a normal fluid and superfluid, and interpreted the superfluid component as Bose condensed helium atoms [7]. Landau presented a theory of superfluidity based on the idea of “quasi particles” [8]. He developed a theory of quantum hydrodynamics without any assumption on the statistics of atoms consisting the liquid, and strongly opposed London and Tisza’s idea. After the long controversy on the connection between BEC and superfluidity, London and Tisza’s idea was supported by most of physicists. However, the relevance of BEC and superfluidity was still unclear due to the lack of microscopic theory of liquid $^4$He, because perturbation theory was not applicable for strongly interacting helium atoms.

On the other hand, theories for a weakly interacting dilute bose gas (WIDBG) had developed without any real experimental system. In 1947, Bogoliubov reported the first microscopic theory of WIDBG based on the assumption of BEC [9]. He calculated the excitation spectrum and showed that it has a phonon spectrum for small momentum, which ensures the stability of superfluidity. Pitaevskii developed Bogoliubov’s theory to an inhomogeneous case to study a vortex line in a Bose condensate [10]. He introduced a concept of macroscopic wave function and derived the famous Gross-Pitaevskii equation for the wave function $\Psi(r, t)$ [10], which was also derived independently by Gross [11]. The generalization of the methods of quantum field theory for WIDBG was also developed by Beliaev [12]. Experimental effort had been also continued to realize BEC in a WIDBG in many systems, e.g., spin-polarized hydrogen, excitons in Cu$_2$O, and cold gases of alkali atoms [13].
In 1995, BEC of trapped atomic gases was realized by Cornell and Wiemann at Boulder [14], and Ketterle at MIT [15]. In these experiments, alkali atoms are confined in a magnetic trap and cooled down to extremely low temperatures of the order of microkelvin. Experimentalists combined laser cooling and evaporative cooling technique, and finally succeeded in reaching the temperatures and densities for achieving BEC [16, 17]. The atomic gas is kept in a metastable state to avoid relaxing to the solid phase in equilibrium. Diluteness and weak interaction are necessary for long lifetime to observe BEC in this system. This experimental success has provided a novel system for studying BEC, superfluidity, and many other phenomena concerning basic concepts of quantum physics. It has opened a new area of physics called “cold atom”, which is still growing rapidly and attracting interest from all areas of physics.

BEC of trapped atomic gases has many features which distinguishes this system from other BEC systems. First of all, BEC can be observed directly by experiments. For instance, the velocity distribution of atoms taken by means of expansion method has clearly shown the appearance of a condensate below the transition temperature [16]. Thus, one can see the amplified matter wave by his own eyes. Furthermore, a lot of quantitative information can be extracted from simple spatial images of atomic cloud. A sequence of in situ observation has shown collective excitations of a condensate [18]. From a theoretical point of view, this system provides a testing ground for many-body theories of WDBG, and we can develop the theory by comparing with experimental data. A great advantage of this system is that the atomic gas can be easily manipulated by electromagnetic field, and one can study novel physics of inhomogeneous Bose gas, for instance, studies of BEC in a harmonic trap and optical lattice have revealed new aspects of Bose condensates. Moreover, experimental parameters can be changed and controlled in a wide range with unprecedented precision. Recent experimental success of Feshbach resonance [19] allows one to study strongly interacting atoms.

1.2 BEC in an optical lattice

An optical lattice is a spatially periodic potential induced by the ac Stark effect of interfering laser beams. It has been widely used from the early stage of the research of ultracold quantum gases [20]. An optical lattice is an artificial perfect crystal for atoms, which is an ideal system for studying solid-state physics phenomena with more tunability of parameters than in solid.

The first experiment of Bose condensates in an optical lattice was reported by Anderson and Kasevich [21]. They observed interference of atomic wave tunneling from a condensate confined in a vertically oriented one dimensional optical lattice in analogy with
CHAPTER 1. INTRODUCTION

a pulsed mode-locked photon laser. This experiment has also offered the possibility of observing Bloch oscillation and Landau-Zener tunneling between different energy bands in an optical lattice. These problems were addressed and realized in Refs. [22, 23]. The result of Anderson and Kasevich’s experiment can be interpreted in terms of ac Josephson effect, and it is a manifestation of coherence of Bose condensate in an optical lattice. After this experiment, Josephson junction arrays were realized and Josephson oscillation was observed in Ref. [24].

Remarkable progress has been made in the study of strongly interacting atomic regime. The possibility for investigating the superfluid-Mott insulator transition in this system was first suggested theoretically by [25]. The observation of number squeezed states was reported in [26] and the superfluid-Mott insulator transition was achieved by Greiner et al. [27]. This experimental success has proved the usefulness of optical lattice for studying strongly correlated systems and opened up a new direction for this research field.

Bose condensates in an optical lattice are also predicted to show novel superfluid states. Wu and Niu found that a moving condensate in an optical lattice exhibits instability called dynamical instability due to the appearance of an imaginary part of the excitation spectrum [28]. This result was also obtained by Smerzi et al. by using tight binding model [29]. The observation of dynamical instability was recently reported in [30]. A characteristic feature of the condensate band structure called swallow tail was reported in [31, 32].

Dynamics of a condensate in an optical lattice has also attracted attention and been investigated theoretically and experimentally. A shift of the oscillation frequency in the presence of the optical lattice was observed [33] and the experimental result has shown a good agreement with the prediction of the renormalized mass theory of Krömer et al. [34]. The damping of the condensate oscillation at finite temperatures was observed in [35]. It is worth noting that the thermal cloud stays locked at the center of the trap due to its incoherent nature in the presence of the optical lattice, while the condensate moves and oscillates through the lattice [35].

Theoretically, Bogoliubov type excitation in an optical lattice has been studied. The excitation spectrum was calculated and the phonon dispersion at long wavelengths was addressed in [36, 37, 38, 39, 40, 41, 42]. The Bragg spectroscopy for a condensate in an optical lattice was suggested to investigate the excitation spectrum [43]. Recently, Störfle et al. prepared a condensate in a three-dimensional optical lattice and studied the property of a condensate by a Bragg spectroscopy type experiment [44]. They studied the excitation spectrum in the strongly interacting regime and observed a broad continuum of excitations which requires an interpretation beyond the Bogoliubov theory [44].

After the first realization of BEC, magnetic traps have been used in BEC experiments for producing Bose-Einstein condensates by providing trapping potentials and allowing
for forced evaporative cooling [16, 17]. In 1998, BEC was achieved in an optical trap using the dipole force between atoms and a laser field [45]. The optical trap has been developed to avoid the limitation of magnetic trap. It allows more precise spatial and temporal manipulation of Bose condensates than magnetic trap. One of the important advantages of optical trap is that atoms in all hyperfine spin states can be trapped, while atoms in one hyperfine spin state can be trapped in a magnetic trap due to the Zeeman energy. This results in the generation of spinor Bose condensates in an optical trap [46, 47], which have no other example in other BEC systems. Spinor Bose condensates have shown novel properties due to spin degrees of freedom such as spin excitations [48, 49], topological spin textures [48, 50, 51, 52, 53], and fragmented BEC [54]. If a Bose condensate is loaded in an optical lattice after it is produced in an optical trap, we can study superfluid-Mott insulator transition of spinor bosons. In fact, several unique properties of spin-1 bosons in an optical lattice have been predicted by Demler and Zhou [55]. They proposed several new phases of superfluid and Mott insulating states and discussed the possibility of exotic fractionalized phases [55].

1.3 Outline

The primary aim of this thesis is to study 1) collective excitations of Bose condensates and damping of these excitations in a uniform optical lattice, and 2) the superfluid-Mott insulator transition of spinor Bose condensates.

As for the topic 1), collective excitation is a key concept for understanding various properties of Bose condensates, e.g., dynamics, thermodynamics, and response to an external field [56]. The excitation spectrum also plays a crucial role for the superfluid-Mott insulator transition, since the spectrum has different dispersion forms characterizing each phase. In the superfluid phase, the excitation spectrum has a linear dispersion for small momentum and it ensures the stability of superfluidity. In the Mott insulator phase, the spectrum has a finite gap, and the system exhibits insulating property. Recent experiments of Bose condensates in an optical lattice have shown remarkable damping of collective excitations [35, 44, 57]. This experimental result has not been explained yet and it motivates us to study the Landau and Beliaev dampings of excitations in a uniform optical lattice.

As for the topic 2), in addition to the fact that spinor Bose condensates have novel properties which is absent in spin-0 Bose condensates as we mentioned above, it is well known that spin degrees of freedom provides rich physics for strongly correlated systems [58]. If we consider the superfluid-Mott insulator transition of spinor bosons, we can expect new superfluid and Mott insulator phases due to spin degrees of freedom and
phase transitions between them. Spinor bosons in an optical lattice can also provide a new system to study various type of spin Hamiltonians. We derive the effective spin-Hamiltonian which describes the Mott insulator phase of spin-1 bosons in an optical lattice.

The outline of this thesis is as follows:

In Chapter 2, we study collective excitation of Bose condensates in a uniform optical lattice. We deal with deep and shallow optical lattices separately. For a deep optical lattice, we introduce a Bose-Hubbard tight-binding model and discuss the Bloch-Bogoliubov excitation. We discuss the Bogoliubov type excitation using the Gross-Pitaevskii approximation. We consider the effect of the thermal cloud and discuss the Landau damping due to coupling to thermal excitations and Beliaev damping due to spontaneous decay of excitations. For a shallow lattice, the time-independent Gross-Pitaevskii equation and the Bogoliubov equations are solved treating the lattice potential as a perturbation and the spectrum of Bloch-Bogoliubov excitation is analytically derived.

In Chapter 3, we study the superfluid-Mott insulator transition of spin-1 bosons with an antiferromagnetic interaction in an optical lattice at zero temperature. We discuss the phase diagram of the ground state using the Bose-Hubbard model of spin-1 bosons. Extending the mean-field theory developed in Refs. [38, 59] to study the superfluid-Mott insulator transition of spin-0 bosons to the spin-1 case, we calculate the phase boundaries between superfluid and Mott insulator phases. We also calculate the phase diagram using the Gutzwiller variational wave function comparing it with the result of the mean-field theory.
Chapter 2

Condensate excitations in optical lattices

This chapter is organized as follows. In Sec. 2.1, we briefly review the interaction of an atom with a laser field. In Sec. 2.2, we introduce the Bose-Hubbard tight-binding model which describes Bose gases in a deep optical lattice. In Sec. 2.3, we discuss the generalized discrete Gross-Pitaevskii equation and derive the excitation spectrum of the Bloch-Bogoliubov excitation. The characteristic change in the Bloch-Bogoliubov excitation dispersion relation as a function of the dimensionless interaction parameter $\alpha = U n^0 / J$ is pointed out. In Sec. 2.4, we introduce the Hartree-Fock-Bogoliubov-Popov theory for optical lattices, and calculate the condensate fraction and $\alpha$ as a function of the optical lattice depth and temperature. We also calculate the phonon velocity of the Bloch-Bogoliubov excitation as a function of the lattice depth. In Sec. 2.5, we calculate the Beliaev and Landau damping of Bloch-Bogoliubov excitations. In Sec. 2.6, we consider Bose condensates in a weak optical lattice and calculate the excitation spectrum treating the lattice potential as a perturbation. We give some concluding remarks of this chapter in Sec. 2.7. This chapter is based on the results reported in Refs. [60, 61].

2.1 Interaction of atoms with a laser field

An optical lattice is produced by interfering laser beams. It is a good example of how laser beam can be used for manipulating atomic matter wave. We start with a review of the force on an atom produced by a laser field and derive the effective potential for atoms in the presence of a laser beam [56].

In a laser field which has a much longer wavelength than the typical atomic size, the
laser-atom interaction can be treated in the dipole approximation as

\[ U(r, t) = -\hat{d} \cdot E(r, t), \quad (2.1) \]
\[ E(r, t) = E(r)e^{-i\omega t} + c.c., \quad (2.2) \]

where \( \hat{d} \) is the electric dipole moment operator, and \( E(r, t) \) is an electric field of the laser beam oscillating with the frequency \( \omega \). This interaction induces an electric dipole moment on the atom oscillating with the same frequency as the laser field. Thus, the expectation value of the dipole moment can be written as

\[ \langle \hat{d} \rangle = \alpha(\omega)E(r, t). \quad (2.3) \]

\( \alpha(\omega) \) is the dipole polarizability of the atom given by

\[ \alpha(\omega) = \frac{1}{\hbar} \sum_n \frac{|\langle n|\hat{d} \cdot e|0\rangle|^2}{\omega_n^2 - (\omega + i\eta)^2}, \quad (2.4) \]

where \( e \) is the unit vector in the direction of the electric field \( E(r) \), \( |0\rangle \) is the electronic ground state of the atom, and the summation is taken over all the excited states \( |n\rangle \). \( \hbar \omega_n \) is the excitation energy from the ground state \( |0\rangle \) to the excited state \( |n\rangle \), and \( \eta \) is an infinitely small positive number. In the second order perturbation theory, the energy change of the system due to the polarization is

\[ V(r) = -\frac{1}{2}\alpha(\omega)|E(r, t)|^2, \quad (2.5) \]

where the bar indicates a time average. This energy change can be regarded as an effective potential for the atom. If we take \( E(r, t) \) as a retro-reflected standing wave field along the \( x \)-direction,

\[ E(r, t) = E_0 e^{i\omega t} \left( e^{-i\omega t} + c.c. \right), \quad (2.6) \]

Eq. (2.5) reduces to

\[ V(r) = -\alpha(\omega)E_0^2 \cos^2 kx. \quad (2.7) \]

Equation (2.7) expresses a periodic potential with a period \( a = \pi/k \) along the \( x \)-direction. It is also possible to create a two and three dimensional lattice potentials with additional laser beams. The well depth of an optical lattice can be tuned by changing the intensity of the electric field. Usually, an optical lattice potential is described as

\[ V(r) = sE_R \cos^2 kx, \quad (2.8) \]

where \( s \) is the dimensionless parameter describing the optical lattice strength in units of the photon recoil energy \( E_R \equiv \hbar^2 k^2/2m \) describing the energy acquired by the atom after absorbing a photon with momentum \( \hbar k \), \( m \) being the mass of a single atom.
2.2 Bose-Hubbard Model

We consider bosonic atoms in an optical lattice potential

\[ V_{op}(r) = sE_R \sum_{i=1}^{d} \sin^2(kx_i), \quad (2.9) \]

where \( s \) is the usual dimensionless parameter describing the depth of the optical lattice in units of the photon recoil energy \( E_R = \hbar^2 k^2 / 2m \). \( d \) is the dimension of the optical lattice and \( a = \frac{\pi}{d} = \frac{3}{2} \) is the lattice period. We only consider simple cubic lattices used in recent experiments [27, 44]. Expanding the optical lattice potential around the minima of the potential wells, the well trap frequency is given by \( \omega_s = s^{1/2} \hbar k^2 / m \).

In recent experiments of atomic gases trapped in an optical lattice, atoms are loaded into an optical lattice after a Bose condensate is produced in a magnetic trap. Thus, atoms are confined in a combined potential of harmonic trap and optical lattice. We neglect, to a first approximation, the effect of a confining harmonic trap along the direction of the optical lattice, but consider the effect of the harmonic trap perpendicular to the optical lattice potential.

Here, we call attention to the recent technique [44, 57, 62, 63, 64] of producing a two-dimensional array of long, tightly confined condensate tubes by loading a condensate into a deep 2D optical lattice potential, which prevents atoms from hopping between different tubes. With an additional 1D optical lattice potential along a tube, an ideal 1D lattice system is realized [44, 57]. One can also have an ideal 2D lattice system by loading a condensate into a deep 1D optical lattice and a shallow 2D optical lattice. We assume this experimental setup for 1D and 2D systems. We also assume that the laser intensity determining the depth of the optical lattice wells is large enough to make the atomic wave functions well localized on the individual sites (tight-binding approximation). The energy gap between the first and the second excitation bands is large compared to the chemical potential and thermal energy \( (\mu, 2k_B T \ll sE_R / 2) \), and thus only the first band is occupied.

Within a tight-binding approximation, the effective Hamiltonian is the Bose-Hubbard model [25, 65] as

\[ H = -J \sum_{\langle j, l \rangle} (a_j^\dagger a_l + a_l^\dagger a_j) + \frac{1}{2} U \sum_j a_j^\dagger a_j^\dagger a_j a_j, \quad (2.10) \]

where \( a_j \) and \( a_j^\dagger \) are destruction and creation operators of atoms on the \( j \)-th lattice site. \( \langle j, l \rangle \) represents nearest neighbor pairs of lattice sites. The first term describes the kinetic
energy due to the hopping of atoms between sites. The hopping matrix element $J$ is given by

$$J = - \int dr w_j^*(r) \left( - \frac{\hbar^2 \nabla^2}{2m} + V_{op}(r) \right) w_l(r),$$  \hspace{1cm} (2.11)

where $w_j(r)$ is a function localized on the $j$-th lattice site, and $m$ is the atomic mass. $J$ is independent of the lattice indices $j$ and $l$ in a uniform system. Approximating the localized function as the ground state wave function of a harmonic oscillator with frequency $\omega_s$ at the potential minima of the $j$-th site $w_j(r) = \left( \frac{m\omega_s}{\pi \hbar} \right)^{1/4} \exp \left( -\frac{m\omega_s}{2\hbar} (r - r_j)^2 \right)$, one obtains

$$J \sim \left[ \left( \frac{\pi}{4} - \frac{1}{2s^{1/2}} \right) - \frac{1}{2} \left( 1 + e^{-s^{-1/2}} \right) \right] (sE_R)e^{-\pi^2 s^{1/2}/4}. \hspace{1cm} (2.12)$$

Here,

$$e^{-\pi^2 s^{1/2}/4} = \exp \left( -\frac{\pi}{4} \frac{\sqrt{2m(sE_R)}}{\hbar} a \right)$$ \hspace{1cm} (2.13)

can be interpreted as a WKB factor for tunneling in an optical lattice potential which has height $sE_R$ and well width $a$. Note that the height of the lattice potential $sE_R$ and the lattice period $a$ are independent parameters, since the former is determined by the intensity of the laser and the latter is determined by the wave vector of the laser (see Eq. (2.7)). From Eq. (2.13), one finds that, if the height lattice potential $sE_R$ is fixed and the lattice period is increased, $J$ decreases exponentially.

The second term in Eq. (2.10) describes the interaction between atoms when they are at the same site. We assume that atoms can move along $x$ direction in 1D case and in $xy$ plane in 2D case. The on-site interaction $U$ depends on the dimensionality of the optical lattice. $U$ is given by [25]

$$U = g \int dr_\perp |\phi_\perp(r_\perp)|^4 \int dx |w_j(x)|^4, \hspace{1cm} (1D) \hspace{1cm} (2.14)$$

$$= g \int dz |\phi_\parallel(z)|^4 \int dx dy |w_j(x, y)|^4, \hspace{1cm} (2D) \hspace{1cm} (2.15)$$

$$= g \int dr |w_j(r)|^4, \hspace{1cm} (3D) \hspace{1cm} (2.16)$$

where $g = 4\pi\hbar^2 a_0/m$ and $a_0$ is the s-wave scattering length. $\phi_\perp(r_\perp) = (\frac{m\omega_\perp}{\pi \hbar})^{1/2} \exp \left( -\frac{m\omega_\perp}{2\hbar} r_\perp^2 \right)$ and $\phi_\parallel(z) = (\frac{m\omega_\parallel}{\pi \hbar})^{1/4} \exp \left( -\frac{m\omega_\parallel}{2\hbar} z^2 \right)$ are the ground state wave functions of the harmonic
2.3. BLOCH-BOGOLIUBOV EXCITATION

trap with the frequencies $\omega_\perp$ and $\omega_\parallel$ in one and two dimensional cases. Approximating the localized function $w_j$ as a simple Gaussian, one obtains [25]

$$\frac{U}{E_R} \sim \frac{g}{(2\pi)^{3/2}a^2 l} = \frac{2^{3/2}a_0 a^2}{\pi^{3/2}a^2 \frac{3}{8}}, \quad (1D) \quad (2.17)$$

$$\sim \frac{g}{(2\pi)^{3/2}a^2 l^2} = \frac{2^{3/2}a_0}{\pi^{1/2}a^2} \frac{1}{8}, \quad (2D) \quad (2.18)$$

$$\sim \frac{g}{(2\pi)^{3/2}l^3} = \frac{2^{3/2}\pi^{1/2}a_0}{a} \frac{3}{8}, \quad (3D) \quad (2.19)$$

where $l = \sqrt{\hbar/m\omega}$, $a_\perp = \sqrt{\hbar/m\omega_\perp}$, and $a_\parallel = \sqrt{\hbar/m\omega_\parallel}$ are the width of the Gaussian wave functions of the harmonic well potential and confining potential.

Although the Bose-Hubbard model Eq. (2.10) has been studied in other systems for the last two decades [65, 66], the great advantage of an optical lattice is that one can change the ratio between the hopping matrix element $J$ and the on-site interaction $U$ by the intensity of the laser beam. Therefore, one can study the Bose-Hubbard model in a wide range of parameter regime in a single experiment. It was emphasized by Jaksch for the first time in Ref. [25].

