Internal Josephson Oscillations for Distinct Momenta Bose-Einstein Condensates

Master Thesis

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Abstract

The internal Josephson oscillations between an atomic Bose-Einstein condensate (BEC) and a molecular one are studied for atoms in a square optical lattice subjected to a staggered gauge field. The system is described by a Bose-Hubbard model with complex and anisotropic hopping parameters, which are different for each species, atoms and molecules. When the flux per plaquette for each species is small, the system oscillates between two conventional zero-momentum condensates. However, there is a regime of parameters where Josephson oscillations between a vortex-carrying atomic condensate (finite momentum BEC) and a conventional zero-momentum molecular condensate may be realized. The experimental observation of the oscillations between these qualitatively distinct BEC’s is possible with state of the art Ramsey interference techniques.
## Contents

1 Introduction 2  

2 Preliminaries 4  

2.1 Atoms in Optical Lattices 4  
2.2 Bose-Hubbard Model 5  
  2.2.1 Superfluid to Mott-Insulator Transition 6  
  2.2.2 Global Phase Invariance 13  
2.3 Staggered Vortex Superfluid 13  
  2.3.1 Finite Momentum Superfluid 17  

3 Molecule Formation in Optical Lattices 24  

3.1 Feshbach Resonances in Optical Lattices 24  
3.2 Two Particle Scattering 27  
  3.2.1 Scattering in the Generalized Bose-Hubbard model 31  

4 Bogoliubov Theory for Atoms and Molecules 34  

4.1 Condensation of Molecules 34  
4.2 Condensation of Atoms and Molecules 36  
4.3 Condensation of Atoms and Molecules in the Generalized Bose-Hubbard  
  Model 39  

5 Conclusion 46  

A Bloch States and Band Structure 49  

B Wannier Functions and Periodic Potentials 54  

C Approximate Values for Hopping and Interaction Parameters 56  

D Time-Ordered Two-Particle Correlation Functions 58
Chapter 1

Introduction

The ability of controlling the dynamics of complex quantum systems would open the perspectives for both, fundamental and applied physics realizations. A high degree of quantum coherence is a crucial requirement for the implementation of quantum logic devices, for instance.

The Josephson effect allows one to measure the degree of coherence between different quantum states. In addition to the spatial Josephson effect, where two superconductors are coupled by a weak link and particles in different reservoirs do not interact, there is also the internal Josephson effect, where particles in different internal states do interact. In this case, the internal states act as the two reservoirs and an external magnetic field provides the weak link between them, similar to the tunneling coupling through a barrier in the spatial Josephson effect.

An external magnetic field may couple different spin states, as originally reported by Rabi [1], who studied the time dependent dynamics of a spin subject to an external time-varying magnetic field, or connect atomic and molecular states in ultracold Bose-Einstein condensates (BECs). Indeed, a quantum superposition of two chemically different species (atoms and molecules), each one in a zero-momentum ground state, has been observed by means of Ramsey-like interference experiments for BECs in a trap [2, 3], and the data showed a good agreement with theoretical predictions [4, 5]. Later, an atomic Bose gas in an optical lattice was investigated theoretically [6], and the zero temperature phase diagram, showing the filling fraction per site $n$ versus the detuning $\delta$ was determined in a regime near the Feshbach resonance.

It was shown recently that a synthetic local magnetic flux, alternating in sign between neighboring plaquettes in a two-dimensional (2D) square optical lattice, can be generated by counter-propagating bichromatic light fields, with the frequency of one laser component slightly dephased with respect to the other [7, 8]. This configuration gives rise to an interesting single-particle spectrum, with two inequivalent Dirac cones and a minimum energy that depends on the value of the flux $\phi$ per plaquette. For $\phi < \pi/4$, bosons loaded into this lattice condense at zero momentum, whereas for $\phi > \pi/4$ a finite angular momentum BEC takes place, which carries a vortex-antivortex lattice [8]. This setup thus opens the possibility to realize two different types of condensate upon varying the flux. In addition, when manipulating the interactions in the system by means of a Feshbach resonance, a bound state of two bosonic atoms (a molecule) can occur, thus raising even further the parameter space for the realization of different BECs: indeed,
each type of particles, atoms (species 1) and molecules (species 2) can, in principle, condense either at zero or at finite angular momentum.

In this thesis, we propose a way to realize a quantum superposition of different species with different momenta, zero for the atomic condensate and finite for the molecular one. This work represents a step further in the precise control of ultracold systems and the realization of more complex BECs. As in the spatial Josephson problem, there are three regimes for the internal one, depending on the strength of the coupling between the internal states [9]. If the coupling between the states (external field) is much stronger than the interactions between the same species, the system is said to be in the Rabi regime, where large oscillations in the density of each internal state take place. In the opposite limit, when the external field is extremely weak, the system is in the Fock regime: density oscillations are negligible and the phase difference between the two states evolves freely. Between these two regimes there is the Josephson regime, where the density imbalance between the two internal states undergoes small oscillations, similar to the spatial Josephson effect.

The remainder of this thesis is structured as follows: In chapter 2, we review the possibility of trapping ultracold bosonic atoms in optical lattices through the Stark effect. We then give a brief introduction to the Bose-Hubbard model, that is used to describe cold atoms in optical lattices in the tight binding regime and review the two phases the system can realize, a uniform superfluid state and the so-called Mott-insulating state. We will introduce the above mentioned generalization of the Bose-Hubbard model with a staggered flux and explore the finite-momentum superfluid phase that is made accessible thereby, in addition to the two phases of the conventional Bose-Hubbard model.