2.3 Bloch-Bogoliubov excitation

Since our major interest in this chapter is in the condensate excitations, it is important to make a clear distinction at the outset between (a) The Bloch-Bogoliubov excitations associated with linearized fluctuations of an equilibrium Bose condensate and (b) The stationary states of the time-independent Gross-Pitaevskii equation for the Bose order parameter. In a continuum model, the latter states can be described by the eigenfunction (we use a 1D system for illustration)

$$\Phi_0^0(x) = e^{ikx}u_k(x), \quad (2.20)$$

where the condensate Bloch function satisfies the usual periodicity condition $u_k(x) = u_k(x + na)$, where $n$ is an integer. Physically, $\Phi_k^0(x)$ corresponds to a solution of the Gross-Pitaevskii equation with a superfluid flow in the periodic potential with the condensate quasi-momentum $k$. Recent theoretical literature (see, for example, Refs. [31], [32]) has reported extensive studies of such condensate Bloch states, including their energy band structure and stability. The former question (a) can be studied by considering the dynamic fluctuations $\delta \Phi_k(x, q)$ around the equilibrium state $\Phi_0^0(x)$, with the generalized Bogoliubov
excitation energy $E_q(k)$. These excitations are also described by a quasi-momentum $q$ in the first Brillouin zone and will be referred to as the Bloch-Bogoliubov excitations of the optical lattice. The thermal cloud of non-condensate atoms which is present at finite temperatures is described as a gas of these Bloch-Bogoliubov excitations. As emphasized in the literature [56], one must not confuse the energy bands of these Bloch-Bogoliubov excitations $E_q(k)$ with the condensate energy bands or Bloch eigenstates described by Eq. (2.20). That is, we must distinguish between the condensate energy band and excitation energy band. In our tight-binding model, the analogue of Eq. (2.20) is

$$\Phi_0^0(l) = e^{ikla} \sqrt{n^c(k)}, \quad (2.21)$$

where $l$ is an integer. While one could generalize our analysis, we only consider the Bose condensate in the $k = 0$ Bloch state, in which case Eq. (2.21) reduces to

$$\Phi_{k=0}^0(l) = \sqrt{n^c0}.$$  \quad (2.22)

Here $n^c0$ gives the number of condensate atoms trapped in each well of the optical lattice.

The Bose-Hubbard model Eq. (2.10) has been used for describing the superfluid-Mott insulator transition [25]. In this chapter, in order to investigate the collective excitations of a Bose condensate in an optical lattice, we restrict ourselves to the superfluid solutions of Eq. (2.10). We start with the Heisenberg equation of motion for $a_j(t)$ (we set $\hbar = 1$ from now on),

$$i \frac{d}{dt} a_j(t) = [a_j(t), H] = -J \sum_{\langle lj \rangle} a_l(t) + U a_j^\dagger(t) a_j(t) a_j(t), \quad (2.23)$$

where $\langle l \rangle$ means that $l$ runs over the nearest neighbor sites of site $j$. In the presence of Bose condensation, we can write

$$a_j(t) = \Phi_j(t) + \tilde{\psi}_j(t), \quad \Phi_j(t) = \langle a_j(t) \rangle, \quad (2.24)$$

where the angular bracket with an operator inside means to take an average with respect to a broken symmetry nonequilibrium ensemble. $\Phi_j$ is the condensate wave function at site $j$, and $\tilde{\psi}_j$ is the non-condensate field operator (with $\langle \tilde{\psi}_j \rangle = 0$). This non-condensate operator $\tilde{\psi}_j$ satisfies the usual equal-time Bose commutation relations,

$$[\tilde{\psi}_j, \tilde{\psi}_j^\dagger] = \delta_{jl}, \quad [\tilde{\psi}_j, \tilde{\psi}_l] = [\tilde{\psi}_j^\dagger, \tilde{\psi}_l^\dagger] = 0.$$  \quad (2.26)
The equation for the condensate wave function is obtained by taking an average of the Heisenberg equation Eq. (2.23). We extend recent work to finite temperatures including the effect of the non-condensate atoms. In the present analysis, we restrict ourselves to the Popov approximation [39, 67, 68] which corresponds to neglecting the off-diagonal non-condensate density \( m_j(t) = \langle \hat{\psi}_j(t) \hat{\psi}_j(t) \rangle \). We also neglect the three-field correlation function \( \langle \hat{\psi}_j(t) \hat{\psi}_j(t) \hat{\psi}_j(t) \rangle \) which gives rise to collisional exchange of atoms in the condensate and non-condensate. We are left with a generalized form of the discrete Gross-Pitaevskii equation which includes the mean-field of non-condensate atoms

\[
\frac{i}{\hbar} \frac{d}{dt} \Phi_j(t) = -J \sum_{\langle l \rangle} \Phi_l(t) + U(n^c_j(t) + 2\tilde{n}_j(t))\Phi_j(t).
\]

(2.27)

Here, \( n^c_j(t) \) is the number of condensate atoms on the \( j \)-th lattice site and \( \tilde{n}_j(t) = \langle \hat{\psi}_j(t) \hat{\psi}_j(t) \rangle \) is the number of the non-condensate atoms on the site. The time-dependent Hartree-Fock mean field \( 2U\tilde{n}_j(t) \) arises from the non-condensate atoms. Equation (2.27) reduces to the usual discrete Gross-Pitaevskii equation [24, 29, 39] when all the atoms are assumed to be in the condensate (i.e., if we set \( \tilde{n}_j = 0 \)).

Introducing phase and amplitude variables, \( \Phi_j(t) = \sqrt{n^c_j(t)} e^{i\theta_j(t)} \), Eq. (2.27) is equivalent to

\[
\frac{d n^c_j(t)}{dt} = -2J \sum_{\langle l \rangle} \sqrt{n^c_j(t)n^c_l(t)} \sin(\theta_l(t) - \theta_j(t)),
\]

(2.28)

\[
\frac{d \theta_j(t)}{dt} = J \sum_{\langle l \rangle} \sqrt{\frac{n^c_j(t)}{n^c_l(t)}} \cos(\theta_l(t) - \theta_j(t)) - U(n^c_j(t) + 2\tilde{n}_j(t))
\]

\[
\equiv -\varepsilon^c_j(t).
\]

(2.29)

Equation (2.28) is the continuity equation for the condensate and Eq. (2.29) is the Josephson equation. The energy of a condensate atom \( \varepsilon^c_j(t) \) reduces to the equilibrium chemical potential \( \mu_{c0} \) of the condensate in static thermal equilibrium (\( \theta_j \) is independent of \( t \) and \( j \), \( n^c_j \) and \( \tilde{n}_j \) are independent of \( t \) and \( j \))

\[
\mu_{c0} = -zJ + U(n^{c0}(T) + 2\tilde{n}^0(T)).
\]

(2.30)

Here \( z \) is the number of the nearest neighbor sites. \( n^{c0} \) and \( \tilde{n}^0 \) are the numbers of the condensate and non-condensate atoms per site in equilibrium. The solution of Eq. (2.29) in static equilibrium is given by \( \theta_0(t) = -\mu_{c0} t/\hbar \). From Eq. (2.28), one finds that the Josephson current between the \( j \)-th and \( l \)-th lattice sites is

\[
J_j(t) = 2J \sqrt{n^c_j(t)n^c_l(t)} \sin(\theta_l(t) - \theta_j(t)).
\]

(2.31)
The Bloch-Bogoliubov excitation spectrum for a uniform optical lattice is easily obtained from the above equations [29, 37, 39, 41, 52]. Considering small fluctuations from equilibrium, \( n_j(t) = n^c_0 + \delta n^c_j(t) \), \( \theta_j(t) = \theta_0 + \delta \theta_j(t) \) and \( \tilde{n}_j(t) = \tilde{n}^0 + \delta \tilde{n}_j(t) \), Eqs. (2.28) and (2.29) reduce to
\[
\frac{d\delta n^c_j(t)}{dt} = -2Jn^c_0 \sum_{(l)} (\delta \theta_l(t) - \delta \theta_j(t)),
\]
\[
\frac{d\delta \theta_j(t)}{dt} = \frac{J}{2n^c_0} \sum_{(l)} (\delta n^c_l(t) - \delta n^c_j(t)) - U (\delta n^c_j(t) + 2\delta \tilde{n}_j(t)).
\]

Ignoring the non-condensate atom term \( \tilde{n}_j = \delta \tilde{n}_j = 0 \), the solution of these coupled equations are the normal modes
\[
\delta \theta_j(t) = \delta \theta(q)e^{i(q \cdot r_j - E_q t)}, \quad \delta n^c_j(t) = \delta n^c(q)e^{i(q \cdot r_j - E_q t)}.
\]

The Bloch-Bogoliubov excitation energy in an optical lattice is given by the well-known expression [37, 38, 39]
\[
E_q = \sqrt{\epsilon^0_q (\epsilon^0_q + 2U n^c_0)},
\]
\[
\epsilon^0_q = 4J \sum_{i=1}^d \sin^2 \frac{q_i a}{2}.
\]

For small \( q \), this spectrum is phonon-like \( E_q \simeq cq \), with the phonon velocity
\[
c = \sqrt{2Ja^2Un^c_0} = \sqrt{\frac{Un^c_0}{m^*}},
\]
where \( m^* \equiv 2Ja^2 \) is an effective mass of atoms in the first excitation band of the optical lattice [34, 41, 42]. The linear dispersion of Eq. (2.35) for small \( q \) reflects the superfluidity of Bose condensates in an optical lattice [56]. This \( T = 0 \) excitation spectrum in 1D case is shown in Fig. 2.1 for two values of the dimensionless interaction parameter \( \alpha \equiv Un^c_0/J \).

We call attention to an important feature of the dispersion relation \( E_q \) in Fig. 2.1, considered as a function of the interaction parameter \( \alpha \). For \( \alpha < 6 \), the excitation spectrum \( E_q \) bends up before bending over as, \( q \) approaches the Brillouin zone boundary. This behavior is analogous to the so called “anomalous dispersion” of the phonon spectrum in superfluid \(^4\text{He} \) [69, 70, 71]. For \( \alpha \geq 6 \), in contrast, the spectrum always simply bends
2.4 Popov approximation

In this section, we calculate the condensate fraction $n_0/n$ and the parameter $\alpha \equiv U n_0/J$ as a function of the optical lattice depth $s$ and the temperature.

Substituting $a_j$ by $\Phi_j + \tilde{\psi}_j$ in $K \equiv H - \mu N$, where $N = \sum_j a_j^\dagger a_j$ is the total number

Figure 2.1: The Bloch-Bogoliubov excitation spectrum $E_q$ in a 1D optical lattice plotted as a function of the quasi-momentum $q$ in the first Brillouin zone. The spectrum is plotted for $\alpha < 6$ and $\alpha > 6$. The dotted lines give the low $q$ phonon dispersion relation $E_q = cq$.

over as one leaves the low $q$ (phonon) region. This feature plays a crucial role when we consider damping processes in optical lattices. The excitation spectrum in 2D and 3D optical lattices also exhibit this kind of spectrum. However, the critical value of $\alpha$ depends on the direction of the excitation $q$, since simple square 2D and cubic 3D optical lattices do not have rotational symmetry. The crucial effect of this anomalous dispersion on damping processes will be discussed in Sec. 2.5.
Here, we use the Hartree-Fock-Bogoliubov-Popov approximation [39, 67, 68] which takes into account the third and fourth order terms of $\tilde{\psi}_j$, $\tilde{\psi}^\dagger_j$ within a mean-field approximation, but neglect terms involving the anomalous averages $\langle \tilde{\psi}_j \tilde{\psi}_j \rangle$ and $\langle \tilde{\psi}^\dagger_j \tilde{\psi}_j \tilde{\psi}_j \rangle$, namely we use

\begin{align}
K_3 & \approx 2U \sum_j \tilde{n}_j \left( \Phi_j^* \tilde{\psi}_j + \Phi_j \tilde{\psi}^\dagger_j \right), \\
K_4 & \approx 2U \sum_j \tilde{n}_j \tilde{\psi}^\dagger_j \tilde{\psi}_j. 
\end{align}
Within this approximation, we have

\[ K = K_0 + K_1' + K_2', \]  
\[ K_1' = \sum_j \left[ \left( -J \sum_{\langle l \rangle} \Phi_l - \mu \Phi_j + U(n_j^c + 2\tilde{n}_j)\Phi_j \right) \tilde{\psi}_j^\dagger \right. \]
\[ + \left. \left( -J \sum_{\langle l \rangle} \Phi_l^* - \mu \Phi_j^* + U(n_j^c + 2\tilde{n}_j)\Phi_j^* \right) \tilde{\psi}_j \right], \]  
\[ K_2' = -J \sum_{\langle j,l \rangle} \left( \tilde{\psi}_j^\dagger \tilde{\psi}_l + \tilde{\psi}_l^\dagger \tilde{\psi}_j \right) - \mu \sum_j \tilde{\psi}_j^\dagger \tilde{\psi}_j 
+ \frac{U}{2} \sum_j \left( \Phi_j^2(\tilde{\psi}_j^l)^2 + 4n_j\tilde{\psi}_j^l\tilde{\psi}_j + (\Phi_j^*)^2(\tilde{\psi}_j^l)^2 \right), \]  

where \( n_j \equiv n_j^c + \tilde{n}_j = |\Phi_j|^2 + 2\langle \tilde{\psi}_j^l \tilde{\psi}_j^l \rangle \). The coefficients of the linear terms in \( \tilde{\psi} \) and \( \tilde{\psi}^\dagger \) in Eq. (2.47) identically vanish using the fact that \( \Phi_j \) is a stationary solution of the generalized Gross-Pitaevskii equation Eq. (2.27). As a result, \( K_1' = 0 \). As we discussed in Section 2.3, we consider a Bose condensate in static thermal equilibrium in the \( k = 0 \) Bloch state, and hence \( \Phi_j = \sqrt{n_0^c} \). Using the value of the condensate chemical potential in thermal equilibrium given in Eq. (2.30), the remaining term \( K_2' \) in Eq. (2.48) reduces to

\[ K_2' = -J \sum_{\langle j,l \rangle} \left( \tilde{\psi}_j^l \tilde{\psi}_l + \tilde{\psi}_l^l \tilde{\psi}_j \right) + (zJ + Un_0^c) \sum_j \tilde{\psi}_j^l \tilde{\psi}_j 
+ \frac{U}{2} \sum_j \left( n_0^c(\tilde{\psi}_j^l)^2 + n_0^c(\tilde{\psi}_j^l)^2 \right). \]  

We next introduce Fourier components,

\[ \tilde{\psi}_j = \frac{1}{\sqrt{I_d}} \sum_{q \neq 0} a_q e^{iqr_j}, \]  

where the number of lattice sites in one direction is denoted by \( I \) and hence the total number of sites is \( I_d \). Substituting Eq. (2.50) into Eq. (2.49), one finds

\[ K_2' = \sum_{q \neq 0} (c_q^0 + Un_0^c)a_q^\dagger a_q + \frac{Un_0^c}{2} \sum_{q \neq 0} (a_q^\dagger a_{-q}^\dagger + a_q a_{-q}). \]  

We can diagonalize \( K = K_0 + K_2' \) by a Bogoliubov transformation,

\[ \alpha_q = u_q a_q + v_q a_{-q}^\dagger, \]
\[ \alpha_{-q}^\dagger = v_{-q}^* a_q + u_{-q}^* a_{-q}^\dagger. \]
If we assume that $\alpha_q$ and $\alpha_q^\dagger$ obey the usual Bose commutation relations, we obtain the following conditions for $u_q$ and $v_q$.

$$|u_q|^2 - |v_q|^2 = 1.$$  

(2.53)

From the condition for the diagonalization of $K$, we find that $u_q$ and $v_q$ have to satisfy the following equation,

$$Un^c(\alpha_q^2 + \alpha_q^\dagger) - 2(\alpha_q^0 + Un^c)u_qv_q = 0.$$  

(2.54)

Solving both Eq. (2.53) and Eq. (2.54), one can easily derive the parameters for the Bogoliubov transformation (we take $u_q$ and $v_q$ real),

$$u_q^2 = \frac{1}{2} \left( \frac{\tilde{E}_q}{E_q} + 1 \right), \quad v_q^2 = \frac{1}{2} \left( \frac{\tilde{E}_q}{E_q} - 1 \right),$$  

(2.55)

where $E_q$ is identical to the Bloch-Bogoliubov spectrum given by Eq. (2.35). We have here introduced the Hartree-Fock excitation spectrum

$$\tilde{E}_q \equiv [\epsilon_0(q) + 2U(n^c + \tilde{n}^0)] - \mu_{c0}$$

$$= 4J \sum_i \sin^2\left( \frac{q_i d}{2} \right) + Un^c.$$  

(2.56)

Putting all these results together, we have

$$K = K_0 + \sum_{q \neq 0} \left( \tilde{E}_q v_q^2 - Un^c u_q v_q \right) + \sum_{q \neq 0} E_q \alpha_q^\dagger \alpha_q$$

$$= -\frac{UN_0}{2}(n^c + 4\tilde{n}^0) + \frac{1}{2} \sum_{q \neq 0} \left( E_q - \tilde{E}_q \right) + \sum_{q \neq 0} E_q \alpha_q^\dagger \alpha_q.$$  

(2.57)

Here $N_0 = n^c I^d$ is the total number of condensate atoms. The Bloch-Bogoliubov-Popov excitation spectrum $E_q$ appearing in Eq. (2.57) is identical to Eq. (2.35), except that now $n^c(T)$ is the temperature-dependent number of condensate atoms in any given lattice well. The Bloch-Bogoliubov-Popov excitation spectrum can be obtained by ignoring the non-condensate fluctuation ($\delta n_j = 0$) but keeping the temperature-dependent number of condensate atoms $n^c(T)$ as given by Eq. (2.32) and Eq. (2.33). We thus assume that the thermal cloud is always in static equilibrium, when dealing with the time-dependent density fluctuations $\delta n_j^c(t)$ of the condensate. Our assumption is based on the experimental report Ref. [35] where a static thermal cloud was observed in an optical lattice.
In the following, we call Bloch-Bogoliubov-Popov excitation simply as Boch-Bogoliubov excitation.

It is easy to verify that $E_q$ in Eq. (2.35) reduces to the Hartree-Fock energy $\tilde{E}_q$ in the limit $J \gg U n^0$, i.e., when $\alpha \ll 1$. This Hartree-Fock limit corresponds to setting the Bogoliubov amplitudes $u^2_q = 1$, $v^2_q = 0$ in Eq. (2.55). In dealing with Bose gases trapped in harmonic potentials, one can always use this Hartree-Fock approximation [72] for the excitations describing the thermal cloud as long as the kinetic energy of the atoms ($\sim k_B T$) is much larger than the interaction energy ($U n^0$). In contrast, apart from the limiting case of $\alpha \ll 1$, we must always use the full Bogoliubov spectrum $E_q$ to describe the thermal cloud composed of excitations in the first band of an optical lattice.

Expressing $\tilde{n}^0(T)$ in terms of these Bloch-Bogoliubov-Popov excitations, we have

$$n = n^0 + \frac{1}{I_d} \sum_{q \neq 0} \langle a_q^\dagger a_q \rangle = n^0 + \frac{1}{I_d} \sum_{q \neq 0} \left[ (u^2_q + v^2_q) f^0(E_q) + v^2_q \right], \tag{2.58}$$

where the number of lattice sites in one direction is $I$ and $f^0(E_q) = \left[ \exp(\beta E_q) - 1 \right]^{-1}$ is the usual Bose distribution function. The number of condensate atoms $n^0$ at a site is found by solving Eq. (2.58) self-consistently for a fixed value of the total number of atoms per site $n$. The condensate fraction $n^0/n$ in a $d$-dimensional optical lattice is shown in Fig. 2.2. We take $n = 2$ and use the parameters from Ref. [44]. The spurious finite jump in the condensate atom number $n^0$ at the transition temperature $T_c$ is an inherent problem of the Bogoliubov theory in a uniform gas (see, for example, Ref. [73]).

Strictly speaking, there are no solutions of Eq. (2.58) at finite temperature for an infinite optical lattice in 1D and 2D because of the divergent contribution from excitations with small momentum, in accordance with the well-known Mermin-Wagner-Hohenberg theorem [74]. However, for the finite systems discussed in this chapter, this divergence is removed. That is, Eq. (2.58) has a solution describing a finite value of the condensate $n^0(T)$ below $T_c$.

In Fig. 2.3, we plot the parameter $\alpha = U n^0/J$ as a function of the temperature for several values of the optical depth $s$. The parameter $\alpha$ and the results in Fig. 2.3 will play an important role in the discussion of the damping of condensate excitations. Since we limit our discussion to the first energy band of the optical lattice, our results only apply when $\mu, k_B T \ll \frac{s E_R}{2}$. Higher excitation bands would be thermally populated and would have to be considered if we consider lower values of $s$.

The phonon velocity $c = \sqrt{2Ja^2U n^0}$ depends on the optical depth $s$ and the temperature through $J(s)$, $U(s)$, and $n^0(s, T)$. Figure 2.4 shows the phonon velocity as a
Figure 2.2: The condensate fraction \( \frac{n^c}{n} \) in \( d \)-dimensional optical lattice as a function of temperature. The height of the optical lattice potential (in units of \( E_R \)) is denoted by \( s \).
Figure 2.3: The dimensionless interaction parameter $\alpha = \frac{U n^c(T)}{J}$, plotted as a function of temperature, for several values of the optical well depth $s$. The number of condensate atoms at a lattice site $n^c(T)$ is given in Fig. 2.2. The dashed line shows the critical value $\alpha_c = 6d$ above which there is no damping, where $d$ is the dimension of the optical lattice.
function of $s$ at $T = 0$. It decreases exponentially as $s$ increases reflecting the change of $J(s)$. The phonon velocity is normalized by the recoil velocity defined by $v_R \equiv \frac{k}{m}$.

![Figure 2.4: The phonon velocity of Bloch-Bogolubov excitation as a function of the optical height $s$ at $T = 0$. $v_R$ is the recoil velocity $k/m$.](image)

2.5 Damping of condensate excitations

In this section, we discuss damping of condensate excitations in an optical lattice. In Sec. 2.5.1, we derive a formal expression for the damping of Bloch-Bogoliubov excitations using the thermal Green’s function formalism. In Sec. 2.5.2, we use this expression to calculate the Landau damping of Bloch-Bogoliubov excitations in a 1D lattice. Section 2.5.3 extends this analysis to 2D and 3D optical lattices. In Sec. 2.5.4, we discuss the Beliaev damping in a 1D lattice.

2.5.1 Green’s function technique

In this section, we take $K_B \equiv K_0 + K_1 + K_2$ in Eq. (2.43) as the bare zeroth-order Hamiltonian and treat $K_3$ as a perturbation. We use the simplest Bogoliubov theory to diagonalize $K_B$ [38]. We neglect the fourth order term in the fluctuation $K_4$. The chemical potential for $K_B$ is given by $\mu_{B0} = -zJ + Un^c_0$ (from the condition $K_1 = 0$). $K_2$ can
be diagonalized by the Bogoliubov transformation Eq. (2.52) and one obtains the same expression as Eq. (2.57).

Using Eq. (2.50) and Eq. (2.52), $K_3$ can be re-written in terms of the Bogoliubov quasiparticles

\[
K_3 = \frac{1}{2} \sum_{p_1,p_2,p_3 \neq 0} M_{p_1,p_2,p_3} \left( \alpha_{p_3}^\dagger \alpha_{p_1} \alpha_{p_2} + \alpha_{p_2}^\dagger \alpha_{p_1} \alpha_{p_3} \right)
\]

\[
+ \sum_{p_1,p_2,p_3 \neq 0} L_{p_1,p_2,p_3} \left( \alpha_{p_3}^\dagger \alpha_{p_1}^\dagger \alpha_{p_2} - \alpha_{p_1} \alpha_{p_2} \alpha_{p_3} \right),
\]

\[
(2.59)
\]

where $G$ is a reciprocal lattice vector. The Kronecker delta $\delta_{p_1+p_2+p_3+G}$ expresses the conservation of quasi-momentum of the three excitation scattering processes (Umklapp processes are associated with $G \neq 0$).

The thermal Green’s function is defined by (see e.g., [75])

\[
G_q(\tau_1 - \tau_2) \equiv -\langle T\tau \left( \alpha_q(\tau_1) \alpha_{q}^\dagger(\tau_2) \right) \rangle,
\]

\[
(2.62)
\]

where

\[
\alpha_q(\tau) \equiv e^{K\tau} \alpha_q e^{-K\tau}, \quad \alpha_{q}^\dagger(\tau) \equiv e^{K\tau} \alpha_{q}^\dagger e^{-K\tau}.
\]

\[
(2.63)
\]

The angular bracket $\langle \ldots \rangle$ indicates to take an average for thermal equilibrium and $T$ means the usual time ordered product of operators. Fourier transformation of this imaginary time Green’s function is given by

\[
G_q(\tau) = \frac{1}{\beta} \sum_{\omega_n} G_q(i\omega_n) e^{-i\omega_n \tau},
\]

\[
(2.64)
\]

where $\omega_n$ is the boson Matsubara frequency $\omega_n \equiv \frac{2n\pi}{\beta}$ ($n$ is an integer), and the momentum sum is taken over the first Brillouin zone of the optical lattice. The zero-th order Green’s function is given by

\[
G^0_q(i\omega_n) = \frac{1}{i\omega_n - E_q},
\]

\[
(2.65)
\]
where $E_q$ is the Bloch-Bogoliubov excitation energy given in Eq. (2.35).

The second-order self-energy terms are given by the usual diagrams in Fig. 2.5. Figure 2.5 (a) describes a condensate excitation of (quasi) momentum $\mathbf{q}$ being absorbed by an excitation $\mathbf{p}_2$ of the optical lattice thermal gas, lending to a thermal excitation with momentum $\mathbf{p}_1$, which is the Landau damping process [76, 77]. Figure 2.5 (b) describes a condensate excitation of momentum $\mathbf{q}$ decaying into two excitations with momentums $\mathbf{p}_1$ and $\mathbf{p}_2$, which is the Beliaev damping process [56, 69]. These diagrams give the second-order self-energy of the Bogoliubov excitation

$$
\Sigma^L_q(i\omega_n) = \Sigma^L_q(i\omega_n) + \Sigma^B_q(i\omega_n),
$$

$$
\Sigma^L_q(i\omega_n) = -\frac{1}{\beta} \sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{q}, \mathbf{p}_2; \mathbf{p}_1}|^2 G^0_{\mathbf{p}_1}(i\omega_l) G^0_{\mathbf{p}_2}(i\omega_l - i\omega_n),
$$

$$
\Sigma^B_q(i\omega_n) = -\frac{1}{2\beta} \sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{p}_1, \mathbf{p}_2; \mathbf{q}}|^2 G^0_{\mathbf{p}_1}(i\omega_l) G^0_{\mathbf{p}_2}(i\omega_n - i\omega_l). \tag{2.66}
$$

The summation over Matsubara frequencies is calculated by the well-known formula (see Ref. [75])

$$
\sum_{\omega_n} g(\omega_n) = -\frac{\beta}{2\pi i} \oint_C dz g(z) f^0(z), \tag{2.67}
$$

where $f^0(z)$ is the Bose distribution function and the contour encircles the poles of $g(z)$. Using Eq. (2.67), we obtain

$$
\Sigma^L_q(i\omega_n) = -\sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{q}, \mathbf{p}_2; \mathbf{p}_1}|^2 \frac{f^0(E_{\mathbf{p}_1}) - f^0(E_{\mathbf{p}_2})}{i\omega_n - (E_{\mathbf{p}_1} - E_{\mathbf{p}_2})}, \tag{2.68}
$$

$$
\Sigma^B_q(i\omega_n) = -\frac{1}{2} \sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{p}_1, \mathbf{p}_2; \mathbf{q}}|^2 \frac{1 + f^0(E_{\mathbf{p}_1}) + f^0(E_{\mathbf{p}_2})}{i\omega_n - E_{\mathbf{p}_1} - E_{\mathbf{p}_2}}. \tag{2.69}
$$

The damping of excitations is given by the imaginary part of the self-energy

$$
\Gamma_q = -\text{Im} \Sigma_q(E_q + i\delta), \tag{2.70}
$$

where the limit $\delta \to +0$ is understood. This gives the damping of Bogoliubov excitations in an optical lattice,

$$
\Gamma_q = \Gamma^L_q + \Gamma^B_q, \tag{2.71}
$$

$$
\Gamma^L_q = \pi \sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{q}, \mathbf{p}_2; \mathbf{p}_1}|^2 [f^0(E_{\mathbf{p}_2}) - f^0(E_{\mathbf{p}_1})] \delta(E_q - E_{\mathbf{p}_1} + E_{\mathbf{p}_2}), \tag{2.72}
$$

$$
\Gamma^B_q = \frac{\pi}{2} \sum_{\mathbf{p}_1, \mathbf{p}_2 \neq 0} |M_{\mathbf{p}_1, \mathbf{p}_2; \mathbf{q}}|^2 [1 + f^0(E_{\mathbf{p}_1}) + f^0(E_{\mathbf{p}_2})] \delta(E_q - E_{\mathbf{p}_1} - E_{\mathbf{p}_2}). \tag{2.73}
$$
The Landau damping $\Gamma^L_q$ is expected to be dominant at higher temperatures where there are thermally excited quasiparticles. In contrast, the Beliaev damping $\Gamma^B_q$ is due to a decay process and can arise in the absence of thermally-excited excitations. The Beliaev damping is possible even at $T = 0$ [i.e., $f^0(E_p) = 0$] and is expected to be dominant at low temperatures.

2.5.2 Landau damping in a 1D optical lattice

In this subsection, we calculate the Landau damping in an optical lattice. First of all, we consider the case for a 1D optical lattice.

The energy conservation condition $E_q + E_p = E_{q+p+G} = E_{q+p}$ in Eq. (2.72) needs to be satisfied for the Landau damping to occur. To find a solution of the energy conservation condition, we follow the graphical method in Ref. [78]. The solution of the energy conservation condition $E_q + E_p = E_{q+p}$ for the 1D optical lattice is illustrated in Fig. 2.6.
Figure 2.6: The Bloch-Bogoliubov excitation energy $E_q$ in a 1D optical lattice for $\alpha < 6$. The intersection of the two dispersion curves at $p + q$ is the place where the energy conservation condition is satisfied.

[78]. First, we draw an excitation spectrum and mark $q$ on the line. Then we draw the spectrum line again with $q$ as an origin. If those two lines intersect, solutions consistent with the energy conservation condition for three-excitation process exist. The intersection can be taken as $(q + p, E_q + E_p = E_{q+p})$. Clearly, the condition for these two dispersion curves to have intersections requires that the dispersion relation $E_q$ first bends up as $q$ increases, before bending over. From Fig. 2.1, we see that the dispersion relation $E_q$ has this feature only for $\alpha < 6$. We conclude that the Landau damping of excitations can occur only when $\alpha < 6$. If the intersection $(q + p, E_q + E_p)$ is outside of the first Brillouin zone, it has to be reduced in the first Brillouin zone by subtracting a reciprocal lattice vector $G_n = \frac{2\pi n}{a}$ (n is an integer), corresponding to an Umklapp process [78].

Figure 2.3 shows that $\alpha$ increases as $s$ increases at low temperatures. We can expect the sudden disappearance of the damping for $3 < s < 3.5$ when $k_B T \approx 0.02E_R$. For fixed $s$, $\alpha$ decreases as the temperature increases, since the number of condensate atoms $n^{c0}(T)$ decreases. If $\alpha > 6$ at low temperatures, one can observe the sudden appearance of the damping when $T$ is close to $T_c$.

The values of $(q, p)$ satisfying the energy conservation condition for 1D optical lattice are shown in Fig. 2.7. For a given value of $q$, we see that as $\alpha \to 6$, the value of $p$ decreases to zero. There is no solution for $\alpha > 6$, indicating the disappearance of the damping for an excitation $E_q$ with any value of $q$. In Fig. 2.7, the curves of the solution
of the energy conservation condition never go across the dashed line $q + p = \pi / a$. Thus Umklapp scattering processes ($G_n \neq 0$) do not contribute to Landau damping in our present single band model.

![Figure 2.7: The values $(q, p)$ satisfying the energy conservation condition $E_q + E_p = E_{q+p}$, for several values of the interaction parameter $\alpha$.](image)

When the excitation $q$ has a wavelength much larger than the thermal excitation $p$ (i.e., when $q \ll p, \pi / a$), one finds $\frac{dE_p}{dp} = c$ from the energy conservation condition $E_q + E_p = E_{q+p}$ in Eq. (2.72) where $c$ is the phonon velocity in Eq. (2.37). The Landau damping of the excitation $E_q = cq$ comes from absorbing a thermal excitation $E_p$ with a group velocity equal to the phonon velocity $c$ [77]. From $\frac{dE_p}{dp} = c$,

$$\frac{dE_p}{dp} = 4Ja \left( \frac{E_p}{E_q} \right) \sin \frac{pa}{2} \cos \frac{pa}{2}$$

$$= c$$

$$= \sqrt{2Ja^2 Un^c}. \quad (2.74)$$

Eq. (2.74) reduces to

$$16X^2 + 8(\alpha - 2)X + (\alpha^2 - 6\alpha) = 0, \quad (2.75)$$
CHAPTER 2. CONDENSATE EXCITATIONS IN OPTICAL LATTICES

where $X \equiv \sin^2 \frac{pa}{2}$. The unique value of $p_0$ such that $\frac{dE_p}{dp_0} = c$ is found to be given by the condition

$$\sin^2 \left( \frac{p_0 a}{2} \right) = -\frac{1}{4}(\alpha - 2) + \sqrt{\frac{1}{4}(\alpha + 2)}.$$  

This expression is only valid for $\alpha$ smaller than 6, such that $p_0 \gg q$.

For $q \ll p$, by using the following approximations,

$$u_q \simeq \sqrt{\frac{U n^{c_0}}{2cp}} \left( 1 + \frac{cp}{2U n^{c_0}} \right),$$
$$v_q \simeq \sqrt{\frac{U n^{c_0}}{2cp}} \left( 1 - \frac{cp}{2U n^{c_0}} \right),$$

$$u_{q+p} \simeq u_p - \frac{J \sin(pa) (U n^{c_0})^2}{2u_p} \frac{E_p}{E_p^3} qd,$$
$$v_{q+p} \simeq v_p - \frac{J \sin(pa) (U n^{c_0})^2}{2v_p} \frac{E_p}{E_p^3} qd,$$

the matrix element in Eq. (2.72) reduces to

$$M_{q,p+q+p} \approx 2U \sqrt{\frac{n^{c_0}}{I}} \left[ (u_p u_{q+p} + v_p v_{q+p} - v_p u_{q+p} - u_p v_{q+p} - u_p v_{q+p}) u_q - (u_p u_{q+p} + v_p v_{q+p} - u_p v_{q+p}) v_q \right]$$

$$\simeq 2U \sqrt{\frac{n^{c_0}}{I}} \left( \frac{E_p^0}{E_p} + \frac{U n^{c_0}}{2E_p} - \frac{(U n^{c_0})^2 J a}{c \sin pa} \right) \sqrt{\frac{c q}{2U n^{c_0}}}.$$  

From the energy conservation condition

$$c = \frac{dE_p}{dp} = \frac{\tilde{E}_p}{E_p} 2Ja \sin pa,$$

one finds (the analogue of Eq. (10.76) in Ref. [77])

$$M_{q,p+q+p} = U \left( \frac{E_p^0}{E_p} + \frac{E_p}{E_p^3} \right) \left( \frac{q}{2m^*c} \right)^{1/2} N_{c_0}^{1/2} \frac{N_{c_0}^{1/2}}{I},$$

where $N_{c_0} = n^{c_0}I$. Using the delta function for energy conservation to integrate over $p$, the Landau damping is given by

$$\Gamma_q = \frac{\alpha}{8(\alpha + 2)} \left( \frac{E_{p_0}}{E_p^0} \right)^3 \left( \frac{E_p^0}{E_{p_0}} + \frac{E_{p_0}}{E_p} \right)^2 \frac{\beta J U q a}{\sinh^2 \frac{\beta E_{p_0}}{2}}.$$  

(2.84)
2.5. DAMPING OF CONDENSATE EXCITATIONS

One finds that $\Gamma_q$ diverges at $\alpha = 6$, because $p_0 \to 0$ as $\alpha \to 6$ (see Eq. (2.76)). The expression of the Landau damping Eq. (2.72) obtained from the lowest order perturbation breaks down when $E_q \lesssim \Gamma_q$ for $\alpha \lesssim 6$. We need to take into account the finite linewidth of the spectrum $E_q$ by considering higher order processes [79]. The calculation of the Landau damping when $\alpha \sim 6$ with higher order perturbation remains as a future work.

2.5.3 Landau damping in 2D and 3D optical lattices

Next, we discuss the energy conservation condition of three-excitation process in a 2D optical lattice. In order to investigate the solution of the energy conservation condition, we imagine a surface in a three dimensional space which satisfies the Bloch-Bogoliubov dispersion relation $(q_x, q_y, E_q)$. Then, we draw a new dispersion $E_q$ in the three dimensional space, with a point on the surface $(q_1x, q_1y, E_{q_1})$ as an origin. That is, we draw a surface $(q_x, q_y, E_{q-q_1} + E_{q_1})$. If those two surfaces intersect, the energy conservation condition $E_{q_1} + E_{q_2} = E_{q_1+q_2}$ is satisfied, the intersection being given by $(q_1 + q_2x, q_1 + q_2y, E_{q_1+q_2})$. For this condition to be satisfied, the surface $(q_x, q_y, E_q)$ has to be above the other surface $(q_x, q_y, E_{q-q_1} + E_{q_1})$ around $(q_{1x}, q_{1y}, E_{q_1})$. Since the Bloch-Bogoliubov spectrum is phonon like $E_q \simeq cq$ for small $q$, the maximum gradient of $E_q$ at $(q_{1x}, q_{1y}, E_{q_1})$ must be greater than $c$. Since $|\nabla_q E_q|_{q=q_1}$ is the maximum gradient of $E_q$ at $q_1$, this condition is equivalent to the requirement

$$|\nabla_q E_q|_{q=q_1} = 2Ja \frac{E_{q_1}}{E_{q_1}} \sqrt{\sin^2 q_{1x}a + \sin^2 q_{1y}a} > c.$$  \hspace{1cm} (2.85)

Eq. (2.85) is the 2D version of the condition for the Bloch-Bogoliubov spectrum of a 1D optical lattice to have anomalous dispersion. If Eq. (2.85) is satisfied, a solution of the energy conservation condition $E_{q_1} + E_{q_2} = E_{q_1+q_2}$ exists. An excitation $E_{q_1}$ can then decay into $E_{q_1+q_2}$ by absorbing $E_{q_2}$ (Landau), or an excitation $E_{q_1+q_2}$ can decay into two excitations $E_{q_1}$ and $E_{q_2}$ (Beliaev).

The condition for such a $q_1$ to exist is that the maximum value of $|\nabla_q E_q|$ as a function of $(q_x, q_y)$ is greater than $c$. Owing to $|\nabla_q E_q|_{q=0} = c$, we only need to consider the condition that $|\nabla_q E_q|$ takes its maximum at $q \neq 0$. When $|\nabla_q E_q|$ has its maximum
value,
\[
|\nabla q E_q| = \frac{2Ja^2 \sin q_x a}{\sqrt{\sin^2 q_x a + \sin^2 q_y a}} \times \left( \frac{\hat{E}_q}{E_q} \begin{pmatrix} \cos q_x a \\ \cos q_y a \end{pmatrix} - \frac{2JU^2(n_c^0)^2}{E_q^3} (\sin^2 q_x a + \sin^2 q_y a) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right)
\]
\[
= 0. \tag{2.86}
\]

From Eq. (2.86), \(|\nabla q E_q|\) has its maximum value when \(\cos q_x a = \cos q_y a\), i.e., \(q_x = \pm q_y\). If we assume \(q_x = q_y\), Eq. (2.86) reduces to
\[
\sin^2 q_x a = \frac{-(3\alpha - 4) + \sqrt{5\alpha^2 + 24\alpha + 16}}{16}. \tag{2.87}
\]

From Eq. (2.87), one sees that \(\sin^2 q_x a\) decreases as \(\alpha\) increases, vanishing when \(\alpha = 12\). Therefore, we conclude that the Landau damping when \(\alpha = 12\) is due to excitations with momentum \(q_x = \pm q_y\) and all damping processes in a 2D optical lattice will vanish when \(\alpha > 12\). Figure 2.3 shows that the disappearance of the damping can be observed in a 2D optical lattice for \(s = 5 \sim 6\). This analytical result is confirmed by numerically solving the energy conservation condition.

The condition for the disappearance of damping in a 3D optical lattice can be derived by generalizing the procedure described above for a 2D optical lattice. One sees that \(|\nabla q E_q|\) has its maximum when \(\cos q_x a = \cos q_y a = \cos q_z a\), i.e., \(q_x = \pm q_y = \pm q_z\) and
\[
\sin^2 q_x a = \frac{-3(\alpha - 2) + \sqrt{5\alpha^2 + 36\alpha + 36}}{24}. \tag{2.88}
\]

One finds that \(\sin^2 q_x a \to 0\) when \(\alpha \to 18\), and damping in a 3D optical lattice vanishes when \(\alpha \geq 18\). As for the 1D and 2D cases, Fig. 2.3 shows that this prediction can be checked for \(s = 7 \sim 9\). As in the 2D case, Landau damping when \(\alpha = 18\) only occurs for an excitation with momentum \(q_x = \pm q_y = \pm q_z\).

We next calculate the Landau damping in Eq. (2.72) for a 2D optical lattice. We consider the damping of long wavelength phonon \(q\). By using the approximation for the long wavelength phonon \(E_q \sim cq\) and \(E_{q+p} \sim E_q + \nabla_p E_p \cdot q\), the energy conservation condition \(E_q + E_q = E_{q+p}\) can be written as
\[
\frac{\alpha}{2} \left( q_x^2 + q_y^2 \right) = \frac{F_p^2}{E_p} \left( \sin^2(p_x a) q_x^2 + 2 \sin(p_x a) \sin(p_y a) q_x q_y + \sin^2(p_y a) q_y^2 \right). \tag{2.89}
\]
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Figure 2.8: The solution of the energy conservation condition $E_q + E_p = E_{q+p}$ for a 2D optical lattice, with $q_x > 0$ and $q_y = 0$. $p_0$ is defined in Eq. (2.76) and we note $p_0 \to 0$ as $\alpha \to 6$.

When $q_x > 0$ and $q_y = 0$, Eq. (2.89) can be solved easily. Defining $X \equiv \sin^2 \frac{p_x a}{2}$ and $Y \equiv \sin^2 \frac{p_y a}{2}$, the solution of Eq. (2.89) is

$$Y = - \left( X + \frac{\alpha}{4} \right) + \frac{1}{4} \sqrt{\frac{\alpha^3}{8X^2 - 8X + \alpha}}.$$  

One can confirm that Eq. (2.90) reduces to Eq. (2.76) when $Y = 0$.