In chapter 3, we review the possibility of molecule formation in optical lattices. In addition to the concept of Feshbach resonances in optical lattices, we also look at the formation of diatomic molecules through energy conservation in the lattice, made accessible by applying two-particle scattering theory. Specifically, we utilize scattering theory to predict the existence of molecular states in the generalized model with a staggered flux.

In chapter 4, we utilize Bogoliubov theory to determine the excitation spectrum of a system that contains both a molecular and an atomic Bose-Einstein condensate. We will see that an internal Josephson effect takes place in the system, leading to oscillations between the densities of atomic and molecular condensates. Specifically, we extract the Josephson frequency describing these oscillations, for both a model resembling the conventional Bose-Hubbard model as well as for the generalized model incorporating a staggered flux. The latter case is interesting in particular, since it will give rise to oscillations between the densities of atomic and molecular condensates of distinct momenta.
Chapter 2

Preliminaries

2.1 Atoms in Optical Lattices

Let us consider a standing wave that is produced by two counterpropagating laser beams, given by \( E(x, t) = \hat{\epsilon} E(x) \cos(\omega t) \), where \( \hat{\epsilon} \) is the polarization vector. We want to calculate the interaction of this field with an atom through the AC-Stark effect, following the treatment in Ref. [10]. The dipole moment of an atom with \( n \) electrons is given by

\[
D = -e \sum_{i=1}^{n} \mathbf{r}_i,
\]

where we sum over the position vectors \( \mathbf{r}_i \) that point from the nucleus of the atom to the electron indexed by \( i \). The interaction Hamiltonian of the atom with the field is given by

\[
H_{\text{int}} = -D \cdot \mathbf{E}.
\]

If we restrict our attention to alkali atoms like rubidium, the significant contribution to the interaction will be given by the valence electrons and we can neglect the contribution of the electrons in the closed shells, because those contributions will average out to yield a zero potential. Applying perturbation theory to \( H_{\text{int}} \) according to

\[
H_{\text{int}} \approx H^{(0)} + H^{(1)} + H^{(2)} + ...
\]

We find that the first order perturbation \( H^{(1)} = \langle g|H_{\text{int}}|g \rangle \) is zero, because the ground state \( |g \rangle \) of the alkali atoms has positive parity, while the parity of \( D \) is odd. Thus, the first correction comes from the second order perturbation. It is given by

\[
E_{\text{int}}^{(2)} = \frac{1}{4} \sum_{l \neq g} |\langle l|D \cdot \hat{\epsilon}|g \rangle|^2 \left( \frac{1}{E_l - E_g - \hbar \omega} + \frac{1}{E_l - E_g + \hbar \omega} \right) |E(x)|^2 \cos^2(\omega t),
\]

where the two terms in the sum correspond to emission and absorption of a photon with the energy \( \hbar \omega \) by the atom in question. This can be written as

\[
E_{\text{int}}(x, t) \approx V_0 |E(x, t)|^2.
\]
This result is very useful, because now we can set up a d-dimensional optical potential, for example by producing a standing wave with a number of counter-propagating lasers, which interact with the alkali atoms through the corresponding interaction Hamiltonian

\[ V_{\text{optic}} = V_0 \sum_{i=1}^{d} \cos^2(kx_i), \quad (2.1) \]

where \( k \) is given in terms of the wavelength \( \lambda \) of the lasers in question according to \( k = 2\pi/\lambda \) and \( d \) denotes the dimension of the optical lattice. In this manner, we can build an optical lattice that has the potential to trap alkali atoms on particular lattice sites. Depending on the depth of the lattice-potential \( V_0 \) they will be more or less likely to tunnel between different sites, as we will see.

### 2.2 Bose-Hubbard Model

The motion of bosonic atoms in an optical lattice set up by the potential (2.1) in the tight-binding approximation can be described by the Bose-Hubbard model (see Appendix B),

\[ H = H_0 + H_U = -J \sum_{<i,j>} a_i^\dagger a_j^\dagger a_j a_i + \frac{U}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i, \quad (2.2) \]

with the bosonic creation and annihilation operators \( a_i^\dagger \) and \( a_i \). We sum over the lattice sites that we denote here by \( i \) or \( j \), and the \( <i,j> \) in the first sum indicates that we sum over all neighboring pairs of lattice sites in the system. The first term in the Hamiltonian \( H_0 \) corresponds to the kinetic energy of the atoms and describes hopping between neighboring lattice sites. The hopping strength \( J \) describes the amount of energy gained by an atom by tunneling between neighboring lattice sites and the interaction parameter \( U \) gives the interaction strength between two particles on the same site. If

![Figure 2.1: Schematic plot of the motion of atoms in an optical lattice described by the Bose-Hubbard model. Included are the hopping parameter \( J \), the interatomic interaction strength \( U \) and the depth of the lattice, \( V_0 \).](image)

we approximate the optical potential on each lattice site as harmonic oscillators (see Appendix C), we can estimate the hopping and interaction parameters \( J \) and \( U \),

\[ J = d\sqrt{V_0 E_R} e^{-\frac{\pi^2}{4} \frac{V_0}{E_R}}, \]

\[ U = \frac{4\pi \hbar^2}{m} \frac{1}{(2\pi)^{d/2}} \frac{a_s}{l}, \]
where $V_0$ is the amplitude of the optical potential and $E_R$ the recoil energy,

$$E_R = \frac{(2\pi \hbar)^2}{2m} \frac{1}{\lambda^2},$$

which is the amount of energy that an atom initially at rest picks up after absorbing one photon from the lattice laser. Here, $m$ denotes the mass of the atom, $l = \sqrt{\hbar/m\omega}$ the oscillator length and $a_s$ the s-wave scattering length of the atoms. A more careful treatment involving the calculation of the corresponding Wannier functions shows that the harmonic approximation underestimates the hopping parameter. A schematic plot of the concepts described by the Bose-Hubbard model is shown in Figure 2.1.

### 2.2.1 Superfluid to Mott-Insulator Transition

The Bose-Hubbard Hamiltonian describes two phases, a superfluid phase and the so-called Mott-insulator phase. If the hopping term $J$ is much larger than $U$, the energy corresponding to hopping between the sites will be far greater than that corresponding to the on-site interaction energy, in which case we are dealing with a superfluid. If $U$ is much larger than $J$, the condensate freezes and hopping between the sites is negligible, in which case we have a Mott insulator. It is therefore sensible to assume that there should be a critical value of $U/J$ at which the transition between the two phases occurs. We want to determine this critical value, following the procedure used in Ref. [11].

Let us write the Bose-Hubbard Hamiltonian in the grand canonical representation by adding a chemical potential $\mu$,

$$H = -J \sum_{<i,j>} a_i^\dagger a_j - \mu \sum_i a_i^\dagger a_i + \frac{U}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i.$$

Using the mean-field approximation $\langle a_i \rangle = \Psi$, $\langle a_i^\dagger \rangle = \Psi^\dagger$ we find that

$$a_i^\dagger a_j \approx \Psi^* a_j + a_i^\dagger \Psi - |\Psi|^2.$$

The Hamiltonian now reads

$$H_{\text{eff}} = zJ|\Psi|^2N - zJ \sum_i \left( \Psi^* a_i + a_i^\dagger \Psi \right) + \frac{U}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i - \mu \sum_i a_i^\dagger a_i,$$

where $z$ equals the number of nearest neighbors and $N$ the total number of lattice sites in the system. Now, we perform the substitution

$$U \rightarrow zJU, \quad \mu \rightarrow zJ\mu, \quad n_i = a_i^\dagger a_i,$$

and write

$$H_{\text{eff}} = zJ \sum_i H_i,$$

with

$$H_i = \frac{U}{2} n_i(n_i - 1) - \mu n_i - \Psi^* a_i - a_i^\dagger \Psi + |\Psi|^2.$$
We write this as

\[ H_i = H_0 + \Psi V_1 + \Psi^* V_2, \]

where

\[ H_0 = \frac{U}{2} n_i(n_i - 1) - \mu n_i + |\Psi|^2, \quad V_1 = -a_i^\dagger, \quad V_2 = -a_i. \]

Now, define \( E_g^{(0)} \) as the unperturbed ground-state energy with \( g \) particles per site, corresponding to \( H_0 \), given by

\[ E_g^{(0)} = \frac{U}{2} g(g - 1) - \mu g \equiv c_0, \quad (2.3) \]

and write the second order perturbation correction to the ground state energy as

\[ E_g^{(2)} = |\Psi|^2 \sum_{n \neq g} \frac{|\langle n | V_i | g \rangle|^2}{E_g^{(0)} - E_n^{(0)}}, \]

where \( |n \rangle \) is the unperturbed wave function with \( n \) particles. The interaction \( V_i \) couples states with one atom more or less than there are in the ground state, so we find

\[ E_g^{(2)} = |\Psi|^2 \left[ g \frac{g}{U(g - 1) - \mu} + \frac{g + 1}{\mu - Ug} \right] \equiv c_2 - 1, \]

and therefore we can now write

\[ E_g(\Psi) = c_0 + c_2 |\Psi|^2 + O(|\Psi|^4), \]

because the expansion in odd powers of \( \Psi \) is zero. The Mott-insulator to superfluid transition is a second-order phase transition, which is therefore expected to occur when \( c_2 = 0, \)

\[ c_2 = \frac{g}{U(g - 1) - \mu} + \frac{g + 1}{\mu - Ug} + 1 = 0, \]

where the factor +1 originates from the \( |\Psi^2| \) term in \( H_0 \). We find

\[ \mu_{\pm} = \frac{1}{2} [U(2g - 1) - 1] \pm \frac{1}{2} \sqrt{U^2 - 2U(2g + 1) + 1}. \quad (2.4) \]

The characteristic form of the values for the chemical potential \( \mu \) as a function of the interatomic interaction strength \( U \), that can be seen in Figure 2.2, are called Mott lobes. Now, equate \( \mu_{+} \) and \( \mu_{-} \) to find the point of smallest \( U \),

\[ U_c = 2g + 1 + \sqrt{(2g + 1)^2} - 1. \]

Shift back to

\[ U \rightarrow U \frac{U}{zJ}, \]

7
and choose the ground state with $g = 1$ particle per site to see that

$$U_c / zJ \approx 5.83,$$

at the Mott-insulator to superfluid transition. We thus found the critical value of $U / J$ that we were looking for. For a larger value of $U / J$ the system is expected to be in the Mott-insulator phase, whereas for smaller values it is in the superfluid phase.