Equation (2.90) is plotted in Fig. 2.8 for several values of $\alpha$. We see that as $\alpha \to 6$ the line in the $(p_x, p_y)$ plane which satisfies the energy conservation condition shrinks and vanishes when $\alpha > 6$. Therefore, the Landau damping of an excitation with $q_y = 0$ disappears when $\alpha > 6$. $p_0$ in Fig. 2.8 is given by Eq. (2.76).

For a long wavelength phonon $q$ with $q_x = q_y > 0$, we solve the energy conservation condition numerically. The solution is shown in Fig. 2.9. There is no solution when $\alpha > 12$ as we expected. Figures 2.8 and 2.9 clearly show that the threshold value of $\alpha$ for the disappearance of damping strongly depends on the direction of $q$ due to the anisotropy of 2D square lattice. This result also holds for 3D square lattice. As for the 1D case, $\Gamma_q$ becomes larger than $E_q$ around the threshold value of $\alpha$ in 2D and 3D cases. We cannot use the expression of the Landau damping Eq. (2.72) and have to extend it
2.5.4 Beliaev damping in a 1D optical lattice

We discuss the Beliaev damping of the Bloch-Bogoliubov excitation in this subsection. The Beliaev damping is due to spontaneous decay of an excitation into two excitations. This decay process needs to satisfy the energy conservation condition $E_q = E_{q-p} + E_p$. We focus on a 1D case in the following.

In Fig. 2.10, the solution of the energy conservation condition for 1D optical lattice $E_q = E_{q-p} + E_p$ is shown in a $(q, p)$ plane. As predicted in Subsection 2.5.2, one finds that the curve of the solution shrinks as $\alpha$ increases and vanishes when $\alpha > 6$, which indicates the disappearance of the Beliaev damping for $\alpha > 6$.

For a fixed value of $\alpha < 6$, we see that the Beliaev damping is possible only when $q$ is between the threshold momenta $q_0$ and $q_c$. At the threshold momenta $q_0$ and $q_c$, two excitations $E_q$ and $E_{q-p}$ created by the decay of an excitation $E_q$ have the same velocity, which was first pointed out by Pitaevskii for the phonon excitation of superfluid $^4$He.
Two excitations have the same quasi-momentum \( q_c/2 \) and energy \( E_{q_c/2} \) at \( q = q_c \). At \( q = q_0 \), one of the generated excitations is a phonon having the sound velocity \( c \). Therefore, the other one also has the velocity equal to the sound velocity \( c \).

In addition to Landau damping and Beliaev damping, one also has intercollisional damping arising from two body collisions which transfer atoms between the condensate and thermal cloud at finite temperatures [72, 80]. This process also involves the energy conservation condition for three-excitation process. Thus, the intercollisional damping also disappears when \( \alpha \geq 6d \) in a \( d \)-dimensional optical lattice.

![Figure 2.10: The solution of the energy conservation condition \( E_q = E_p + E_{q-p} \) for Beliaev damping in a 1D optical lattice.](image)

### 2.6 Perturbation theory for a weak lattice potential

We deal with a condensate in a weak optical lattice potential in this section. One can gain more substantial picture of Bloch-Bogoliubov excitation by considering condensates in a weak optical lattice. In this regime, the tight binding approximation is not valid, since the wave function on each site is not well localized.

We discuss a condensate at \( T = 0 \) within the Gross-Pitaevskii mean-field theory [56]. The depletion of the condensate increases as the depth of the optical lattice increases, and
the superfluid-Mott insulator transition arises at a critical value of the lattice strength. If a large number of atoms are trapped in each lattice site, the transition to the Mott insulator phase is expected to take place for very large intensity of the lattice strength, and there is a wide range of parameter region where the effect of the depletion can be neglected and the Gross-Pitaevskii mean-field theory is valid. In current experiments of elongated condensate loaded in a 1D optical lattice [21, 22, 33], the number of atoms per lattice site is of the order of thousand. We apply our theory to these experiments. We restrict ourselves to a 1D case, but the theory we present in this section can be extended to 2D and 3D optical lattices.

The order parameter of a Bose condensate in static equilibrium $\Phi_0(x)$ obeys the time-independent Gross-Pitaevskii equation,

$$\left(-\frac{1}{2m} \frac{d^2}{dx^2} + V_{\text{op}}(x)\right) \Phi_0(x) + g|\Phi_0(x)|^2 \Phi_0(x) = \mu \Phi_0(x). \tag{2.91}$$

For convenience, we use a different definition of an optical lattice potential $V_{\text{op}}(x)$ from the form used in the previous sections. Here, $V_{\text{op}}(x)$ is defined as

$$V_{\text{op}}(x) = V_0 \cos Gx, \tag{2.92}$$

where $G = \frac{2\pi}{a}$ is a reciprocal lattice vector, and $a$ is a lattice constant. The order parameter is normalized in a unit cell of the optical lattice as

$$\int_0^a dx |\Phi_0(x)|^2 = n_c, \tag{2.93}$$

where $n_c$ is the number of condensate atoms per site.

We use the Thomas-Fermi approximation for the Gross-Pitaevskii equation [36, 42]. Neglecting the kinetic energy term in Eq. (2.91), one obtains

$$n_0(x) = |\Phi_0(x)|^2 = \frac{1}{g} (\mu - V_{\text{op}}(x)). \tag{2.94}$$

The Thomas-Fermi approximation is valid when the density varies in space on a length scale much larger than the healing length [42]. From Eq. (2.93), the chemical potential is given by $\mu = \frac{gn_c}{a}$.

The collective excitation of a Bose condensate corresponds to the fluctuation of the order parameter $\Phi(x,t)$ around the stationary solution of Eq. (2.91),

$$\delta \Phi(x,t) = e^{-i\mu t} \sum_j \left( u_j(x)e^{-i\omega_j t} - v_j(x)^*e^{i\omega_j t} \right), \tag{2.95}$$
2.6. PERTURBATION THEORY FOR A WEAK LATTICE POTENTIAL

where \( \omega_j \) is the energy of the excitation in an eigenstate labeled by \( j \). \( u_j(x) \) and \( v_j(x) \) are the Bogoliubov transformation coefficients describing the amplitudes of an excitation in particle and hole states.

\( u_j(x) \) and \( v_j(x) \) fulfill the Bogoliubov equations [56, 83],

\[
\begin{align*}
\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + V_{\text{op}}(x) + 2g|\Phi_0(x)|^2 - \mu \right] u_j(x) - g\Phi_0(x)^2 v_j(x) &= \omega_j u_j(x), \quad (2.96) \\
\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + V_{\text{op}}(x) + 2g|\Phi_0(x)|^2 - \mu \right] v_j(x) - g(\Phi_0(x)^*)^2 u_j(x) &= -\omega_j v_j(x), \quad (2.97)
\end{align*}
\]

where \( u_j(x) \) and \( v_j(x) \) satisfy the normalization and orthogonality conditions

\[
\int dx (u_i(x)u^*_j - v_i(x)v^*_j) = \delta_{ij}. \quad (2.98)
\]

Note that the Bogoliubov equations are linear equations, i.e., \((u_{1j} + u_{2j}, v_{1j} + v_{2j})\) is a solution of Eqs. (2.96) and (2.97) when \((u_{1j}, v_{1j})\) and \((u_{2j}, v_{2j})\) are solutions.

Using the Thomas-Fermi approximation Eq. (2.94), Eqs. (2.96) and (2.97) reduce to

\[
\begin{align*}
\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + (\mu - V_{\text{op}}(x)) \right] u_j(x) - (\mu - V_{\text{op}}(x)) v_j(x) &= \omega_j u_j(x), \quad (2.99) \\
\left[ -\frac{1}{2m} \frac{d^2}{dx^2} + (\mu - V_{\text{op}}(x)) \right] v_j(x) - (\mu - V_{\text{op}}(x)) u_j(x) &= -\omega_j v_j(x). \quad (2.100)
\end{align*}
\]

Expanding \( u_j(x) \) and \( v_j(x) \) by plane waves,

\[
\begin{align*}
u_j(x) &= \sum_q u_{j,q} e^{iqx}, \quad (2.101) \\
v_j(x) &= \sum_q v_{j,q} e^{iqx}. \quad (2.102)
\end{align*}
\]

Eqs. (2.99) and (2.100) reduce to the equations for \( u_{j,q} \) and \( v_{j,q} \), which can be combined in a single matrix equation:

\[
\left( \mathbf{\hat{L}}_q - \omega_j \mathbf{\hat{\sigma}} \right) \mathbf{\hat{\Psi}}_{j,q} - \frac{V_0}{2} \mathbf{\hat{A}} \left( \mathbf{\hat{\Psi}}_{j,q+G} + \mathbf{\hat{\Psi}}_{j,q-G} \right) = 0, \quad (2.103)
\]
where

\[ \hat{L}_q \equiv \begin{pmatrix} \varepsilon_q + \mu & -\mu \\ -\mu & \varepsilon_q + \mu \end{pmatrix}, \quad (2.104) \]

\[ \hat{\Psi}_{j,q} \equiv \begin{pmatrix} u_{j,q} \\ v_{j,q} \end{pmatrix}, \quad (2.105) \]

\[ \hat{A} \equiv \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad (2.106) \]

\[ \hat{\sigma} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2.107) \]

and \( \varepsilon_q = \frac{q^2}{2m} \). Equation (2.103) couples \( \hat{\Psi}_{j,q} \) with \( \hat{\Psi}_{j,q \pm G} \) by the optical lattice potential and the potential formed by the condensate. The diagonal matrix elements of \( \hat{A} \) couple the particle amplitudes \( u_{j,q} \) with \( u_{j,q + G} \), and the hole amplitudes \( v_{j,q} \) with \( v_{j,q + G} \). The off-diagonal matrix elements of \( \hat{A} \) couple \( u_{j,q} \) with \( v_{j,q + G} \), and \( v_{j,q} \) with \( v_{j,q + G} \). For fixed \( q \) in the first Brillouin zone, the set of coefficients \( \hat{\Psi}_{j,q + nG} \) (\( n \) is an integer) are coupled to each other by Eq. (2.103). Therefore, a normal mode labelled by a quasi-momentum \( q \) and a band index \( l \) is formed by a superposition of plane waves with wave vectors different from \( q \) by a reciprocal lattice vector,

\[ \left( \begin{array}{c} u_{l,q}(x) \\ v_{l,q}(x) \end{array} \right) = \sum_n \hat{\Psi}_{j,q + nG} e^{i(q+nG)x} = e^{iqx} \hat{f}_{l,q}(x), \quad (2.108) \]

Thus, \( j \) is specified by the band index \( l \) and quasi-momentum \( q \). \( \hat{f}_{l,q}(x) \) is given by

\[ \hat{f}_{l,q}(x) = \sum_n \hat{\Psi}_{j,q + nG} e^{inGx}. \quad (2.109) \]

Therefore, \( u_{l,q}(x) \) and \( v_{l,q}(x) \) satisfy the Bloch theorem,

\[ \hat{f}_{l,q}(x + a) = \hat{f}_{l,q}(x). \quad (2.110) \]

Equation (2.108) describes the wave function of a Bloch-Bogoliubov excitation.

Without the optical lattice potential, (i.e., \( V_0 = 0 \)), the excitation spectrum can be obtained by the condition \( \det |\hat{L}_q - \omega_q| = 0 \), and one obtains the famous Bogoliubov excitation spectrum,

\[ \omega_q = \sqrt{\varepsilon_q(\varepsilon_q + 2\mu)} \equiv E_q, \quad (2.111) \]
where the chemical potential is given by $\mu = gn_0$ in the absence of the lattice potential.

In the following, we solve Eq. (2.103) treating the optical lattice potential as a perturbation. We apply the perturbation theory for Schrödinger equation with a periodic potential (see e.g. Chapter 9 of Ref. [84]) to the Bogoliubov equations.

First, we consider the case where the unperturbed state is not degenerate. The unperturbed state is a Bogoliubov excitation in a uniform system with the energy $E_q$, and the unperturbed wave function is given by

$$\hat{\Psi}_{j,q} \neq 0, \quad \hat{\Psi}_{j,q+nG} = 0 \quad (n \neq 0).$$  \hfill (2.112)

We consider such a $q$ that the unperturbed energy $E_q$ is far from the value of $\pm E_{q+nG}$ compared with $V_0$, i.e., $|E_q \pm E_{q+nG}| \gg V_0$. We assume that only $\hat{\Psi}_{j,q}$ and $\hat{\Psi}_{j,q\pm G}$ are nonzero and neglect other coefficients in the presence of a weak lattice potential as a perturbation, since they are expected to have corrections in higher order in $V_0$ than $\hat{\Psi}_{j,q\pm G}$. From Eq. (2.103) $\hat{\Psi}_{j,q\pm G}$ can be written as

$$\hat{\Psi}_{j,q\pm G} = \frac{V_0}{2} \left( \hat{L}_q - \omega_j \hat{\sigma} \right)^{-1} \hat{A} \hat{\Psi}_{j,q},$$  \hfill (2.113)

where

$$\left( \hat{L}_q - \omega_j \hat{\sigma} \right)^{-1} = \frac{1}{E_q^2 - \omega_j^2} \begin{pmatrix} \varepsilon_q + \mu + \omega_j & \mu \\ \mu & \varepsilon_q + \mu - \omega_j \end{pmatrix}. $$  \hfill (2.114)

Substituting Eqs. (2.113) and (2.114) into Eq. (2.103) using

$$\hat{A} \left( \hat{L}_q - \omega_j \hat{\sigma} \right)^{-1} \hat{A} = \frac{2\varepsilon_q}{E_q^2 - \omega_j^2} \hat{A},$$  \hfill (2.115)

Eq. (2.103) reduces to

$$\left[ \left( \hat{L}_q - \omega_j \hat{\sigma} \right) - \left( \frac{V_0}{2} \right)^2 \left( \frac{2\varepsilon_{q+G}}{E_{q+G}^2 - \omega_j^2} + \frac{2\varepsilon_{q-G}}{E_{q-G}^2 - \omega_j^2} \right) \hat{A} \right] \hat{\Psi}_{j,q} = 0. $$  \hfill (2.116)

The excitation spectrum can be obtained from the condition that Eq. (2.116) has a non-trivial solution. Here, we approximate $\omega_j$ in the denominator of the second term in the square brackets of Eq. (2.116) as the unperturbed excitation energy $E_q$. The spectrum of Bloch-Bogoliubov excitation is given by

$$\omega_q = \sqrt{\varepsilon_q \left( \varepsilon_q + 2\mu - \frac{V_0^2}{2} (M_{q+G} + M_{q-G}) \right)},$$  \hfill (2.117)
where

\[ M_{q \pm G} = \frac{2 \varepsilon_{q \pm G}}{E_{q \pm G}^2 - E_q^2}. \]  

(2.118)

The spectrum Eq. (2.117) is linear for small \( q \). This is a manifestation of the superfluidity of Bose condensate in a shallow optical lattice. This result is consistent with the excitation spectrum of the Bose-Hubbard model Eq. (2.35) and the spectrum obtained by numerically solving the Gross-Pitaevskii-Bogoliubov equations [36, 41]. When \( q \) is much smaller than the reciprocal lattice vector \( G \) and the inverse of the healing length \( 1/\xi \) (the healing length \( \xi \) is defined by \( \xi \equiv \frac{1}{\sqrt{2m\mu}} \)), Eq. (2.117) can be approximated as a phonon spectrum \( \omega_q \sim cq \), where the phonon velocity of the Bloch-Bogoliubov excitation is given by

\[ c = \sqrt{\frac{1}{m} \left( \mu - \frac{V_0^2}{\varepsilon_G + 2\mu} \right)}. \]  

(2.119)

Equation (2.119) shows that the phonon velocity decreases as the strength of the lattice potential \( V_0 \) increases. This is consistent with the behavior of the phonon velocity obtained by the Bose-Hubbard model Eq. (2.37) (see Fig. 2.4). One also finds that the phonon velocity increases when the lattice spacing \( a \) increases and \( \varepsilon_G \) decreases. This result is not consistent with Eq. (2.37), since the hopping matrix element \( J \) decreases exponentially as \( a \) increases which results in the decrease of the sound velocity.

When the lattice constant is much larger than the healing length i.e., \( a \gg \xi \), the phonon velocity reduces to

\[ c = \sqrt{\frac{\mu}{m} \left( 1 - \frac{V_0^2}{2\mu^2} \right)}. \]  

(2.120)

Equation (2.120) was first derived by Berg-Sørensen and Mølmer by solving the Bogoliubov equations by another approximation in Ref. [36]. Taylor and Zaremba also derived Eq. (2.120) using thermodynamic relations [42].

The degeneracy between the unperturbed state \( \hat{\Psi}_{j,q} \) and the intermediate state \( \hat{\Psi}_{j,q \pm G} \) occurs when \( E_q = E_{q \pm G} \) (\( q = \pm \frac{G}{2} \)) at the Brillouin zone edge. In this case, the denominator of Eq. (2.118) becomes zero and the above perturbation theory is invalid. In this case, we have to solve Eq. (2.103) for the degenerate modes precisely. From Eq. (2.103), we consider the following coupled equations for the degenerate modes:

\[ \left( \hat{\mathcal{L}}_q - \omega_j \hat{\sigma} \right) \hat{\Psi}_{j,q} - \frac{V_0}{2} \hat{A} \hat{\Psi}_{j,q-G} = 0, \]  

(2.121)

\[ \left( \hat{\mathcal{L}}_q - \omega_j \hat{\sigma} \right) \hat{\Psi}_{j,q-G} - \frac{V_0}{2} \hat{A} \hat{\Psi}_{j,q} = 0. \]  

(2.122)
Substituting Eq. (2.122) into Eq. (2.121), one obtains
\[
\left[ \left( \hat{\mathcal{L}}_q - \omega_j \hat{\sigma} \right) - \frac{V_0^2}{2} \frac{\varepsilon_{q-G}}{E_{q-G}^2 - \omega_j^2} \right] \hat{\Psi}_{j,q} = 0. \tag{2.123}
\]

The excitation spectrum can be obtained from the above matrix equation, which yields
\[
\omega_q = \sqrt{\frac{1}{2} (E_q^2 + E_{q-G}^2)} \pm \frac{1}{2} \sqrt{(E_q^2 - E_{q-G}^2)^2 + 4V_0^2\varepsilon_q\varepsilon_{q-G}}. \tag{2.124}
\]

The sign in the square root in Eq. (2.124) indicates the spectrum in the upper and lower Bogoliubov bands. At \( q = \frac{G}{2} \), Eq. (2.124) reduces to
\[
\omega_{\frac{G}{2}} = \sqrt{\frac{E_{\frac{G}{2}}^2}{4} \pm V_0 \varepsilon_{\frac{G}{2}}} \tag{2.125}
\]
\[
\sim E_{\frac{G}{2}} \pm \frac{V_0}{2} \frac{\varepsilon_{\frac{G}{2}}}{E_{\frac{G}{2}}}. \tag{2.126}
\]

Thus, the band gap between the first and second Bogoliubov bands is given by
\[
\Delta = \sqrt{\frac{\varepsilon_G}{\varepsilon_G + 8\mu} V_0}. \tag{2.127}
\]

Equation (2.127) shows that \( \Delta \) is smaller than the band gap of ideal atoms in the lattice potential \( V_0(x) \). It indicates that \( \Delta \) decreases as the interaction between atoms increases or \( \mu \) increases. One finds that the \( \Delta \) increases as the lattice spacing \( a \) is decreased and \( \varepsilon_G \) is increased. When the optical lattice potential changes slowly compared to the healing length, i.e. \( \mu \gg \varepsilon_G \), Eq. (2.127) reduces to
\[
\Delta = \sqrt{\frac{\varepsilon_G}{8\mu} V_0}. \tag{2.128}
\]

This result was first obtained by Berg-Sørensen and Mølmer [36]. The numerical solution of the Bogoliubov equations in the presence of an optical lattice potential has been obtained in Refs. [36, 43].

The spectrum of the Bloch-Bogoliubov excitation Eqs. (2.117) and (2.124) are shown in Fig. (2.11). Equation (2.117) is plotted around \( q = 0 \), and Eq. (2.124) is plotted around the edge of the first Brillouin zone \( q = \pm \frac{G}{2} \). The chemical potential is taken from experiments of Florence’s group [24] as \( \mu = 0.5E_R \).
2.7 Summary

In this chapter, we have studied the collective excitations of Bose condensates in an optical lattice. Collective excitation is an important concept for understanding many properties of Bose condensate in a lattice system such as dynamics, stability and quantum phase transition. An optical lattice allows one to study various properties of Bose condensates in a lattice system with a wide parameter regime.

First, we discussed Bose-Einstein condensates in a deep optical lattice with the Bose-Hubbard tight-binding model. We generalized recent work for a condensate at zero temperature to finite temperatures taking account of the presence of non-condensate atoms. We derived the Bloch-Bogoliubov excitation spectrum at finite temperatures on the basis of the static Popov approximation which assumes that the condensate moves in a static mean-field produced by the non-condensate atoms. We calculated the number of condensate atoms in each lattice well \( n^0 \) as a function of the temperature and the well depth of the optical lattice within the Popov approximation, and used the result in the calculation of the dimensionless interaction parameter \( \alpha = Un^0/J \), phonon velocity, and the Landau and Beliaev damping of Bloch-Bogoliubov excitations. For damping processes to occur, the dispersion relation of the Bloch-Bogoliubov excitations \( E_q \) must initially bend upward as the quasi-momentum \( q \) increases. This is referred to as “anomalous dispersion” and
is also the source of 3-phonon damping of long wavelength phonons in superfluid $^{4}\text{He}$. We found that this condition leads to a dramatic disappearance of all damping processes of phonon modes in a $d$-dimensional optical lattice when $\alpha > 6d$. From the calculation of $\alpha$, we estimated the temperature and the well depth where the sudden change of the damping can be observed.