The same calculation can be performed using an alternative procedure, first laid out in [11]. We consider the action corresponding to the Bose-Hubbard Hamiltonian

$$S[a^*, a] = \int_0^{\hbar \beta} d\tau \left[ \sum_i a_i^*(\tau) \left( \hbar \partial_\tau - \mu \right) a_i(\tau) - \sum_{i,j} J_{ij} a_i^*(\tau) a_j(\tau) + \frac{U}{2} \sum_i a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau) \right] \right. \left. - \sum_{i,j} J_{ij} \left[ a_i^*(\tau) \Psi_j(\tau) + \Psi_i^*(\tau) a_j(\tau) \right] + \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau) \right] \right].$$

We would like to decouple the hopping between different sites, therefore we perform a Hubbard-Stratonovitch transformation by introducing the order-parameter fields $\Psi$ and $\Psi^*$. This is done by inserting

$$1 = \int D\Psi^* D\Psi \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar \beta} d\tau \sum_{i,j} \left[ \Psi_i^*(\tau) - a_i^*(\tau) \right] J_{ij} \left[ \Psi_j(\tau) - a_j(\tau) \right] \right\},$$

which amounts to replacing the action $S[a^*, a]$ by a new action $S[a^*, a, \Psi^*, \Psi]$, given by

$$S[a^*, a, \Psi^*, \Psi] = S[a^*, a] + \int_0^{\hbar \beta} d\tau \sum_{i,j} \left[ \Psi_i^*(\tau) - a_i^*(\tau) \right] J_{ij} \left[ \Psi_j(\tau) - a_j(\tau) \right],$$

so that we arrive at

$$S[a^*, a, \Psi^*, \Psi] = \int_0^{\hbar \beta} d\tau \left\{ \sum_i a_i^*(\tau) \left[ \hbar \partial_\tau - \mu \right] a_i(\tau) + \frac{U}{2} \sum_i a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau) \right. \left. - \sum_{i,j} J_{ij} \left[ a_i^*(\tau) \Psi_j(\tau) + \Psi_i^*(\tau) a_j(\tau) \right] + \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau) \right\}.$$
We denote the action for $J_{ij} = 0$ (corresponding to no hopping between the sites) by $S^{(0)}$ and integrate over the fields $a_i$ and $a_i^*$ to arrive at

$$\exp \left\{ -\frac{S}{\hbar} \right\} = \exp \left\{ -\frac{1}{\hbar} \int_0^{h\beta} d\tau \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau) \right\}$$

$$\times \int D a^* D a e^{-\frac{1}{\hbar} S^{(0)}[a^*,a]} \exp \left\{ -\frac{1}{\hbar} \int_0^{h\beta} d\tau \left[ -\sum_{i,j} J_{ij} (a_i^*(\tau) \Psi_j(\tau) + \Psi_i^*(\tau) a_j(\tau)) \right] \right\}.$$ 

Let us define the average of a functional $A[a^*,a]$ as

$$\langle A[a^*,a] \rangle_{S^{(0)}} = \int D a^* D a A[a^*,a] e^{-\frac{1}{\hbar} S^{(0)}[a^*,a]}.$$ 

We can now expand the exponential according to

$$\int D a^* D a e^{-\frac{1}{\hbar} S^{(0)}[a^*,a]} e^{M[a^*,a]} = \langle 1 \rangle_{S^{(0)}} + \langle M[a^*,a] \rangle_{S^{(0)}} + \frac{\langle M[a^*,a]^2 \rangle_{S^{(0)}}}{2} + \ldots$$

We will use

$$\langle a_i \rangle_{S^{(0)}} = \langle a_i^* \rangle_{S^{(0)}} = 0,$$

to see that the terms in the expansion which are linear in the fields $a$ and $a^*$ do not contribute. Re-exponentiation yields

$$S^{(2)}[\Psi^*,\Psi] = -\frac{1}{2\hbar} \left\langle \left( \int_0^{h\beta} d\tau \sum_{i,j} J_{ij} [a_i^*(\tau) \Psi_j(\tau) + \Psi_i^*(\tau) a_j(\tau)] \right)^2 \right\rangle_{S^{(0)}}$$

$$+ \int_0^{h\beta} d\tau \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau)$$

$$= -\frac{1}{2\hbar} \left\langle \int_0^{h\beta} d\tau \int_0^{h\beta} d\tau' \sum_{i,j,i',j'} J_{ij} J_{i'j'} [a_i^*(\tau) \Psi_j(\tau)$$

$$+ \Psi_i^*(\tau) a_j(\tau)] [a_i^*(\tau) \Psi_j(\tau) + \Psi_i^*(\tau) a_j(\tau)] \right\rangle_{S^{(0)}}$$

$$+ \int_0^{h\beta} d\tau \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau).$$

We know about the unperturbed system that the particles cannot hop to another lattice site, thus

$$\langle a_i a_j \rangle_{S^{(0)}} = \langle a_i^* a_j^* \rangle_{S^{(0)}} = 0,$$

$$\langle a_i^* a_j \rangle_{S^{(0)}} = \langle a_i a_j^* \rangle_{S^{(0)}} = \langle a_i^* a_i \rangle_{S^{(0)}} = \delta_{i,j},$$

9
and we find

\[ S^{(2)}[\Psi^*, \Psi] = \int_{0}^{\hbar \beta} d\tau \left\{ \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau) \right. \]

\[ \left. - \frac{1}{\hbar} \int_{0}^{\hbar \beta} d\tau' \sum_{i,j,k,j'} J_{ij} J_{ij'} \Psi_j^*(\tau) \langle a_i(\tau) a_{i'}^*(\tau') \rangle S(0) \Psi_{j'}(\tau') \right\}, \]

where we made use of the fact that \( J_{ij} = J_{ji} \). From now on, we will consider only nearest-neighbor hopping. As we already know, the first term in \( S^{(2)} \) can then be written as

\[ \sum_{i,j} J_{ij} \Psi_i^*(\tau) \Psi_j(\tau) = \sum_{k} 2J \Psi_k(\tau) \Psi_k^*(\tau) \sum_{j=1,d} \cos(d_i k_j). \]