Next, we discussed Bose condensates in a weak optical lattice potential. Since the Bose-Hubbard tight-binding model is not valid for a weak lattice potential, we started from the Gross-Pitaevskii mean-field theory. We used the Thomas-Fermi approximation for the time-independent Gross-Pitaevskii equation and solved the Bogoliubov equations treating the lattice potential as a perturbation. We derived the analytical expression of the spectrum of the Bloch-Bogoliubov excitation. The analytical expressions of the phonon velocity $c$ and the band gap between the first and second excitation bands $\Delta$ were also obtained. We found that the phonon velocity $c$ decreases as the lattice strength or the lattice spacing increase, and that the band gap $\Delta$ increases as the lattice spacing decreases.
Chapter 3

Superfluid-Mott insulator transition of spin-1 bosons

This chapter is organized as follows. In Sec. 3.1, using a tight-binding approximation, we introduce the Bose-Hubbard model for spin-1 atoms in an optical lattice. In Sec. 3.2, we study the Mott insulator (MI) phase in the limit of small kinetic energy $t = 0$, where $t$ is the hopping matrix element between the nearest neighbor sites (we will use $t$ as a hopping matrix element instead of $J$ in this chapter for avoiding confusion with the spin exchange constant of the effective spin Hamiltonian in Sec. 3.4). In Sec. 3.3, we calculate the phase boundary between the superfluid (SF) and MI phases by using a perturbative mean-field theory. We also determine the symmetry of the order parameter in the SF phase. We show the phase diagram of the spin-1 Bose-Hubbard model and discuss the even-odd dependence of the MI phase. In Sec. 3.4, we derive an effective spin Hamiltonian for the MI phase with one atom on each lattice site and discuss the spin order. In Sec. 3.5, we study the spin-1 Bose-Hubbard model by a variational method with a Gutzwiller-type wave function. We discuss the first-order SF-MI transition at a part of the phase boundary and the possibility for observing the first order transition by measuring magnetization in experiment. In Sec. 3.6, we summarize our results. Some details of our calculations in Sec. 3.3 is given in Appendix A and Appendix B. The result of this chapter is based on Refs. [85, 86].
CHAPTER 3. SUPERFLUID-MOTT INSULATOR TRANSITION OF SPIN-1 BOSONS

3.1 Model

We consider bosonic atoms with hyperfine spin $F = 1$ trapped in a combined potential of an optical lattice and an optical trap. We start with the following Hamiltonian [48, 49],

$$ H = \int \! d\mathbf{r} \left( -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{op}}(\mathbf{r}) + V_{\text{ho}}(\mathbf{r}) - \mu \right) \psi_{\alpha}(\mathbf{r}) $$

$$ + \frac{c_0}{2} \int \! d\mathbf{r} \psi_{\alpha}^\dagger(\mathbf{r}) \psi_{\beta}(\mathbf{r}) \psi_{\alpha}(\mathbf{r}) $$

$$ + \frac{c_2}{2} \int \! d\mathbf{r} \psi_{\alpha}^\dagger(\mathbf{r}) \psi_{\beta}^\dagger(\mathbf{r}) \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\gamma\delta} \psi_{\delta}(\mathbf{r}) \psi_{\beta}(\mathbf{r}), \quad (3.1) $$

Here $\psi_{\alpha}(\mathbf{r})$ is a field operator for an atom in a hyperfine state $|F, m_F = \alpha\rangle$ ($\alpha = 1, 0, -1$). $M$ is the mass of the atom and $\mu$ is the chemical potential. $V_{\text{op}}(\mathbf{r}) = V_0 \sum_{l=1}^d \sin^2(kx_l)$ is a periodic potential of a $d$-dimensional optical lattice with a lattice period $a = \pi/k$, where $k = 2\pi/\lambda$ is the wave vector of the laser beam. $V_{\text{ho}}(\mathbf{r})$ is an external harmonic potential of the optical trap. $\mathbf{F}_{\alpha\beta}$ are the following spin-1 matrices,

$$ F_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F_y = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (3.2) $$

The two-body interaction potential between atoms is assumed to be given by an effective pseudopotential,

$$ V(\mathbf{r}_1 - \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \left( c_0 + c_2 \mathbf{F}_1 \cdot \mathbf{F}_2 \right). \quad (3.3) $$

This assumption is valid when the $s$-wave scattering contribution is not frozen out at low temperatures. The coefficient is $c_0 = (g_0 + 2g_2)/3$, where $g_F = 4\pi \hbar^2 a_F/M$. $a_F$ is an $s$-wave scattering length for two colliding atoms with total hyperfine spin $F$. From the symmetry of the bosonic wave function, scattering with total spin $F = 1$ is prohibited. The second term of the right hand side of Eq. (3.1) describes the spin-independent interaction, and the third term of the right hand side of Eq. (3.1) is the spin-dependent interaction. The coefficient $c_2 = (g_2 - g_0)/3$ is proportional to the difference of the scattering lengths $a_2 - a_0$. The spin-dependent interaction is ferromagnetic when $c_2 < 0$ (i.e., $a_2 < a_0$) and antiferromagnetic when $c_2 > 0$ (i.e., $a_2 > a_0$). In this chapter, we consider the case of an antiferromagnetic interaction like $^{23}$Na [48].

The energy eigenstates of a single atom in a periodic potential are Bloch states. Any Bloch function $\phi_{nk}(\mathbf{r})$ ($n$ is the band index and $k$ is the quasi-momentum) can be written
as a linear combination of Wannier functions \[ \phi_{n\mathbf{k}}(\mathbf{r}) = \sum_i e^{i\mathbf{r}_i \cdot \mathbf{k}} w_n(\mathbf{r} - \mathbf{r}_i), \]
where \( w_n(\mathbf{r} - \mathbf{r}_i) \) is the Wannier function around \( i \)-th lattice site for \( n \)-th energy band. A set of Wannier functions with all \( n \) and \( \mathbf{r}_i \) form a complete orthogonal set. We consider a deep optical lattice potential and assume that the band gap between the first and second bands is larger than the chemical potential. Therefore, we consider only the lowest energy band in the following. We also assume that the Wannier function of the lowest energy band \( w_0(\mathbf{r} - \mathbf{r}_i) \) is well localized in the \( i \)-th lattice site. Expanding a field operator by the Wannier functions of the lowest energy band,

\[ \psi_{\alpha}(\mathbf{r}) = \sum_i a_{i\alpha} w_0(\mathbf{r} - \mathbf{r}_i), \]

Eq. (3.1) reduces to a tight-binding Bose-Hubbard model for spin-1 bosons in an optical lattice,

\[
H = -t \sum_{\langle i,j \rangle} \sum_{\alpha} (a_{i\alpha}^\dagger a_{j\alpha} + a_{j\alpha}^\dagger a_{i\alpha}) - \sum_i \sum_{\alpha} (\mu - \epsilon_i) a_{i\alpha}^\dagger a_{i\alpha}
+ \frac{1}{2} U_0 \sum_{i} \sum_{\alpha,\beta} a_{i\alpha}^\dagger a_{i\beta} a_{i\beta}^\dagger a_{i\alpha}
+ \frac{1}{2} U_2 \sum_{i} \sum_{\alpha,\beta,\gamma,\delta} a_{i\alpha}^\dagger a_{i\gamma}^\dagger F_{\alpha\beta} \cdot F_{\gamma\delta} a_{i\beta} a_{i\delta}. \tag{3.4}
\]

Here \( \langle i,j \rangle \) expresses a summation over all the sets of the nearest neighbor sites. \( a_{i\alpha} \) and \( a_{i\alpha}^\dagger \) are destruction and creation operators for an atom at site \( i \) with hyperfine spin \( \alpha \). \( t \) is the hopping matrix element between adjacent sites \( i \) and \( j \), and is defined as

\[
t \equiv -\int d\mathbf{r} w_0^* (\mathbf{r} - \mathbf{r}_i) \left( -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{op}}(\mathbf{r}) \right) w_0(\mathbf{r} - \mathbf{r}_j). \tag{3.5}
\]

Note that \( t \) is independent of the site indices \( i \) and \( j \) even in the presence of the harmonic potential, since the Wannier function \( w_0(\mathbf{r} - \mathbf{r}_j) \) changes only through the difference \( \mathbf{r} - \mathbf{r}_j \). In Eq. (3.4), \( U_0 \) is the on-site spin-independent interaction and \( U_2 \) is the on-site spin-dependent interaction. \( U_F \) \((F = 0, 2)\) is defined by

\[
U_F \equiv c_F \int d\mathbf{r} |w_0(\mathbf{r} - \mathbf{r}_i)|^4. \tag{3.6}
\]

\( \epsilon_i \) describes the energy offset of each lattice site, due to the external harmonic potential

\[
\epsilon_i \equiv \int d\mathbf{r} V_{\text{ho}}(\mathbf{r}) |w_0(\mathbf{r} - \mathbf{r}_i)|^2. \tag{3.7}
\]

The first three terms in Eq. (3.4) are a natural generalization of the usual expression for a single component Bose gas, Eq. (2.10). The fourth term is new and describes additional interaction which arises for spin-1 bosons.
We consider the case of $^{23}\text{Na}$ atoms with an antiferromagnetic interaction i.e., $c_2 > 0$ and $U_2 > 0$ (see Eq. (3.6)). The scattering lengths of $^{23}\text{Na}$ are $a_0 = (46 \pm 5)a_B$ and $a_2 = (52 \pm 5)a_B$, where $a_B$ is the Bohr radius [48, 87]. We take $U_2/U_0 = 0.04$ in our calculation. In the following analysis, we neglect the effect of the harmonic potential and hence set $\epsilon_i = 0$.

### 3.2 Mott insulating phase in the limit of $t = 0$

We start from the Mott insulating state in the limit of $t = 0$. In this case, the Hamiltonian Eq. (3.4) is diagonal with respect to lattice sites,

$$ H = \sum_i H_i^0, $$

$$ H_i^0 = -\mu \hat{n}_i + \frac{1}{2} U_0 \hat{n}_i(\hat{n}_i - 1) + \frac{1}{2} U_2 (\hat{S}_i^2 - 2\hat{n}_i). $$

Here, we define a spin operator $\hat{S}_i = a_{i\alpha}^\dagger F_{\alpha\beta} a_{i\beta}$ and a number operator for each spin component $\hat{n}_{i\alpha} \equiv a_{i\alpha}^\dagger a_{i\alpha}$. $\hat{n}_i \equiv \sum_{\alpha=\pm1,0} \hat{n}_{i\alpha}$ is the total atom number operator. Note that the single site Hamiltonian Eq. (3.9) is studied in Refs. [54] and [88] in connection with a spin-1 Bose condensate in a harmonic trap.

Each component of the spin operator is given by

$$ \hat{S}_{ix} = \frac{1}{\sqrt{2}} \left( a_{i1}^\dagger a_{i0} + a_{i0}^\dagger a_{i1} + a_{i-1}^\dagger a_{i0} + a_{i0}^\dagger a_{i-1} \right), $$

$$ \hat{S}_{iy} = \frac{1}{\sqrt{2}} \left( -a_{i1}^\dagger a_{i0} + a_{i0}^\dagger a_{i1} - a_{i1}^\dagger a_{i-1} + a_{i-1}^\dagger a_{i0} \right), $$

$$ \hat{S}_{iz} = \hat{n}_{i1} - \hat{n}_{i-1}. $$

One can show that $\hat{S}_{i\mu}$ ($\mu = x, y, z$) obeys the usual angular momentum commutation relation $[\hat{S}_{i\nu}, \hat{S}_{i\rho}] = i\epsilon_{\nu\rho\lambda} \hat{S}_{i\lambda}$. Using Eqs. (3.10), (3.11) and (3.12), one obtains

$$ \hat{S}_i^2 = 2\hat{n}_{i1}\hat{n}_{i0} + 2\hat{n}_{i0}\hat{n}_{i-1} + \hat{n}_{i1} + 2\hat{n}_{i0} + \hat{n}_{i-1} $$

$$ + \hat{n}_{i1}^2 - 2\hat{n}_{i1}\hat{n}_{i-1} + \hat{n}_{i-1}^2 + 2a_{i1}^\dagger a_{i1}^\dagger a_{i0}^\dagger a_{i0}^\dagger + 2(a_{i0}^\dagger)^2 a_{i1}^\dagger a_{i-1}. $$

The last two terms in Eq. (3.13) mix different spin components without changing the total net spin.

One can show that $\hat{S}_i^2$, $\hat{S}_{iz}$ and $\hat{n}_i$ commute with each other. Therefore, an eigenstate of the single site Hamiltonian Eq. (3.9) is described by $|S_i, m_i; n_i \rangle$, where the eigenvalue
of each operator is given by

\[
\begin{align*}
\hat{S}^2_i |S_i, m_i; n_i\rangle &= S_i(S_i + 1) |S_i, m_i; n_i\rangle, \\
\hat{S}^z_i |S_i, m_i; n_i\rangle &= m_i |S_i, m_i; n_i\rangle, \\
\hat{n}_i |S_i, m_i; n_i\rangle &= n_i |S_i, m_i; n_i\rangle.
\end{align*}
\]

(3.14) (3.15) (3.16)

From the commutation relation of the spin operators, \( m_i \) satisfies \(-S_i \leq m_i \leq S_i\). Using Eqs. (3.14), (3.15) and (3.16), the eigenvalue of the single site Hamiltonian Eq. (3.9) is

\[
H^0_i |S_i, m_i; n_i\rangle = E^{(0)}(S_i, n_i) |S_i, m_i; n_i\rangle,
\]

(3.17)

\[
E^{(0)}(S, n) = -\mu n + \frac{1}{2} U_0 n(n-1) + \frac{1}{2} U_2 [S(S+1) - 2n].
\]

(3.18)

Since the orbital part of the wave function in one lattice site is a product of the Wannier function for all atoms, it is symmetric under the permutation of any two atoms. The spin part of the wave function also has to be symmetric because of Bose statistics. Therefore, \( S_i \) has to be even \((S_i = 0, 2, 4, ..., n_i)\) when \( n_i \) is even, and \( S_i \) has to be odd \((S_i = 1, 3, 5, ..., n_i)\) when \( n_i \) is odd. The rigorous proof of these results is given in Ref. [89]. It is convenient to express \(|S_i, m_i; n_i\rangle\) by the creation operator \( a^\dagger_{m_i} \) for later calculations. One can show [54]

\[
\begin{align*}
|S_i, S_i; n_i\rangle &= \frac{1}{\sqrt{f(Q, S_i)}} (a^\dagger_{1})^{S_i} (\Theta^\dagger_i)^Q |\text{vac}\rangle \\
Q &= \frac{n_i - S_i}{2} \\
f(Q, S_i) &= \frac{S_i! Q! 2^Q (2Q + 2S_i + 1)!!}{(2S_i + 1)!!},
\end{align*}
\]

(3.19) (3.20) (3.21)

where \( \Theta_i \equiv a^2_{i0} - 2a_{i1}a_{i-1} \) and \( \Theta^\dagger_i \equiv a^2_{i0} - 2a_{i1}a_{i-1}^\dagger \). \( \Theta_i \) and \( \Theta^\dagger_i \) are destruction and creation operators of a spin-singlet pair which is made up of two bosons and carries no spin. They satisfy the commutation relation \([\Theta_i, \Theta^\dagger_i] = 4\hat{n}_i + 6\). Other states \(|S_i, m_i; n_i\rangle\), with \( m_i < S_i \), can be obtained by operating \( \hat{S}_z^+ \) to \(|S_i, S_i; n_i\rangle\). \( \hat{S}_z^+ \) and \( \hat{S}_z^- \) are rising and lowering operators of \( z \)-component of spin eigenvalue defined as

\[
\begin{align*}
\hat{S}_z^+ &\equiv \hat{S}_{xz} + i\hat{S}_{yz} = \sqrt{2}(a_{i1}^\dagger a_{i0} + a_{i0}^\dagger a_{i-1}), \\
\hat{S}_z^- &\equiv \hat{S}_{xz} - i\hat{S}_{yz} = \sqrt{2}(a_{i0}^\dagger a_{i1} + a_{i-1}^\dagger a_{i0}).
\end{align*}
\]

(3.22) (3.23)

Since we are considering an antiferromagnetic interaction (i.e., \( U_2 > 0 \)), the ground state of \( H^0_i \) has the minimum total spin \( S_i \). Therefore, the Mott insulating state with an
even number atoms per site is $|0_i, 0_i; n_i\rangle$ with $n_i/2$ singlet pairs. This is referred to as the spin singlet insulator in Ref. [55]. The Mott insulating state with odd number atoms is $|1_i, m_i; n_i\rangle$ and it has spin $S = 1$ on each lattice site. In this state, one atom cannot make a singlet pair on a lattice site. This difference between the MI states with even and odd number of atoms per site plays an important role for the stability of the MI phase against the transition to the SF phase. The ground state has also minimum energy for $n_i$. The condition that $E^{(0)}(0, n_i)$ is minimum is $E^{(0)}(1, n_i - 1) > E^{(0)}(0, n_i)$ and $E^{(0)}(1, n_i + 1) > E^{(0)}(0, n_i)$. The condition that $E^{(0)}(1, n_i)$ is minimum is $E^{(0)}(0, n_i - 1) > E^{(0)}(1, n_i)$ and $E^{(0)}(0, n_i + 1) > E^{(0)}(1, n_i)$. From Eq. (3.18), we find that the ground state has even $n_i$ when $(n_i - 1)U_0 - 2U_2 < \mu < n_iU_0$ and odd $n_i$ when $(n_i - 1)U_0 < \mu < n_iU_0 - 2U_2$.

### 3.3 Perturbative mean-field approximation

To study the SF-MI transition, we use the perturbative mean-field approximation which was developed for the Bose-Hubbard model for spin-0 bosons [38, 59]. For the Bose-Hubbard model for spin-0 bosons, this approximation gives results that are in good agreement with quantum Monte Carlo simulations [90, 91].

We now consider the case of finite $t$ to study the transition to the SF phase. We introduce the superfluid order parameter $\psi_\alpha \equiv \langle a_{i\alpha} \rangle = \sqrt{n_s} \zeta_\alpha$, where $n_s$ is the number of condensate atoms in each lattice site and $\zeta_\alpha$ is a normalized spinor $\sum_{\alpha = \pm 0} \zeta_\alpha^* \zeta_\alpha = 1$ [48]. The site dependence of the order parameter is neglected to consider only the phase transition to the ground state of the SF phase. Neglecting the second order fluctuation, one obtains

$$a_{i\alpha}^\dagger a_{j\alpha} \sim (\psi_\alpha^* a_{i\alpha}^\dagger + \psi_\alpha a_{j\alpha}^\dagger) - \psi_\alpha^* \psi_\alpha.$$  \hfill (3.24)

Using this approximation, the hopping term can be simplified to

$$-t \sum_{(i,j)} \sum_{\alpha} a_{i\alpha}^\dagger a_{j\alpha} + a_{j\alpha}^\dagger a_{i\alpha} \sim -zt \sum_i \sum_{\alpha} (\psi_\alpha^* a_{i\alpha} + \psi_\alpha a_{i\alpha}^\dagger) + zt N_s \sum_{\alpha} \psi_\alpha^* \psi_\alpha, \hfill (3.25)$$

where $z \equiv 2d$ is the number of nearest neighbor sites of a single site in $d$-dimensional optical lattice, and $N_s$ is the total number of the lattice sites. Using this approximation,
the Hamiltonian Eq. (3.4) reduces to

\[ H = \sum_i H_i^{\text{mf}}, \]  
\[ H_i^{\text{mf}} = H_i^0 + V_i + zt \sum_\alpha \psi_\alpha^* \psi_\alpha, \]  
\[ V_i = -zt \sum_\alpha (\psi_\alpha^* a_{i\alpha} + \psi_\alpha a_{i\alpha}^*). \]

Here, \( V_i \) describes the transfer of atoms between the \( i \)-th site and the condensate \( \psi_\alpha \).

We treat \( V_i \) as a small perturbation, assuming \( t \) is small. The ground state of the non-perturbative Hamiltonian \( H_i^0 \) is \( |0_i, 0; n_i\rangle \) for even \( n_i \) and \( |1_i, m_i; n_i\rangle \) for odd \( n_i \). In the following subsections, we calculate the ground state energy in each case using the perturbation theory. Since the effective Hamiltonian Eq. (3.26) is diagonal with respect to the site, we drop the site index in the following.