The part of \( S^{(2)} \) that is quadratic in \( J_{ij} \) now amounts to double-jumps. We find that

\[ \sum_{i,j,j',j''} J_{ij} J_{ij'} \Psi_j^*(\tau) \langle a_i(\tau) a_{i'}^*(\tau') \rangle S(0) \Psi_{j'}(\tau') \]

\[ = \sum_i \langle a_i(\tau) a_i^*(\tau') \rangle S(0) \sum_{j,j'} J_{ij} J_{ij'} \Psi_j^*(\tau) \Psi_{j'}(\tau') \]

\[ = \sum_i J^2 \langle a_i(\tau) a_i^*(\tau') \rangle S(0) \sum_{j} \left\{ z \Psi_j^*(\tau) \Psi_j(\tau') \right. \]

\[ \left. + z \Psi_j^*(\tau) \Psi_{j\pm \{2\}}(\tau') + z \Psi_j^*(\tau) \Psi_{j\pm \{2\}}(\tau') \right\}. \]

The first term denotes a jump in one direction followed by a jump back, the second term denotes two jumps in the same direction and the third term represents two successive jumps in perpendicular directions. We manipulate the double-jumps in yet a different way,

\[ J^2 \sum_{m,j,j',l,j''} \Psi_j^*(\tau) \Psi_{j'}(\tau') \delta_{j,m+\epsilon_l} \delta_{j',m+\epsilon_l'} \]

\[ = \frac{J^2}{N} \sum_{m,j,j',l,l',k,k'} \Psi_k^*(\tau) \Psi_{k'}(\tau') \delta_{j,m+\epsilon_l} \delta_{j',m+\epsilon_l'} e^{ik_j} e^{-ik_j'} \]

\[ = \frac{J^2}{N} \sum_{m,l',k,k'} \Psi_k^*(\tau) \Psi_{k'}(\tau') e^{ik(m+\epsilon_l)} e^{-ik'(m+\epsilon_l')} \]

\[ = J^2 \sum_{l,l',k} \Psi_k^*(\tau) \Psi_k(\tau') e^{ik\epsilon_l} e^{-ik\epsilon_l'} \]

\[ = \sum_k \Psi_k^*(\tau) \Psi_k(\tau') \right\} \]

with \( \epsilon_k = -2J \sum_{j=1,d} \cos(d_i k_j) \). Now we want to treat the time-dependence of the fields by introducing Matsubara frequencies \( \hbar \omega_n = 2\pi n / \hbar \beta \) according to

\[ \Psi_k(\tau) = \frac{1}{\sqrt{\hbar \beta}} \sum_n \Psi_{kn} e^{-i\omega_n \tau}, \quad \Psi_k^*(\tau) = \frac{1}{\sqrt{\hbar \beta}} \sum_n \Psi_{kn}^* e^{i\omega_n \tau}. \]
Introduce an imaginary time-ordering operator $T$ to translate the expectation value of fields into the expectation value of operators,

$$
\langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} = \langle T[a_i(\tau)a_i^*(\tau')] \rangle_{S(0)} = \theta(\tau - \tau') \langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} + \theta(\tau' - \tau) \langle a_i^*(\tau')a_i(\tau) \rangle_{S(0)}.
$$

We already found that the unperturbed energies of the system are given by Eq. (2.3), as long as the condition $U(g - 1) < \mu < Ug$ is fulfilled. Utilizing that (see appendix D)

$$
\langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} = g e^{g_0 - E_0 g (\tau - \tau')/\hbar},
$$

$$
\langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} = (g + 1) e^{-E_0 g (\tau - \tau')/\hbar},
$$

we find that the time ordered two-particle correlation function is given by

$$
\langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} = \theta(\tau - \tau')(1 + g)e^{E_0 g - E_0 g (\tau - \tau')/\hbar}
$$

$$
+ \theta(\tau' - \tau)g e^{E_0 g - E_0 g (\tau - \tau')/\hbar}.
$$

We note that

$$
E_{g+1}^0 - E_g^0 = -\mu/zJ + gU/zJ > 0,
$$

$$
E_g^0 - E_{g-1}^0 = -\mu/zJ + (g - 1)U/zJ < 0.
$$

Putting everything together we find

$$
S^{(2)}[\Psi^*, \Psi] = \int_0^{\hbar^2} d\tau \left\{ \sum_{i,j} J_{ij} \Psi_i^* \Psi_j - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau' \sum_{i,j,j'} J_{ij} J_{i'j'} \Psi_j^*(\tau) \langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} \Psi_{j'}(\tau') \right\}
$$

$$
= \int_0^{\hbar^2} d\tau \left\{ \sum_k |\Psi_k(\tau)|^2 \epsilon_k - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau' \langle a_i(\tau)a_i^*(\tau') \rangle_{S(0)} \sum_k |\Psi_k|^2 \epsilon_k \right\}
$$

$$
= \sum_{n,k} |\Psi_k|^2 \epsilon_k - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau \int_0^{\hbar^2} d\tau' \left[ \theta(\tau - \tau')(1 + g)e^{E_0 g - E_0 g (\tau - \tau')/\hbar} + \theta(\tau' - \tau)g e^{E_0 g - E_0 g (\tau - \tau')/\hbar} \right] \sum_k |\Psi_k|^2 \epsilon_k \epsilon_k.
$$