### 3.3.1 MI state with an even number of atoms

We first consider the SF-MI transition from the MI state with even number of atoms per site. In order to calculate the second order perturbation of the ground state energy, we need to know the matrix element of \( V \) between the ground state \( |0, 0; n\rangle \) and an intermediate state. In Appendix A, we list the results of operating \( a_\alpha \) and \( a_{i\alpha}^\dagger \) on \( |S, m; n\rangle \) needed for the calculations of this section. From Appendix A, we obtain

\[ V|0, 0; n\rangle = -zt \left[ -\sqrt{\frac{n}{3}} \psi_1^* |1, -1; n - 1\rangle + \sqrt{\frac{n + 3}{3}} \psi_1 |1, 1; n + 1\rangle \\
+ \sqrt{\frac{n}{3}} \psi_0^* |1, 0; n - 1\rangle + \sqrt{\frac{n + 3}{3}} \psi_0 |1, 0; n + 1\rangle \\
- \sqrt{\frac{n}{3}} \psi_{-1}^* |1, 1; n - 1\rangle + \sqrt{\frac{n + 3}{3}} \psi_{-1} |1, -1; n + 1\rangle \right]. \]  

(3.29)

The intermediate states are \( |1, m; n \pm 1\rangle \) where \( m = \pm 1, 0 \). From Eq. (3.29), one can easily calculate the matrix element \( \langle 1, m; n \pm 1|V|0, 0; n\rangle \). The ground state energy within the second order perturbation is

\[ E_n(\psi) = E^{(0)}(0, n) + A(n, t, U_0, U_2, \mu) (\tilde{\psi}^\dagger \cdot \tilde{\psi}), \]

\[ A(n, t, U_0, U_2, \mu) = zt + \frac{1}{3} \left( \frac{n + 3}{\mu - U_0 n} + \frac{n}{-\mu + U_0 (n - 1) - 2U_2} \right) (zt)^2, \]  

(3.30)
where $\vec{\psi} \equiv (\psi_1, \psi_0, \psi_{-1})$. Since the value of the order parameter has to be taken to minimize the ground state energy, the ground state is the MI phase with $\vec{\psi} = 0$ when $A > 0$ and SF phase with finite $\vec{\psi} \cdot \vec{\psi}$ when $A < 0$. Therefore, the phase boundary between the SF phase and the MI phase is given by the condition $A = 0$. Solving the equation $A = 0$ for $\mu$, one obtains the phase boundary

$$
\mu_{\pm} = -U_2 + \frac{1}{2}[(2n - 1)U_0 - zt]
\pm \frac{1}{6}
\left[
9U_0^2 + 6(6U_2 - (2n + 3)(zt))U_0
+ (36U_2^2 - 12(2n + 3)(zt)U_2 + 9(zt)^2)
\right]^{1/2}.
$$

(3.31)

In Fig. 3.1, the phase boundaries are shown in the $(t, \mu)$-plane. $\mu_+$ and $\mu_-$ correspond to the upper and lower phase boundaries for a given value of $n$. By equating $\mu_+$ and $\mu_-$, we find the maximum value of $t$ for each Mott lobe to be

$$
z t_c = \frac{U_0 + 2U_2}{3} \left((2n + 3) - \sqrt{4n^2 + 12n}\right).
$$

(3.32)

We note that the expression inside the square root in Eq. (3.31) is always positive when $t < t_c$.

Equation (3.30) cannot determine the symmetry of the superfluid order parameter, since $(\vec{\psi} \cdot \vec{\psi}) = n_s$ is symmetric under the rotation in spin space, and the ground state energy of SF phase is degenerate for any $\zeta_\alpha$. In order to determine the symmetry of the order parameter, we need to calculate the fourth-order perturbation correction [92],

$$
E^{(4)} = \sum_{n,p,q \neq i} \frac{\langle i|V|n\rangle}{E_i^{(0)} - E_n^{(0)}} \frac{\langle n|V|p\rangle}{E_n^{(0)} - E_p^{(0)}} \frac{\langle p|V|q\rangle}{E_p^{(0)} - E_q^{(0)}} \frac{\langle q|V|i\rangle}{E_q^{(0)} - E_i^{(0)}} - E^{(2)} \sum_{n \neq i} \frac{||i|V|n||^2}{(E_i^{(0)} - E_n^{(0)})^2},
$$

(3.33)

where $E^{(l)}$ is the $l$-th order perturbation energy. $|i\rangle$ is the initial state, and $|q\rangle$, $|p\rangle$ and $|n\rangle$ are the intermediate states. From Appendix A, $|q\rangle$ and $|n\rangle$ are $|1, m; n \pm 1\rangle$, and $|p\rangle$ can be $|0, 0; n \pm 2\rangle$, $|2, m; n \pm 2\rangle$ and $|2, m; n\rangle$. The details of the calculation are given in Appendix A. A long but straightforward calculation gives

$$
E_n^{(4)} = B(n, t, U_0, U_2, \mu) n_s^2|\zeta_{-1}^2| + C(n, t, U_0, U_2, \mu) (\vec{\psi} \cdot \vec{\psi})^2,
$$

(3.34)
3.3. PERTURBATIVE MEAN-FIELD APPROXIMATION

Figure 3.1: Phase diagram of the Bose-Hubbard model for spin-1 bosons when $\frac{\mu}{U_0} = 0.04$. The superfluid phase is the polar state. The MI phase with an even number of atoms per site is the $S = 0$ state (spin singlet insulator) and the MI phase with an odd number of atoms per site has spin $S = 1$ at each lattice site.
where $B$ and $C$ are

$$B(n, t, U_0, U_2, \mu) = -\frac{n(zt)^4}{15\Delta E^{(0)}(1, n - 1)\Delta E^{(0)}(0, n - 2)\Delta E^{(0)}(2, n - 2)\Delta E^{(0)}(2, n)}$$

$$\times\left[(n + 3)\Delta E^{(0)}(0, n - 2)^2 + 6(n + 3)U_2\Delta E^{(0)}(0, n - 2) + 15(n + 1)U_2^2\right]$$

$$-\frac{(n + 3)(zt)^4}{15\Delta E^{(0)}(1, n + 1)\Delta E^{(0)}(0, n + 2)\Delta E^{(0)}(2, n + 2)\Delta E^{(0)}(2, n)}$$

$$\times\left[n\Delta E^{(0)}(0, n + 2)^2 + 4nU_2\Delta E^{(0)}(0, n + 2) + 5(n + 2)U_2^2\right]$$

$$-\frac{2n(n + 3)(zt)^4}{15\Delta E^{(0)}(1, n + 1)\Delta E^{(0)}(1, n - 1)\Delta E^{(0)}(2, n)}, \quad (3.35)$$

$$C(n, t, U_0, U_2, \mu) = -\frac{2}{15}\left[\frac{n(n - 2)}{\Delta E^{(0)}(1, n - 1)^2\Delta E^{(0)}(2, n - 2)} + \frac{(n + 3)(n + 5)}{\Delta E^{(0)}(1, n + 1)^2\Delta E^{(0)}(2, n + 2)}\right](zt)^4$$

$$+\frac{n(n + 3)}{45}\left[\frac{1}{\Delta E^{(0)}(1, n - 1)} + \frac{1}{\Delta E^{(0)}(1, n + 1)}\right]^2(zt)^4$$

$$+\frac{n}{9}\left[\frac{n}{\Delta E^{(0)}(1, n - 1)} + \frac{n + 3}{\Delta E^{(0)}(1, n + 1)}\right]\left[\frac{n}{\Delta E^{(0)}(1, n - 1)^2} + \frac{n + 3}{\Delta E^{(0)}(1, n + 1)^2}\right](zt)^4. \quad (3.36)$$

Here $\Delta E^{(0)}(S, l) \equiv E^{(0)}(S, l) - E^{(0)}(0, n) > 0$. If we define the average of spin in the SF phase as

$$\langle F \rangle \equiv \sum_{\alpha, \beta} \zeta_\alpha^* F_{\alpha\beta}\zeta_\beta, \quad (\alpha, \beta = x, y, z), \quad (3.37)$$

we find

$$|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 = 1 - \langle F \rangle^2. \quad (3.38)$$

If the fluctuation of the order parameter $a_\alpha - \psi_\alpha$ can be neglected, we find

$$|\langle \Theta \rangle|^2 = n_\alpha^4|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2. \quad (3.39)$$

The first term on the right-hand side of Eq. (3.34) lifts the degeneracy of the SF phase in spin space. Since $B(n, t, U_0, U_2, \mu)$ is negative, $\langle F \rangle^2$ takes the minimum value in the
ground state, i.e., \( \langle F \rangle = 0 \). Therefore, the superfluid phase is a polar state as in the case of spin-1 Bose condensate with antiferromagnetic interaction in a usual harmonic trap [48, 49]. Since all spinors are related to each other by gauge transformation \( e^{i\theta} \) and spin rotation \( R(\alpha, \beta, \tau) = e^{-iF_z^\alpha} e^{-iF_y^\beta} e^{-iF_z^\tau} \) where \((\alpha, \beta, \tau)\) are the Euler angles, the order parameter in polar state can be written as [48]

\[
\zeta = e^{i\theta} R(\alpha, \beta, \tau) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = e^{i\theta} \begin{pmatrix} -\frac{1}{\sqrt{2}} e^{-i\alpha} \sin \beta & 0 \\ \cos \beta & 0 \\ \frac{1}{\sqrt{2}} e^{i\alpha} \sin \beta \end{pmatrix}.
\]

(3.40)

This fourth-order perturbation result can be understood in physical terms. The processes with \(|p\rangle = |0, 0; n \pm 2\rangle\) make negative contributions to \(B(n, t, U_0, U_2, \mu)\) (see Appendix A) which favors the polar state. Since this \(|0, 0; n \pm 2\rangle\) state has one more (or one less) singlet pair than the ground state, we can understand that the polar state is favorable as a result of the hopping of the singlet pairs.

### 3.3.2 MI state with an odd number of atoms

We next consider the SF-MI transition from the MI phase with odd number of atoms per site. Since the MI state \(|1, m; n\rangle\) has degeneracy for \(m = \pm 1, 0\), we need to solve the usual secular equation

\[
\det \left[ \langle 1, m; n | V E^{(0)}(1, n) - \hat{H}_0 V | 1, m'; n \rangle - E_n^{(2)} \delta_{mm'} \right] = 0
\]

(3.41)

to obtain the second order perturbation energy \(E_n^{(2)}\). In Appendix B, we give the details of the calculation.

Solving Eq. (3.41) yields

\[
E_n^{(2)} = -3(\beta + \delta)(\bar{\psi} \cdot \psi)(zt)^2,
\]

\[
-\frac{1}{2}((\alpha + \gamma) + 7(\beta + \delta))(zt)^2(\bar{\psi} \cdot \psi) \pm \frac{1}{2} \left( (\alpha - \gamma) - 5(\beta - \delta) \right)^2 (\bar{\psi} \cdot \psi)^2
\]

\[
+ 4(3\beta + \gamma - 2\delta)(\alpha - 2\beta + 3\delta)n_s^2|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 \right)^{1/2} (zt)^2,
\]

(3.42)

where \(\alpha = \frac{n+2}{3} \Delta E_{(0)0,n-1}, \beta = \frac{n-1}{15} \Delta E_{(0)1,n-1}, \gamma = \frac{n+1}{3} \Delta E_{(0)0,n+1}, \delta = \frac{n+4}{15} \Delta E_{(0)2,n+1},\) and \(\Delta E_{(0)}(S,l) \equiv E^{(0)}(S, l) - E^{(0)}(1, n) > 0\). It is clear that the ground state energy corresponds to the lower sign of Eq. (3.42). Since \(3\beta + \gamma - 2\delta\) and \(\alpha - 2\beta + 3\delta\) can be
written as

\[
3\beta + \gamma - 2\delta = \frac{1}{15\Delta E^{(0)}(0,n+1)\Delta E^{(0)}(2,n-1)\Delta E^{(0)}(2,n+1)} \times \left[ 3(n-1)\Delta E^{(0)}(0,n+1)^2 + 3(n-1)\left(\Delta E^{(0)}(2,n-1) + 3U_2\right) \times \Delta E^{(0)}(0,n+1) + 15(n+1)U_2\Delta E^{(0)}(2,n-1) \right] > 0, \tag{3.43}
\]

\[
\alpha - 2\beta + 3\delta = \frac{1}{15\Delta E^{(0)}(2,n-1)\Delta E^{(0)}(0,n-1)\Delta E^{(0)}(2,n+1)} \times \left[ 3(n+4)\Delta E^{(0)}(0,n-1)^2 + 3(n+4)\left(\Delta E^{(0)}(2,n+1) + 3U_2\right) \times \Delta E^{(0)}(0,n-1) + 15(n+2)U_2\Delta E^{(0)}(2,n+1) \right] > 0, \tag{3.44}
\]

the ground state energy takes the minimum value when \(|\xi_0^2 - 2\xi_1\xi_{-1}|^2 = 1 - \langle F \rangle^2\) is maximum i.e., when \(\langle F \rangle = 0\). Therefore, the ground state of the superfluid phase is the polar state, the same as in the case of even \(n\).

When \(\langle F \rangle = 0\), the ground state energy is

\[
E = E^{(0)}(1,n) + D(n,t,U_0,U_2,\mu)n_s, \tag{3.45}
\]

\[
D(n,t,U_0,U_2,\mu) = zt[1 - (\alpha + 4\beta + \gamma + 4\delta)(zt)]. \tag{3.46}
\]

The phase boundary between the SF phase and the MI phase for odd-\(n\) can be obtained by solving \(D(n,t,U_0,U_2,\mu) = 0\). We numerically solve this equation and show the result in Fig. 3.1.

### 3.3.3 Phase diagram

Figure 3.1 shows the phase diagram we have obtained from the perturbative mean-field approximation. We have also investigated the phase boundary by numerically diagonalizing the effective Hamiltonian Eq. (3.27). When we assume that the SF phase is a polar state i.e., \(\psi_1 = \psi_{-1} = 0\), the ground state energy as a function of \(\psi_0\) obtained by the numerical diagonalization shows the complete agreement in the small \(\psi_0\) region with the result of the perturbation theory. Therefore, the phase boundary determined by the behavior of the ground state energy in the small \(\psi_0\) region is consistent with Fig. 3.1. Since the perturbation parameter \(zt\psi\) is arbitrarily small near the phase boundary, the
perturbation theory can determine the phase boundary rigorously within the mean field approximation as far as the SF-MI transition is of second order.

In Fig. 3.1, one can see that the MI phase with even $n$ is stabilized against the superfluid phase compared with odd-$n$ case. This is intuitively understood as follows. In the case of the MI state with even-$n$, all atoms are able to form singlet pairs at each site and the boson singlet pairs are strongly localized at a site, since forming singlet pairs prevents the bosons from hopping to the nearest-neighbor sites. However, in the case of MI state with odd-$n$, one of the atoms cannot make a singlet pair and can hop to other sites without breaking singlet pairs. Since the hopping is essential for the superfluid phase, the Mott insulating phase is stabilized when even number atoms are in each lattice site. Equation (3.32) shows that $t_c$ increases as $U_2$ increases. This is consistent with the above considerations since the formation of singlet pairs is energetically more favorable as $U_2$ increases. We have also found that the “even-odd” dependence of the phase boundary smoothly disappears when $U_2$ approaches to 0, where the phase boundary becomes identical to that in Ref. [38] for spin-0 bosons.

We note that if we assume a ferromagnetic inter-atomic interaction ($U_2 < 0$), there seems to be no strong “even-odd” dependence of the phase boundaries since the MI state has the highest spin in each lattice site and singlet pairs are not formed. A detailed comparison between the ferromagnetic and antiferromagnetic cases remains as a future problem. Other possibilities such as fragmented condensates or two-particle pairings [55, 93] could also be studied in this system.

3.4 Spin order in the Mott insulating phase

In this section, we briefly discuss the spin correlation between different sites in the MI state with an odd number of atoms. In the limit $t = 0$, each site has spin-1 in the ground state, but the orientations of those spins have no correlation between them. When $t$ is finite but small enough not to destroy the MI state, those spins begin to have correlations. We derive an effective spin Hamiltonian for the MI state with $n = 1$ when $U_0, U_2 \gg t$ starting from the original Bose-Hubbard Hamiltonian Eq. (3.4). Note that the spin correlation cannot be determined by the effective Hamiltonian Eq. (3.26), since Eq. (3.26) is diagonal with respect to the lattice sites as a result of the mean field approximation.

We start with a two-site problem. We consider neighboring two sites $j, l$ with one
atom on each site. The Hamiltonian is given by

$$H = H_t + H_U,$$  \hspace{1cm} (3.47)

$$H_t \equiv -t \sum_{\alpha=\pm1,0} \left( a_{j\alpha}^\dagger a_{l\alpha} + a_{l\alpha}^\dagger a_{j\alpha} \right),$$  \hspace{1cm} (3.48)

$$H_U \equiv H_0^j + H_0^l.$$  \hspace{1cm} (3.49)

In the limit $t = 0$, the ground state is described as $|1_j, m_j; 1_j \rangle \otimes |1_l, m_l; 1_l \rangle$ and its energy is $E_G \equiv 2E^{(0)}(1, n)$. The ground state has degeneracy for $m_j$ and $m_l$. The second order perturbation energy and wave function can be obtained by calculating the eigenvalue and eigenstate of an operator $P \equiv H_t^{-1} E_G H_t$. We define $|m_j, m_l \rangle \equiv |1_j, m_j; 1_j \rangle \otimes |1_l, m_l; 1_l \rangle$.

Using Eqs. (A.10)~(A.35) in Appendix A, we obtain

$$P|1, 1 \rangle = \frac{4t^2}{-U_0 - U_2} |1, 1 \rangle,$$  \hspace{1cm} (3.50)

$$P|1, 0 \rangle = \frac{2t^2}{-U_0 - U_2} (|1, 0 \rangle + |0, 1 \rangle),$$  \hspace{1cm} (3.51)

$$P|1, -1 \rangle = \frac{t^2}{3} \left[ \frac{2}{-U_0 - U_2} (|1, -1 \rangle + 2|0, 0 \rangle + | -1, 1 \rangle)
\begin{align*}
&\quad - \frac{4}{-U_0 + 2U_2} (|0, 0 \rangle - |1, -1 \rangle - | -1, 1 \rangle) \right],
\right.$$  \hspace{1cm} (3.52)

$$P|0, 0 \rangle = \frac{t^2}{3} \left[ \frac{4}{-U_0 - U_2} (|1, -1 \rangle + | -1, 1 \rangle + 2|0, 0 \rangle)
\begin{align*}
&\quad + \frac{4}{-U_0 + 2U_2} (|0, 0 \rangle - |1, -1 \rangle - | -1, 1 \rangle) \right].
\right.$$  \hspace{1cm} (3.53)

Other results of the operation of $P$ on $a_{j\alpha}^\dagger a_{l\beta}^\dagger |vac \rangle$ can be obtained by changing the sign of the spin +1 and −1 due to the symmetry of the Hamiltonian in spin space. If we define $|S_t, m_t \rangle$ as a state which has the total spin of two sites $S_t$ and the $z$-component of the
3.4. SPIN ORDER IN THE MOTT INSULATING PHASE

total spin \( m_t, |S_t, m_t\rangle \) can be written as

\[
|0, 0\rangle = \frac{1}{\sqrt{3}} (|1, -1\rangle - |0, 0\rangle + |-1, 1\rangle), \\
|1, 1\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle - |0, 1\rangle), \\
|1, 0\rangle = \frac{1}{\sqrt{2}} (|1, -1\rangle - |-1, 1\rangle), \\
|2, 2\rangle = |1, 1\rangle, \\
|2, 1\rangle = \frac{1}{\sqrt{2}} (|1, 0\rangle + |0, 1\rangle), \\
|2, 0\rangle = \frac{1}{\sqrt{6}} (|1, -1\rangle + 2|0, 0\rangle + |-1, 1\rangle).
\]

The operator \( P \) is diagonalized by \( |S_t, m_t\rangle \) as

\[
P|0, 0\rangle = -\frac{4t^2}{U_0 - 2U_2} |0, 0\rangle, \\
P|1, m_t\rangle = 0, \\
P|2, m_t\rangle = -\frac{4t^2}{U_0 + U_2} |2, m_t\rangle.
\]

Thus, the degeneracy of the ground state is lifted up by the perturbation of the hopping term, and the ground state turns out to be a spin singlet state between two sites \( |0, 0\rangle \) when the interaction is antiferromagnetic, i.e., \( U_2 > 0 \). When the interaction is ferromagnetic (\( U_2 < 0 \)), the ground state is the highest spin state \( |2, m_t\rangle \). The operator \( P \) can be replaced by an effective Hamiltonian

\[
\mathcal{H}_{jl} = -J_0 - J_j \hat{S}_j \cdot \hat{S}_l - J_2 \left( \hat{S}_j \cdot \hat{S}_l \right)^2
\]

where \( \hat{S}_j \) is a spin-1 operator. Since the higher order terms \((\hat{S}_j \cdot \hat{S}_l)^n (n \geq 3)\) reduce to linear combinations of \( \hat{S}_j \cdot \hat{S}_l \) and \((\hat{S}_j \cdot \hat{S}_l)^2 \), Eq. (3.63) is a general expression for describing an exchange interaction of spin-1 atoms. Since \( \hat{S}_j \cdot \hat{S}_l \) is diagonal matrix with respect to \( |S_t, m_t\rangle \) as

\[
(\hat{S}_j \cdot \hat{S}_l)|0, 0\rangle = -2|0, 0\rangle, \\
(\hat{S}_j \cdot \hat{S}_l)|1, m_t\rangle = -|1, m_t\rangle, \\
(\hat{S}_j \cdot \hat{S}_l)|2, m_t\rangle = |2, m_t\rangle.
\]
the eigenenergy of $H_{jl}$ is
\[ H_{jl}|0,0\rangle = (-J_0 + 2J_1 - 4J_2)|0,0\rangle, \] (3.67)
\[ H_{jl}|1,m_i\rangle = (-J_0 + J_1 - J_2)|1,m_i\rangle, \] (3.68)
\[ H_{jl}|2,m_i\rangle = (-J_0 - J_1 - J_2)|2,m_i\rangle. \] (3.69)

Comparing Eqs. (3.60)\sim(3.62) with Eqs. (3.67)\sim(3.69), one obtains
\[ J_0 = \frac{4t^2}{3} \left( \frac{1}{U_0 - 2U_2} - \frac{1}{U_0 + U_2} \right), \] (3.70)
\[ J_1 = \frac{2t^2}{U_0 + U_2}, \] (3.71)
\[ J_2 = \frac{2t^2}{3} \left( \frac{1}{U_0 + U_2} + \frac{2}{U_0 - 2U_2} \right). \] (3.72)

Since the second order perturbation energy for a system with more than two sites is given by the summation of the second order perturbation energy for every neighboring two sites, the effective Hamiltonian for the whole system is
\[ H_{eff} = \sum_{j,l} H_{jl} \]
\[ = -J_1 \sum_{<j,l>} S_j \cdot S_l - J_2 \sum_{<j,l>} (S_j \cdot S_l)^2 \]
\[ = -\frac{J_2}{4} \sum_{<j,l>} [(S_j + S_l)^2 - 4][(S_j + S_l)^2 - 4 + \frac{2}{\alpha}], \] (3.73)

where $\alpha \equiv \frac{J_2}{J_1} = \frac{U_0}{U_0 - 2U_2}$. The same effective Hamiltonian has been derived by Imambekov et al. [94]. From the result of the two-site problem, the ground state of the effective Hamiltonian Eq. (3.73) with $U_2 > 0$ is expected to be a dimerized state, where every two sites have a spin-singlet pair. In one dimensional case, the ground state is proved to be a dimerized state with a finite spin excitation gap when $\frac{U_2}{U_0} < 0.5$ [95]. However, if neighboring two sites belong to different singlet pairs, a singlet pair cannot be formed between these two sites and the excited total spin states for these two sites are mixed. This consideration suggests a possible ground state with the excited total spin states for every site. Recently, Yip has shown that the ground state of the effective spin Hamiltonian Eq. (3.73) for two and three dimensional square and cubic lattice are dimerized states by a variational ansatz [96]. In Refs. [94, 97], the possibility of nematic MI phase is pointed out.
3.5 Gutzwiller’s variational method

3.5.1 Gutzwiller wave function

In this section, we study the Bose-Hubbard model for spin-1 bosons Eq. (3.4) with a variational method. We employ the Gutzwiller-type variational wave function (GW) [98, 99] and investigate the phase diagram of the ground state. The GW brings us with a powerful technique for studying strongly correlated Fermi systems, and has been used for the original Hubbard model for electrons [100]. The GW has been also applied to the spinless Bose-Hubbard model Eq. (2.10) [98, 99]. It predicts a second-order SF-MI transition [98, 99], and the phase diagram calculated by the GW shows an exact agreement with that calculated by the perturbative mean-field approximation (PMFA) for spinless bosons [38] which we applied to the spin-1 Bose-Hubbard model in Sec. 3.3.

According to the Gutzwiller ansatz [98], we assume that the ground state wave function of the spin-1 Bose-Hubbard model can be written as a product of single-site wave functions:

\[ |\Psi\rangle = \prod_i |\Phi_i\rangle, \]  

where \(|\Phi_i\rangle\) is the wave function at site \(i\). Since we consider the ground state of a uniform system, \(|\Phi_i\rangle\) is independent of the site index, i.e., \(|\Phi_i\rangle = |\Phi\rangle\). Therefore, we only need to focus on a single site. We drop the site index hereafter.

\(|\Phi\rangle\) can be written as a linear combination of number states as

\[ |\Phi\rangle = \sum_N g(N)|N\rangle, \]  

where \(|N\rangle\) is a state with \(N\) atoms in the site. \(|N\rangle\) can be expanded by the complete set \(|S,m;N\rangle\) introduced in Sec. 3.2. Since \(S + N\) must be even as we noted in Sec. 3.2, we have to distinguish even and odd \(N\) cases. When \(N\) is even (odd), \(S\) can take even (odd) number smaller than \(N\). Thus, the states \(|2n\rangle\) and \(|2n + 1\rangle\) \((n\) is an integer\) can be written as

\[ |2n\rangle = \sum_{S=0}^{2n} f(S,2n)|S,2n\rangle, \]  

\[ |2n + 1\rangle = \sum_{S=1}^{2n+1} f(S,2n + 1)|S,2n + 1\rangle. \]
Here, we define $|S, N \rangle \equiv |S, m = 0; N \rangle$. Without a magnetic field, a complete set required for describing the ground state includes only $|S, m = 0; N \rangle$. It can be numerically confirmed that the ground state energy calculated by the GW with the complete set $|S, m; N \rangle$ $(m = -S, -S + 1 \ldots S)$ is the same as the ground state energy calculated by the GW which includes only $|S, m = 0; N \rangle$ for $N$ up to 6. This is because the ground state in the SF phase is a polar state. In order to obtain the wave function of the ground state, the variational parameters $g(N)$ and $f(S, N)$ are determined to minimize the total energy by Powell’s method \[101\] under the normalization condition

$$\sum_{N}|g(N)|^2 = \sum_{S}|f(S, N)|^2 = 1.$$ (3.78)

We determine the variational parameters $g(N)$ and $f(S, N)$ with $0 \leq N \leq 6$, which is sufficient for the numerical convergence in the parameter regime studied here.

In the SF phase, the order parameter $\psi_\alpha (\alpha = 1, 0, -1)$ is given by

$$\psi_\alpha = \langle \Phi | a_\alpha | \Phi \rangle = \sum_{N} g(N)^* g(N + 1) \langle N | a_\alpha | N + 1 \rangle = \sum_{N} \sum_{S_1, S_2} g(N)^* g(N + 1) f(S_1, N)^* f(S_2, N + 1) \langle S_1, N | a_\alpha | S_2, N + 1 \rangle.$$ (3.79)

Since the $z$-component of the total spin of $|S, N \rangle$ is zero, $\langle S_1, N | a_1 | S_2, N + 1 \rangle = \langle S_1, N | a_{-1} | S_2, N + 1 \rangle = 0$. Thus, the SF phase is a polar state with its order parameter $\psi_1 = \psi_{-1} = 0, \psi_0 \neq 0$.

The average of the hopping term in Eq. (3.4) by $|\Psi \rangle$ is

$$\langle \Psi | H_t | \Psi \rangle = -zt N_{\text{site}} \sum_{\alpha} |\psi_\alpha|^2,$$ (3.80)

where $N_{\text{site}}$ is the number of lattice sites. In the MI state, the order parameter $\psi_\alpha$ vanishes. Therefore, the ground state wave function of the MI phase is determined by the on-site interaction terms in Eq. (3.4), and it reduces to $|0, 0; N \rangle$ for even $N$ and $|1, 0; N \rangle$ for odd $N$.

### 3.5.2 Phase diagram

The phase diagram of the spin-1 Bose-Hubbard model calculated by the GW is shown in Fig. 3.2. The solid and dashed curves are the SF-MI phase boundaries calculated by the GW and the PMFA, respectively. In Fig. 3.2, one can see that the region of the MI state...
3.5. GUTZWILLER'S VARIATIONAL METHOD

Figure 3.2: Phase diagram of the Bose-Hubbard model of spin-1 bosons calculated by the Gutzwiller variational wave function (GW). We set $U_2/U_0 = 0.04$. The solid line is the phase boundary between the SF and MI phases calculated by the GW, and the dashed line is the phase boundary calculated by the perturbative mean-field theory obtained in Sec. 3.3. The inset shows the SF-MI phase boundary for $N = 3$ MI phase when $U_2/U_0 = 0.001$. 
with even number of atoms is modified and becomes smaller than that of the PMFA. We emphasize that the phase boundaries of the two methods coincide for spinless bosons [59]. Therefore, this discrepancy of the phase boundaries is due to the spin degrees of freedom. The region of the MI phase with even number of atoms is still larger than that of the MI phase with odd number of atoms, and the even-odd conjecture predicted by the PMFA in Sec. 3.3 still holds for the phase diagram of the GW.

The phase boundary of the MI state with odd number of atoms appears not to be modified. If we assume smaller $U_2$, the similar change can be seen for the $N \geq 3$ MI region, as well. The inset of Fig. 3.2 shows the phase boundaries obtained by the GW and PMFA for $N = 3$ when $U_2/U_0 = 0.001$. For the $N = 1$ MI phase, the phase boundaries show complete agreement.

The phase diagram of the PMFA can be reproduced by the GW, if the GW is assumed to include only the nonperturbative and intermediate states in the calculation of the second-order perturbation of the PMFA (see Sec 3.3). The phase boundary of the MI state with even number of atoms Eq. (3.4) can be derived analytically by assuming

$$|\Phi\rangle = \sqrt{1 - \epsilon_{2n+1}^2 - \epsilon_{2n-1}^2} |0, 2n\rangle + \epsilon_{2n+1} |1, 2n + 1\rangle + \epsilon_{2n-1} |1, 2n - 1\rangle,$$

(3.81)

where $\epsilon_{2n\pm 1}$ are infinitesimal. $\epsilon_{2n\pm 1}$ can be considered as the coefficients proportional to the order parameter $\psi_\alpha$ and $t$ from the result of PMFA. Thus, one can treat them as infinitesimal parameters near the phase boundary. We can also reproduce the phase boundary of the MI state with odd number of atoms numerically by assuming that the GW only includes $|1, 2n + 1\rangle$, $|0, 2n\rangle$, $|2, 2n\rangle$, $|0, 2n + 2\rangle$, and $|2, 2n + 2\rangle$ and optimize the coefficients of these states.

### 3.5.3 First-order SF-MI transition

In this section, we discuss the reason for the disagreement of the phase boundaries of the GW and PMFA. Hereafter, we call the part of the phase boundary of the GW which does not agree with the phase boundary of the PMFA as the non-perturbative part, and the other part which shows agreement with the phase boundary of the PMFA as the perturbative part.

In Fig. 3.3, the total energy per site $\langle H \rangle$ is shown as a function of $|g(3)|^2$ for various values of $zt/U_0$ for $\mu/U_0 = 1.5$. This parameter regime is across the non-perturbative part of the phase boundary of $N = 2$ MI phase. $|g(3)|^2$ can be regarded as an order parameter of the SF phase, and it is determined from the condition that the total energy takes its minimum value. When $zt/U_0 < 0.184$, $\langle H \rangle$ is minimum at $|g(3)|^2 = 0$ and the ground state is the MI state. When $zt/U_0 > 0.184$, $\langle H \rangle$ is minimum at $|g(3)|^2 \neq 0$, and
Figure 3.3: The total energy per site $\langle H \rangle$ as a function of the superfluid order parameter $|g(3)|$ when $\mu/U_0 = 1.5$ and $U_2/U_0 = 0.04$. Other variational parameters are determined to minimize the energy. The total energy is measured from the energy of the MI state with $N = 2$. 
the ground state becomes the SF phase. One can see that the value of $|g(3)|^2$ minimizing the total energy changes discontinuously. Therefore, the SF-MI phase transition across the nonperturbative part of the phase boundary is of first order.

Figure 3.4 shows the various variational parameters as functions of $\mu/U_0$ along the phase boundary of the $N = 2$ MI phase. Note that these parameters are calculated in the SF phase (only $|g(2)|^2$ is nonzero inside the $N = 2$ Mott phase). The superfluid order parameters $|g(1)|^2$ and $|g(3)|^2$ are finite at the non-perturbative part of the phase boundary ($0.97 < \mu/U_0 < 1.79$), then the phase transition across the non-perturbative part is of first-order. $|g(1)|^2$ and $|g(3)|^2$ vanish on the perturbative part of the phase boundary, and the SF-MI transition becomes second-order. $|f(2, 2)|^2$ and $|f(3, 3)|^2$ are also finite along the non-perturbative part of the phase boundary. This fact indicates that the higher spin states which do not appear in the calculation of the second order perturbation $|S = 2, N = 2\rangle$ and $|S = 3, N = 3\rangle$ are due to the first order phase transition.

If the ratio $U_2/U_0$ is increased, the difference between the phase boundaries calculated by the GW and PMFA disappears, and they coincide completely at a certain value of $U_2/U_0$. The $N = 2$ MI phase boundaries of the GW and PMFA are found to coincide when $U_2/U_0 \sim 0.32$, and the $N = 3$ MI phase boundaries of the GW and PMFA agree when $U_2/U_0 \sim 0.014$.

Figure 3.5 shows the variational parameters at the top of the $N = 2$ Mott lobe in the phase diagram (see Fig. 3.2) as functions of $U_2/U_0$. $zt/U_0$ and $\mu/U_0$ are set as the values corresponding to the top of the $N = 2$ Mott lobe. We note that the top of the Mott lobe stays on the non-perturbative part until the phase boundary of the GW completely coincides with that of the PMFA. $|g(3)|$ and $|g(1)|$ are found to be equal within the numerical errors. The order parameters of the SF phase $|g(1)|^2$ and $|g(3)|^2$ vanish when $U_2 = 0$ and $U_2 \sim 0.32$, and the phase transition becomes second-order when $U_2 = 0$ and $U_2 > 0.32$. $|f(2, 2)|^2$ and $|f(3, 3)|^2$ increase as $U_2/U_0$ decreases and reach their maximum values in the limit of $U_2/U_0 \to 0$. In the limit of $U_0/U_2 \to 0$, the ground state of the SF phase is given by

$$|\Phi\rangle = \sum_N g(N)|N\rangle$$

$$|N\rangle = \frac{1}{\sqrt{N!}}(a_0^\dagger)^N|0\rangle.$$ (3.82)

In Eq. (3.82), $|N = 2\rangle$ and $|N = 3\rangle$ can be rewritten as

$$|N = 2\rangle = \frac{1}{\sqrt{2}}(a_0^\dagger)^2|0\rangle = \frac{1}{\sqrt{3}} \left( |2, 0\rangle + \sqrt{2}|2, 2\rangle \right).$$ (3.83)

$$|N = 3\rangle = \frac{1}{\sqrt{3!}}(a_0^\dagger)^3 = \frac{1}{\sqrt{5}} \left( \sqrt{3}|3, 1\rangle + \sqrt{2}|3, 3\rangle \right).$$ (3.84)
Figure 3.4: The variational parameters of the Gutzwiller wave function as functions of $\mu/U_0$ along the phase boundary of the $N = 2$ MI phase. The black and white circles are for $|g(1)|^2$ and $|g(3)|^2$, and the black and white squares are for $|f(2, 2)|^2$ and $|f(3, 3)|^2$. 
Figure 3.5: The variational parameters of the Gutzwiller wave function as functions of $U_2/U_0$. $zt/U_0$ and $\mu/U_0$ are set as the values corresponding to the top of the $N = 2$ Mott lobe. Here, $|g(3)| = |g(1)|$ within numerical errors. The inset shows the same variational parameters on the $N = 2$ MI phase boundary when $\mu/U_0 = 1.5$. The white circle is for $|g(3)|$. 
3.5. GUTZWILLER’S VARIATIONAL METHOD

From Eqs. (3.83) and (3.84), the variational parameters are expected to be $|f(2,2)|^2 = 2/3$ and $|f(3,3)|^2 = 2/5$ when $U_2 \to 0$, and it is consistent with the result of Fig. 3.5. The inset of Fig. 3.5 shows the variational parameters on the $N = 2$ MI phase boundary when the chemical potential is fixed $\mu/U_0 = 1.5$. We set $zt/U_0$ as the value on the phase boundary for $\mu/U_0 = 1.5$. $|g(3)|$ is different from $|g(1)|$ in this case, and they vanish at $U_2/U_0 \sim 0.15$ where $\mu/U_0 = 1.5$ is on the perturbative part of the phase boundary.

3.5.4 Detection of the first order SF-MI transition

Next, we investigate the possibility of observing the first order SF-MI transition experimentally. We numerically calculate the magnetization (expectation value of the total spin) under a weak magnetic field, and show that a signature of the first-order transition appears.

We consider a uniform magnetic field along the $x$ axis, and add a Zeeman energy term $-g\mu_B B \sum_i S_{xi}$ to the Hamiltonian Eq. (3.4) in order to calculate the magnetization. Here, $g$ is Lande’s $g$-factor, $\mu_B$ is a Bohr magneton, and $B$ is the magnetic field. The quadratic Zeeman term can be neglected, because the magnetic field of the order of mG is sufficient for the measurement of the magnetization [102]. For a uniform magnetic field, the magnetization is site-independent, i.e. $\langle S_{xi} \rangle = \langle S_x \rangle$. In the presence of the magnetic field, we have to include $|S, m; n\rangle$ with $m = -S, -S+1, \ldots, S$ in the GW to prepare a complete set.

Figure 3.6 shows the magnetization as a function of $zt/U_0$ when $U_2/U_0 = 0.04$ and $\mu/U_0 = 1.5$. We set the strength of the magnetic field so that $g\mu_B B/U_0 = 0.005$. It can be clearly seen that $\langle S_x \rangle$ jumps at the boundary of the $N = 2$ MI phase at $zt/U_0 \sim 1.85$. In the MI phase, all atoms make singlet pairs with total spin 0, and energy cost of the order of $U_2$ is needed to break the singlet pairs. Thus, they are stable under the weak magnetic field and have zero magnetization. In the polar SF phase, the excitation spectrum does not have a gap and a finite magnetization can be generated in the weak magnetic field. If the transition is of second order, the superfluid order parameter and the magnetization vanish continuously at the phase boundary. Therefore, the finite jump of the magnetization in Fig. 3.6 can be considered as the result of the first-order phase transition. Magnetization can be measured by Stern-Gerlach type time-of-flight experiment discussed in Ref. [102]. Our prediction can be tested by such experiments.
Figure 3.6: The magnetization $\langle S_x \rangle$ as a function of $zt/U_0$ when $U_2/U_0 = 0.04$ and $\mu/U_0 = 1.5$. We assume a uniform weak magnetic field $g\mu_B B/U_0 = 0.005$. 
3.6 Summary

We have investigated the SF-MI transition of spin-1 bosons in an optical lattice with an antiferromagnetic interaction.

We have calculated the phase boundary between the SF and MI phases using the PMFA and obtained the zero-temperature phase diagram. It was found that all atoms form singlet pairs and have total spin 0 in the MI phase with even number of atoms on each lattice site, while one atom cannot form a singlet pair and each site has the total spin 1 when the MI state has odd number of atoms on each lattice site. We found that the MI phase is strongly stabilized against the SF phase when the number of atoms per lattice site is even compared with the case of the MI phase with an odd number of atoms per site. This is because forming singlet pairs is energetically favorable due to the antiferromagnetic interaction and hopping of atoms is suppressed when the number of atoms per site is even. In an MI phase with an odd number of atoms per site, one atom cannot make a singlet pair and can hop to other sites without the energy cost of breaking a singlet pair. We have determined the order parameter of the SF phase and shown that the SF phase is a polar state as the case for a spin-1 condensate with an antiferromagnetic interaction in a harmonic trap. In order to investigate the spin order of the MI state with odd number of atoms in each site, we derived an effective spin Hamiltonian for the MI with one atom per site.

Next, we have studied the spin-1 Bose-Hubbard model by a variational method with a GW. We have numerically determined the phase boundary of the SF and MI phases and found that the result of the PMFA is modified. The MI phase region obtained by the GW is smaller than that obtained by the PMFA, but the even-odd dependence of the MI phase predicted by the PMFA still holds. It was also found that the SF-MI transition is of first-order at the nonperturbative part of the phase boundary due to higher spin states which are not included in the calculation of the PMFA. We have calculated the magnetization in the presence of a weak magnetic field, and suggested that the first-order transition may be detected by observing the finite jump of the magnetization at the nonperturbative phase boundary by a Stern-Gerlach type experiment.
Chapter 4

Conclusion and outlook

In this thesis, we have studied Bose-Einstein condensates in an optical lattice.

In Chapter 2, we have studied collective excitations of Bose condensates in an optical lattice and their damping. First, we have studied Bose condensates in a deep optical lattice using the tight-binding Bose-Hubbard model. We have extended recent theory for zero temperature to finite temperatures applying the Popov approximation to the Bose-Hubbard model. The spectrum of the Bloch-Bogoliubov excitations at finite temperatures has been derived within the static Popov approximation which neglects the dynamics of the non-condensate atoms. We have calculated the condensate fraction as a function of the temperature and the lattice well depth $s$. We have also discussed the Landau and Beliaev dampings of Bloch-Bogoliubov excitation. The spectrum of Bloch-Bogoliubov excitation $E_q$ must exhibit anomalous dispersion which is bending-up of excitation spectrum at low $q$ for all damping processes including three excitations to occur. In the absence of this feature of the spectrum, the energy conservation condition for the damping process cannot be satisfied and the damping process is prohibited. We have found that the spectrum of Bloch-Bogoliubov excitation in tight-binding approximation exhibits anomalous dispersion when $\alpha = Un^c_0/J < 6d$ where $J$ is the hopping matrix element, $U$ is the on-site interaction, $n^c_0$ is the number of condensate atoms in each lattice site, and $d$ is the dimension of optical lattice. As a consequence, the damping of excitation is absent when $\alpha > 6d$. Using the calculation of the condensate fraction, we have calculated the dimensionless interaction strength $\alpha$ as a function of $s$ and $T$ and estimated the parameter regime where the sudden change of the damping can be observed in experiment. We have derived the spectrum of Bloch-Bogoliubov excitation in a shallow optical lattice by using the Gross-Pitaevskii mean-field theory. The Bogoliubov equations have been solved treating the lattice potential as a perturbation. We have derived the phonon velocity $c$ and the band gap between the first and second excitation bands $\Delta$ which are the extension
In Chapter 2, we have dealt with collective excitation and its damping in a uniform optical lattice. However, most of experiments on Bose-Einstein condensates in an optical lattice have been performed in the presence of a harmonic trap, and the effect of a harmonic trap cannot be ignored. Our theory for a uniform optical lattice is applicable if a Bose condensate could be prepared in an optical lattice with a slowly changing harmonic trap or without a harmonic trap. We believe that our theory can serve as a starting point for understanding recent experiments in the presence of a harmonic trap [35, 57]. Further studies on the topic in Chapter 2 could include the calculation of the Landau and Beliaev dampings around the threshold value of $\alpha \simeq 6d$ considering the linewidth of the spectrum with higher perturbation corrections [79], intercollisional damping of Bloch-Bogoliubov excitations [72, 80, 81], and the calculation of Bloch-Bogoliubov spectrum in a shallow optical lattice with higher order corrections of the lattice potential. As a more important but difficult problem, the description of the superfluid-Mott insulator transition extending the mean-field theory presented in Chapter 2 is still an open problem.