We shift the integration variable $\tau \to \tau - \tau'$ and perform a Matsubara expansion in the second term to see that this is equal to

$$
S^{(2)}[\Psi^*, \Psi] = \sum_{n,k} |\Psi_k|^2 \epsilon_k - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau' \int_0^{\hbar^2} d\tau \sum_{k,n,n'} \frac{|\Psi_k^*|^2}{\hbar} \frac{|\Psi_{k'}|^2}{\hbar} \epsilon_k \epsilon_{k'} \times
$$

$$
\left[ (1 + g)e^{-(E_{g+1}^0 - E_g^0)\tau/\hbar} e^{i\omega_n(\tau + \tau')} + ge^{-(E_{g+1}^0 - E_g^0)\tau/\hbar} e^{i\omega_n(\tau' - \tau)} \right] e^{-i\omega_n\tau'}
$$

$$
= \sum_{n,k} |\Psi_k|^2 \epsilon_k - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau' \sum_{k,n,n'} \frac{|\Psi_k^*|^2}{\hbar} \frac{|\Psi_{k'}|^2}{\hbar} \epsilon_k \epsilon_{k'} e^{i\tau'(\omega_n - \omega_{n'})} \times
$$

$$
\left[ (1 + g)e^{-(E_{g+1}^0 - E_g^0 - i\omega_n)\tau/\hbar} + ge^{-(E_{g+1}^0 - E_g^0 + i\omega_n)\tau/\hbar} \right] e^{-i\omega_n\tau'}
$$

$$
= \sum_{n,k} |\Psi_k|^2 \epsilon_k - \frac{1}{\hbar} \int_0^{\hbar^2} d\tau' \sum_{k,n,n'} \frac{|\Psi_k^*|^2}{\hbar} \frac{|\Psi_{k'}|^2}{\hbar} \epsilon_k \epsilon_{k'} e^{i\tau'(\omega_n - \omega_{n'})} \times
$$

$$
\left[ (1 + g)e^{-(E_{g+1}^0 - E_g^0 - i\omega_n)\tau/\hbar} + ge^{-(E_{g+1}^0 - E_g^0 + i\omega_n)\tau/\hbar} \right] e^{-i\omega_n\tau'}.
$$
Working in the zero-temperature limit $\hbar \beta \to \infty$, the terms $\propto \exp(-\hbar \beta)$ will approach zero, leaving us with

$$S^{(2)}[\Psi^\ast, \Psi] = \sum_{k,n} |\Psi_{kn}|^2 \epsilon_k \left[ 1 - \epsilon_k \left( \frac{g + 1}{-i\hbar \omega_n - \mu + gU} + \frac{g}{i\hbar \omega_n + \mu - (g - 1)U} \right) \right].$$

Now we can substitute $i\omega_n \to \omega$ and equate the remaining factor to zero to get the poles of the Green’s functions,

$$1 - \epsilon_k \left( \frac{g + 1}{-\hbar \omega - \mu + gU} + \frac{g}{\hbar \omega + \mu - (g - 1)U} \right) = 0.$$

Solving this equation for $\hbar \omega$, we get the quasi-particle and quasi-hole dispersion relations

$$\hbar \omega_{p,h} = -\mu + U \left( g - \frac{1}{2} \right) - \frac{\epsilon_k}{2} \pm \frac{1}{2} \sqrt{\epsilon_k^2 - (4g + 2)U \epsilon_k + U^2}.$$

To obtain the gap of the Mott insulator, we subtract $\hbar \omega_h$ from $\hbar \omega_p$ to arrive at the expression,

$$\Delta E_k = \hbar \omega_p - \hbar \omega_h = \sqrt{\epsilon_k^2 - (4g + 2)U \epsilon_k + U^2}.$$

The superfluid to Mott insulator phase transition can then be located at the point where the gap vanishes, found by equating $\Delta E_k = 0$. A plot of the gap as a function of $U/zJ$ for one particle per lattice site is shown in Figure 2.3. We see that the gap is zero below the critical value $U/zJ \approx 5.83$. This is the same value that we found when applying the mean-field approximation. We see that the gap is nonzero for very small values of $U$, a regime where the validity of our approximation seems to break down.

![Figure 2.3](image.png)

**Figure 2.3**: The Mott insulator gap $\Delta E_{k=0}/zJ$ plotted as a function of $U/zJ$ for $g = 1$. 
2.2.2 Global Phase Invariance

We realize that the Bose-Hubbard Hamiltonian (2.2) is invariant under a global $U(1)$ phase transformation according to

$$a_i \rightarrow e^{i\phi} a_i, \quad a_i^\dagger \rightarrow e^{-i\phi} a_i^\dagger.$$ 

In the Mott-insulating phase this phase invariance will remain intact. In this phase, the particles will be localized in space, while their momentum values are smeared out in $k-$space.

On the other hand, in the superfluid phase, there is a macroscopic occupation of the zero-momentum state, according to

$$a_{k=0} \rightarrow \sqrt{N_0},$$

where $N_0$ denotes the condensate number. This breaks the global phase invariance of the Bose-Hubbard model. In the superfluid phase, the atoms can not be localized in real space, but in momentum space we will see a high concentration of atoms at zero momentum. Figure 2.4 illustrates this behavior of the system: in the superfluid phase, corresponding to low values of $U$, the atoms have a common macroscopic wave function that is delocalized in space, but has sharp peaks in momentum space. The strong peak at zero momentum can be attributed to the Bose Einstein condensate. On the other hand, in the Mott insulating phase, corresponding to high values of $U$, we find that the particles are localized in real space, but delocalized in momentum space.