In Chapter 3, we have investigated the superfluid (SF)-Mott insulator (MI) transition of spin-1 bosons with an antiferromagnetic interaction. We have applied the perturbative mean-field theory (PMFA) to the Bose-Hubbard model of spin-1 bosons. Within the PMFA, all atoms form singlet pairs and have total spin 0 in the MI phase with even number of atoms on each lattice site, while one atom cannot form a singlet pair and each site has the total spin 1 in the MI phase with odd number of atoms on each lattice site. The phase boundary between the SF and MI phases has been calculated assuming the phase transition is of second order, and the zero-temperature phase diagram has been obtained. We have found that the MI phase with even number of atoms in each lattice site is strongly stabilized against the SF phase due to the formation of singlet pairs. In the MI phase with odd number of atoms, one atom which is not forming a singlet pair can hop to other sites and the transition to the SF phase occurs for the smaller value of the hopping matrix element than the value for the MI phase with even number of atoms per site. We have also determined the order parameter of the SF phase and shown that the SF phase is a polar state. In order to investigate the spin order of the MI phase with one atom per site, we have derived the effective spin Hamiltonian with a Heisenberg-type exchange term and a quadratic exchange term. We have reexamined the phase diagram of the Bose-Hubbard model of spin-1 bosons with an antiferromagnetic interaction by a variational study with the Gutzwiller-type wave function (GW). We have found that a part of the phase boundary obtained by the PMFA is modified and the MI phase becomes smaller in the new phase diagram obtained by the GW. The SF-MI transition is found to be of first order along the phase boundary obtained by the GW where the phase boundaries of PMFA and GW show a discrepancy. This first order transition is due to the finite
probability density of higher spin states along the phase boundary which reduce kinetic energy. Experiments of spin-1 bosons in an optical lattice have not been done yet. To conclude, we hope that this work will stimulate theoretical studies as well as experiments investigating the SF-MI transition of spin-1 bosons.

We need more detailed studies of the MI phase when the hopping matrix element $t$ is close to the critical value of the SF-MI transition $t_c$, since the MI is always described as the state for $t = 0$ in the mean-field approximation and the Gutzwiller approximation. The competition between the SF-MI transition and the singlet-nematic transition [94] is an open subject. We can apply the Gross-Pitaevskii mean-field theory in Chapter 2 to the Bose-Hubbard model of spin-1 bosons and discuss collective excitation and damping as we did for spinless bosons in Chapter 2. Such a theory would be useful if dynamics of spin-1 Bose condensate would be observed in future experiments.
Appendix A

In this appendix, we show the details of the calculations of the second and fourth order perturbations in Sec. 3.3.1. First, we note the commutation relations between the operators introduced in Sec. 3.2 which can be easily derived from the definitions of the operators in Sec. 3.2,

\[
[S^+, a_1] = -\sqrt{2}a_0, \quad [S^-, a_1] = 0, \quad [S_z, a_1] = -a_1, \quad (A.1)
\]

\[
[S^+, a_0] = -\sqrt{2}a_{-1}, \quad [S^-, a_0] = -\sqrt{2}a_1, \quad [S_z, a_0] = 0, \quad (A.2)
\]

\[
[S^+, a_{-1}] = 0, \quad [S^-, a_{-1}] = -\sqrt{2}a_0, \quad [S_z, a_{-1}] = a_{-1}, \quad (A.3)
\]

\[
[a_1, \Theta^\dagger] = -2a_{-1}^\dagger, \quad [a_0, \Theta^\dagger] = 2a_0^\dagger, \quad [a_{-1}, \Theta^\dagger] = -2a_1^\dagger. \quad (A.4)
\]

By comparing the expressions of \(|S, S; n\rangle\) and \(|S + 1, S + 1; n + 1\rangle\) in Eq. (3.20), we obtain

\[
a_1^\dagger |S, S; n\rangle = \sqrt{\frac{(S + 1)(2Q + 2S + 3)}{2S + 3}} |S + 1, S + 1; n + 1\rangle. \quad (A.5)
\]

By operating \(S^-\) on Eq. (A.5) and using the above commutation relations, the following
relations can be derived

\[
\begin{align*}
a_{\pm 1}|0, 0; n\rangle &= -\sqrt{\frac{n}{3}}|1, \mp 1; n-1\rangle, \quad \text{(A.6)} \\
a_0|0, 0; n\rangle &= \sqrt{\frac{n}{3}}|1, 0; n-1\rangle, \quad \text{(A.7)} \\
a_{\pm 1}^\dagger|0, 0; n\rangle &= \sqrt{\frac{n+3}{3}}|1, \pm 1; n+1\rangle, \quad \text{(A.8)} \\
a_0^\dagger|0, 0; n\rangle &= \sqrt{\frac{n+3}{3}}|1, 0; n+1\rangle, \quad \text{(A.9)} \\
a_{\pm 1}|1, \pm 1; n\rangle &= \sqrt{\frac{n+2}{3}}|0, 0; n-1\rangle - \sqrt{\frac{n-1}{5!!}}|2, 0; n-1\rangle, \quad \text{(A.10)} \\
a_0|1, \pm 1; n\rangle &= \sqrt{\frac{n-1}{5}}|2, \pm 1; n-1\rangle, \quad \text{(A.11)} \\
a_{\mp 1}|1, \pm 1; n\rangle &= -\sqrt{\frac{2(n-1)}{5}}|2, \mp 1; n-1\rangle, \quad \text{(A.12)} \\
a_{\pm 1}|1, 0; n\rangle &= -\sqrt{\frac{n-1}{5}}|2, \mp 1; n-1\rangle, \quad \text{(A.13)} \\
a_0|1, 0; n\rangle &= \sqrt{\frac{n+2}{3}}|0, 0; n-1\rangle + 2\sqrt{\frac{n-1}{5!!}}|2, 0; n-1\rangle, \quad \text{(A.14)} \\
a_{\pm 1}^\dagger|1, \pm 1; n\rangle &= \sqrt{\frac{2(n+4)}{5}}|2, \pm 1; n+1\rangle, \quad \text{(A.15)} \\
a_0^\dagger|1, \pm 1; n\rangle &= \sqrt{\frac{n+4}{5}}|2, \pm 1; n+1\rangle, \quad \text{(A.16)} \\
a_{\mp 1}^\dagger|1, \pm 1; n\rangle &= \sqrt{\frac{n+4}{5!!}}|2, 0; n+1\rangle - \sqrt{\frac{n+1}{3}}|0, 0; n+1\rangle, \quad \text{(A.17)} \\
a_{\pm 1}^\dagger|1, 0; n\rangle &= \sqrt{\frac{n+4}{5!!}}|2, 0; n+1\rangle, \quad \text{(A.18)} \\
a_0^\dagger|1, 0; n\rangle &= 2\sqrt{\frac{n+4}{5!!}}|2, 0; n+1\rangle + \sqrt{\frac{n-1}{3}}|0, 0; n+1\rangle, \quad \text{(A.19)}
\end{align*}
\]
\[ a_{\pm}|2, \pm 2; n\rangle = -\sqrt{\frac{3(n-2)}{7!!}}|3, \pm 1; n-1\rangle + \sqrt{\frac{2(n+3)}{5}}|1, \pm 1; n-1\rangle, \quad (A.20) \]
\[ a_0|2, \pm 2; n\rangle = \sqrt{\frac{n-2}{7}}|3, \pm 2; n-1\rangle, \quad (A.21) \]
\[ a_{\mp}|2, \pm 2; n\rangle = -\sqrt{\frac{3(n-2)}{7}}|3, \pm 3; n-1\rangle, \quad (A.22) \]
\[ a_{\pm}|2, \pm 1; n\rangle = -3\sqrt{\frac{n-2}{7!!}}|3, 0; n-1\rangle + \sqrt{\frac{n+3}{5}}|1, 0; n-1\rangle, \quad (A.23) \]
\[ a_0|2, \pm 1; n\rangle = 2\sqrt{\frac{6(n-2)}{7!!}}|3, \pm 1; n-1\rangle + \sqrt{\frac{n+3}{5}}|1, \pm 1; n-1\rangle, \quad (A.24) \]
\[ a_{\mp}|2, \pm 1; n\rangle = -\sqrt{\frac{2(n-2)}{7}}|3, \pm 2; n-1\rangle, \quad (A.25) \]
\[ a_{\pm}|2, 0; n\rangle = -3\sqrt{\frac{2(n-2)}{7!!}}|3, \mp 1; n-1\rangle + \sqrt{\frac{n+3}{5!!}}|1, -1; n-1\rangle, \quad (A.26) \]
\[ a_0|2, 0; n\rangle = 3\sqrt{\frac{3(n-2)}{7!!}}|3, 0; n-1\rangle + 2\sqrt{\frac{n+3}{5!!}}|1, 0; n-1\rangle, \quad (A.27) \]
\[ a_{\pm}^\dagger|2, \pm 2; n\rangle = \sqrt{\frac{3(n+5)}{7}}|3, \pm 3; n+1\rangle, \quad (A.28) \]
\[ a_0^\dagger|2, \pm 2; n\rangle = \sqrt{\frac{n+5}{7}}|3, \pm 2; n+1\rangle, \quad (A.29) \]
\[ a_{\mp}^\dagger|2, \pm 2; n\rangle = \sqrt{\frac{3(n+5)}{7!!}}|3, \pm 1; n+1\rangle - \sqrt{\frac{2n}{5}}|1, \pm 1; n+1\rangle, \quad (A.30) \]
\[ a_{\pm}^\dagger|2, \pm 1; n\rangle = \sqrt{\frac{2(n+5)}{7}}|3, \pm 2; n+1\rangle, \quad (A.31) \]
\[ a_0^\dagger|2, \pm 1; n\rangle = 2\sqrt{\frac{6(n+5)}{7!!}}|3, \pm 1; n+1\rangle + \sqrt{\frac{n}{5}}|1, \pm 1; n+1\rangle, \quad (A.32) \]
\[ a_{\mp}^\dagger|2, \pm 1; n\rangle = 3\sqrt{\frac{(n+5)}{7!!}}|3, 0; n+1\rangle - \sqrt{\frac{n}{5}}|1, 0; n+1\rangle, \quad (A.33) \]
\[ a_{\pm}^\dagger|2, 0; n\rangle = 3\sqrt{\frac{2(n+5)}{7!!}}|3, \pm 1; n+1\rangle - \sqrt{\frac{n}{15}}|1, \pm 1; n+1\rangle, \quad (A.34) \]
\[ a_0^\dagger|2, 0; n\rangle = 3\sqrt{\frac{3(n+5)}{7!!}}|3, 0; n+1\rangle + 2\sqrt{\frac{n}{15}}|1, 0; n+1\rangle. \quad (A.35) \]
Using above relations, one can calculate the matrix elements in Eq. (3.33). It is convenient to classify the first term of the right hand side of Eq. (3.33) by the second order intermediate state $|p\rangle$. $|p\rangle$ can be $|0,0;n\pm2\rangle$, $|2,m;n\pm2\rangle$ and $|2,m;\rangle$ where $-2 \leq m \leq 2$. If we note the contribution from the processes with $|p\rangle$ to the right hand side of Eq. (3.33) as $E_n^{(4)}(p)$, we obtain

$$E_n^{(4)}(0,0; n+2) + E_n^{(4)}(0,0; n-2) = -\frac{1}{9}\left[ \frac{n(n+1)}{\Delta E(1,n-1)^2\Delta E(0,n-2)} + \frac{(n+2)(n+3)}{\Delta E(1,n+1)^2\Delta E(0,n+2)} \right] \times n^2_s|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2(zt)^4,$$

(A.36)

$$\sum_{-2 \leq m \leq 2} E_n^{(4)}(2,m; n-2) = \frac{2n(n-2)}{45} \frac{1}{\Delta E(1,n-1)^2\Delta E(2,n-2)} \times \left( n^2_s|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 - 3(\vec{\psi}^\dagger \cdot \vec{\psi})^2 \right) (zt)^4,$$

(A.37)

$$\sum_{-2 \leq m \leq 2} E_n^{(4)}(2,m; n) = -\frac{n(n+3)}{45} \left( \frac{1}{\Delta E(1,n+1)} + \frac{1}{\Delta E(1,n-1)} \right)^2 \frac{1}{\Delta E(2,n)} \times \left( 3n^2_s|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 + (\vec{\psi}^\dagger \cdot \vec{\psi})^2 \right) (zt)^4,$$

(A.38)

$$\sum_{-2 \leq m \leq 2} E_n^{(4)}(2,m; n+2) = \frac{2(n+3)(n+5)}{45} \frac{1}{\Delta E(1,n+1)^2\Delta E(2,n+2)} \times \left( n^2_s|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 - 3(\vec{\psi}^\dagger \cdot \vec{\psi})^2 \right) (zt)^4.$$

(A.39)

Here $\Delta E^{(0)}(S, l) \equiv E^{(0)}(S, l) - E^{(0)}(0, n) > 0$. The last term of the right hand side of Eq. (3.33) is

$$\sum_n \frac{|\langle i|\mathbf{V}|n\rangle|^2}{(E_i^{(0)} - E_n^{(0)})^2} = \frac{1}{3} \left( \frac{n+3}{\Delta E(1,n+1)^2} + \frac{n}{\Delta E(1,n-1)^2} \right) (zt)^3(\vec{\psi}^\dagger \cdot \vec{\psi}).$$

(A.40)

Combining Eqs. (A.36)~(A.40), Eqs. (3.34), (3.35) and (3.36) are obtained.
Appendix B

In this appendix, we show the details of the calculation in Sec. 3.3.2. From Eq. (3.41), $E^{(2)}_n$ is the eigenvalue of the matrix

$$M_{m,m'} \equiv \langle 1, m; n | V \frac{1}{E^{(0)}(1, n) - H_0} V | 1, m'; n \rangle \\
= \sum l \langle 1, m; n | V | l \rangle \langle l | V | 1, m'; n \rangle \quad (E^{(0)}(1, n) - E^{(0)}_l). \quad (B.1)$$

Using Eqs. (A.10)~(A.35), operating with $V$ on $|1, m; n \rangle$ yields

$$V | 1, 1; n \rangle = -zt \left[ \psi_1^* \left( \sqrt{\frac{n+2}{3}} | 0, 0; n-1 \rangle - \sqrt{\frac{n-1}{15}} | 2, 0; n-1 \rangle \right) \\
+ \psi_1 \sqrt{\frac{2(n+4)}{5}} | 2, 2; n+1 \rangle \\
+ \psi_0^* \sqrt{\frac{n-1}{5}} | 2, 1; n-1 \rangle + \psi_0 \sqrt{\frac{n+4}{5}} | 2, 1; n+1 \rangle \\
- \psi_{-1}^* \sqrt{\frac{2(n-1)}{5}} | 2, 2; n-1 \rangle \\
+ \psi_{-1} \left( \sqrt{\frac{n+4}{15}} | 2, 0; n+1 \rangle - \sqrt{\frac{n+1}{3}} | 0, 0; n+1 \rangle \right) \right] \quad (B.2)$$

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\[ V|1, 0; n\rangle = -zt \left[ -\psi_1^* \sqrt{\frac{n-1}{5}} |2, -1; n - 1\rangle + \psi_1 \sqrt{\frac{n+4}{5}} |2, 1; n + 1\rangle ight. \\
+ \psi_0^* \left( \sqrt{\frac{n+2}{3}} |0, 0; n - 1\rangle + 2 \sqrt{\frac{n-1}{15}} |2, 0; n - 1\rangle \right) \\
+ \psi_0 \left( 2 \sqrt{\frac{n+4}{15}} |2, 0; n + 1\rangle + \sqrt{\frac{n+1}{3}} |0, 0; n + 1\rangle \right) \\
\left. - \psi_{-1}^* \sqrt{\frac{n-1}{5}} |2, 1; n - 1\rangle + \psi_{-1} \sqrt{\frac{n+4}{5}} |2, -1; n + 1\rangle \right], \quad (B.3) \\

\[ V|1, -1; n\rangle = -zt \left[ -\psi_1^* \sqrt{\frac{2n-2}{5}} |2, -2; n - 1\rangle ight. \\
+ \psi_1 \left( \sqrt{\frac{n+4}{15}} |2, 0; n + 1\rangle - \sqrt{\frac{n+1}{3}} |0, 0; n + 1\rangle \right) \\
+ \psi_0^* \sqrt{\frac{n-1}{5}} |2, 1; n - 1\rangle + \psi_0 \sqrt{\frac{n+4}{5}} |2, 1; n + 1\rangle \\
+ \psi_{-1}^* \left( \frac{n+2}{3} |0, 0; n - 1\rangle - \sqrt{\frac{n-1}{15}} \right) \\
+ \psi_{-1} \sqrt{\frac{2(n+4)}{5}} |2, -2; n + 1\rangle \right]. \quad (B.4) \]
From the above equations, the matrix elements of $M_{m,m'}$ are given by

$$M_{1,1} = -(zt)^2 \left[ \alpha |\psi_1|^2 + \beta (|\psi_1|^2 + 3|\psi_0|^2 + 6|\psi_\text{-1}|^2) 
+ \gamma |\psi_\text{-1}|^2 + \delta (6|\psi_1|^2 + 3|\psi_0|^2 + |\psi_\text{-1}|^2) \right]$$  \hspace{1cm} (B.5)

$$M_{1,0} = -(zt)^2 \left[ \alpha \psi_0^* \psi_{1} - \beta (2\psi_0^* \psi_{1} + 3\psi_0^* \psi_{\text{-1}})
- \gamma \psi_0 \psi_{\text{-1}} + \delta (3\psi_1 \psi_{0}^* + 2\psi_0 \psi_0^* \psi_{\text{-1}}) \right]$$  \hspace{1cm} (B.6)

$$M_{1,-1} = -(zt)^2 \left[ \alpha \psi_1^* \psi_{\text{-1}} + \beta \psi_1 \psi_{\text{-1}}^*
+ \gamma \psi_1 \psi_{\text{-1}}^* + \delta \psi_1 \psi_{\text{-1}}^* \right]$$  \hspace{1cm} (B.7)

$$M_{0,0} = -(zt)^2 \left[ \alpha |\psi_0|^2 + \beta (3|\psi_1|^2 + 4|\psi_0|^2 + 3|\psi_\text{-1}|^2)
+ \gamma |\psi_\text{-1}|^2 + \delta (3|\psi_1|^2 + 4|\psi_0|^2 + 3|\psi_\text{-1}|^2) \right]$$  \hspace{1cm} (B.8)

$$M_{0,-1} = -(zt)^2 \left[ \alpha \psi_0 \psi_{\text{-1}}^* - \beta (3\psi_1 \psi_{0}^* + 2\psi_0 \psi_1^*)
- \gamma \psi_0 \psi_{\text{-1}} + \delta (2\psi_1 \psi_{0}^* + 3\psi_0 \psi_1^*) \right]$$  \hspace{1cm} (B.9)

$$M_{-1,-1} = -(zt)^2 \left[ \alpha |\psi_\text{-1}|^2 + \beta (6|\psi_1|^2 + 3|\psi_0|^2 + |\psi_\text{-1}|^2)
+ \gamma |\psi_1|^2 + \delta (|\psi_1|^2 + 3|\psi_0|^2 + |\psi_\text{-1}|^2) \right]$$  \hspace{1cm} (B.10)

where $\alpha = \frac{n+2}{3} \frac{1}{\Delta E^{(0)}(0,n-1)}$, $\beta = \frac{n-1}{15} \frac{1}{\Delta E^{(0)}(2,n-1)}$, $\gamma = \frac{n+1}{3} \frac{1}{\Delta E^{(0)}(0,n+1)}$, $\delta = \frac{n+4}{15} \frac{1}{\Delta E^{(0)}(2,n+1)}$, and $\Delta E^{(0)}(S,l) \equiv E^{(0)}(S,l) - E^{(0)}(1,n) > 0$. Other matrix elements can be obtained from $M_{m,m'}^* = M_{m,m'}$. 
Bibliography


BIBLIOGRAPHY


[58] A. Auerbach, Interaction Electrons and Quantum Magnetism (Springer-Verlag, 1994).


[61] S. Tsuchiya and A. Griffin (to be published).


BIBLIOGRAPHY

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