Figure 2.4: Schematic plot of the two phases in the Bose-Hubbard model, as simulated with cold atoms, taken from Ref. [12].

2.3 Staggered Vortex Superfluid

We have seen that a standing optical wave can interact with ultracold alkali atoms through a potential of the form (2.1). In the tight binding limit, we found that this system can be described by the Bose-Hubbard Hamiltonian, Eq. (2.2). We know that depending on the relation between the hopping and interaction parameters $J$ and $U$, this system can realize two different phases, the uniform superfluid phase and the Mott-insulating phase. Now we describe a possible generalization of the Bose-Hubbard model.
that is based on a two dimensional, time dependent optical potential that was worked out in Refs. [7], [13] and [8]. Consider a linearly polarized bichromatic light field

\[ E(x, y, t) = e_z|\phi(x, y)| \left[ A_1 e^{iS(x, y)} + A_2 e^{-iS(x, y)} e^{i\Omega t} \right] e^{i\omega t}, \]

where we denote the polarization vector by \( e_z \), the (real) time by \( t \) and where we assume

\[ \phi(x, y) = e^{i\theta/2} \sin(kx) + e^{-i\theta/2} \sin(ky) = |\phi(x, y)| e^{iS(x, y)}, \]

with the phase

\[ S(x, y) = \tan^{-1} \left[ \tan \left( \frac{\theta}{2} \frac{\sin(kx) - \sin(ky)}{\sin(kx) + \sin(ky)} \right) + \frac{\pi}{2} \text{sgn}[\Im(\phi)](1 - \text{sgn}[\Re(\phi)]) \right], \]

where \( \text{sgn}[z] \) denotes the sign of \( z \), \( \Re(\phi) \) the real part of \( \phi \) and \( \Im(\phi) \) the corresponding imaginary part. From now on, we will only consider the case \( \sin \theta = 1 \). This yields

\[ |\phi(x, y)|^2 = [\sin^2(kx) + \sin^2(ky)] . \]

We have seen that the optical potential obeys

\[ V(r) = -\text{Re}(\alpha)I. \]

Here, \( I \) denotes the intensity of the light and \( \alpha \) the polarizability. After integrating over the period of \( \omega \), we find that \( I(x, y) = E(x, y)E^*(x, y) \) can be divided into two parts \( I_L \) and \( I_R \), where \( I_L \) gives rise to a square optical lattice structure like the one in the usual Bose-Hubbard model and \( I_R \) to a so called microrotor potential. These intensities are given by

\[ I_L(x, y) = (A_1^2 + A_2^2)|\phi(x, y)|^2 \equiv -V_1|\phi(x, y)|^2, \]

\[ I_R(x, y, t) = 2A_1A_2|\phi(x, y)|^2 \cos(2S(x, y) - \Omega t) \equiv -KV_1|\phi(x, y)|^2 \cos(2S(x, y) - \Omega t). \]

Following the same procedure that yields the Bose-Hubbard model in the case where only an intensity comparable to \( I_L(x, y) \) is considered, we find for \( I_R(x, y, t) \) a new term denoted by \( H_R \). In second quantized form, this term is given in terms of the Wannier functions \( W(r - r_n) \), \( W^*(r - r_n) \) by the expression

\[ H_R = \sum_{i,j} a_i^\dagger a_j \int dW^*(r - r_i)V_R(r, t)W(r - r_j), \quad (2.6) \]

with

\[ V_R(r, t) = -K\frac{V_1}{2}|\phi(x, y)|^2 e^{i2S} e^{-i\Omega t} + h.c.. \]

A plot of this potential can be seen in Figure 2.5. We see that in the description we chose with basis vectors \( e_x, e_y \) of length \( \lambda/2 \), we find two sublattices, denoted by \( A \) and \( B \), that are inequivalent and arranged in a chessboard pattern, so that by hopping from one lattice site to one of its nearest neighbors we always get into a different sublattice.
Therefore, we will from now on use two different sets of creation and annihilation operators, $a_i^\dagger$ ($a_i$) which will create (annihilate) an atom in the A-sublattice and $b_i^\dagger$ ($b_i$) which will create (annihilate) an atom in the B-sublattice.

But there is a different choice of basis vectors that we can choose to work with. The Bravais lattice $\mathcal{R}$ has basis vectors $R_{\pm} = (\lambda/2)(e_x \pm e_y)$. We can therefore decompose the whole lattice into $(\lambda/2 \times \lambda/2)$ sized plaquettes along these basis vectors, that we denote by $d_1 = (\lambda/2)(e_x + e_y)$, $d_2 = (\lambda/2)(e_x - e_y)$.

Assume we can approximate

$$\int d\mathbf{r} W^* (\mathbf{r} - \mathbf{r}_i) V(\mathbf{r}) W(\mathbf{r} - \mathbf{r}_j) \approx V((\mathbf{r}_i + \mathbf{r}_j)/2) \int d\mathbf{r} W^* (\mathbf{r} - \mathbf{r}_i) W(\mathbf{r} - \mathbf{r}_j),$$

and that it is enough to consider nearest-neighbor and next-nearest neighbor (diagonal) hopping. Denote the corners of each plaquette by 1, 2, 3 and 4, then evaluation of Eq. (2.6) yields

$$H_R \approx \chi_1 \sin(\Omega t) \sum_{\mathbf{r} \in A} \sum_{l=1}^4 (-1)^{l+1} (a_{\mathbf{r}+\mathbf{e}_l}^\dagger b_{\mathbf{r}+\mathbf{e}_l} + h.c.) + \chi_2 \cos(\Omega t)(n_A - n_B), \quad (2.7)$$
where
\[
\begin{align*}
n_A &= \sum_{r \in A} a_r^\dagger a_r, \\
n_B &= \sum_{r \in B} b_r^\dagger b_r,
\end{align*}
\]
\[
\chi_1 = KV_1 \int d\mathbf{r}^2 W^*(x + \frac{\lambda}{4}, y) \left[ \sin^2 \left( \frac{2\pi x}{\lambda} \right) - \cos^2 \left( \frac{2\pi y}{\lambda} \right) \right] W(x - \frac{\lambda}{4}, y),
\]
\[
\chi_2 = 2KV_1 \int d\mathbf{r}^2 |W(x, y)|^2 \cos \left( \frac{2\pi x}{\lambda} \right) \cos \left( \frac{2\pi y}{\lambda} \right).
\]

The second term of Eq. (2.7) breaks the lattice into the two sublattices \( A \) and \( B \) discussed above by associating different time dependent potentials with them. The first resembles the hopping parameter from the original Bose-Hubbard model but is dependent on time as well as hopping direction.

We can rewrite the full Hamiltonian as

\[
H(t) = H_0 + W(t) + H_{\text{int}},
\]

with

\[
\begin{align*}
H_0 &= -J_0 T, \\
T &= \sum_{<i,j>} a_i^\dagger b_j, \\
W(t) &= Q^\dagger e^{i\Omega t} + Q e^{-i\Omega t}, \\
Q &= \frac{1}{2} (\chi_2 \mathcal{N} + i\chi_1 \mathcal{M}), \\
\mathcal{N} &= \sum_{r \in A} (n_r - n_{r+e_1}), \\
\mathcal{M} &= \sum_{r \in A, l=1..4} [(-1)^l+1 a_r^\dagger b_{r+e_l} + h.c.], \\
H_{\text{int}} &= \frac{U_0}{2} \sum_{r \in A \oplus B} n_r (n_r - 1).
\end{align*}
\]

Here, \( U_0 \) denotes the on-site interaction parameter from the conventional Bose-Hubbard model. The single-body Hamiltonian in the noninteracting case is given by \( H_{1B} = H_0 + W(t) \) and its evolution is determined by the time-evolution operator

\[
U_{1B} = T \left\{ \exp \left[ \frac{-i}{\hbar} \int_0^t ds H_{1B}(s) \right] \right\},
\]

where \( T \) denotes the time-ordering operation. The Dyson series corresponding to times \( t \) that are multiples of the revolution time of the microrotor potential \( \tau_{\text{mr}} = \frac{2\pi}{\Omega} \) is given by

\[
U_{1B}(\tau_{\text{mr}}) = 1 + \left( \frac{-i}{\hbar} \right) \int_0^{\tau_{\text{mr}}} ds H_{1B}(s) \\
+ \left( \frac{-i}{\hbar} \right)^2 \int_0^{\tau_{\text{mr}}} ds \int_0^s ds' H_{1B}(s) H_{1B}(s') + O \left[ \left( \frac{-i}{\hbar} \right)^3 \right] \\
= 1 - \frac{i}{\hbar} H_0 \tau_{\text{mr}} - \frac{1}{i\hbar^2 \Omega} \left( [H_0, Q - Q^\dagger] + [Q, Q^\dagger] \right) \tau_{\text{mr}} + O(2B, \tau_{\text{mr}}),
\]

16
where $O(2B, \tau_{mr})$ denotes terms with two or more body character scaling with at least order one in $\tau_{mr}$. We write Eq. 2.8 as

$$U_{1B}(\tau) \approx 1 - \frac{i}{\hbar} H_0^{\text{eff}} \tau_{mr},$$

$$H_0^{\text{eff}} = -J_0 T + \frac{iJ_0 \chi_1}{\hbar \Omega} [T, M] - \frac{i\chi_1 \chi_2}{2\hbar \Omega} [M, N], \quad (2.9)$$

Evaluating the commutators we find

$$[T, M] = \sum_{r,r', l, l'} (-1)^{l+l'} [a^\dagger_r b_{r+e_l} + a_r b^\dagger_{r+e_l}, a^\dagger_{r'} b_{r'+e_l'} + a_{r'} b^\dagger_{r'+e_l'}]$$

$$= \sum_{r,r'} \sum_{l, l'} (-1)^{l+l'} \left[ -b_{r+e_l} b^\dagger_{r'+e_l'} \delta_{r,r'} + a^\dagger_r a_r \delta_{(r+e_l, r'+e_l')} + b_{r+e_l} b^\dagger_{r'+e_l'} \delta_{r,r'} - a_r a^\dagger_r \delta_{(r+e_l, r'+e_l')} \right]$$

$$= 0,$$

$$[M, N] = \sum_{r, r', l} (-1)^{l+l'} \left[ a^\dagger_r b_{r+e_l} + a_r b^\dagger_{r+e_l}, a^\dagger_{r'} b_{r'+e_l} + a_{r'} b^\dagger_{r'+e_l} \right]$$

$$= \sum_r \sum_l (-1)^l \left[ a^\dagger_r b_{r+e_l} - a_r b^\dagger_{r+e_l} + a_r b_{r+e_l} + a^\dagger_r b^\dagger_{r+e_l} \right]$$

$$= 2 \sum_r \sum_l (-1)^l \left[ a^\dagger_r b_{r+e_l} - a_r b^\dagger_{r+e_l} \right],$$

so that Eq. 2.9 finally yields

$$H_0^{\text{eff}} = -J \sum_r \sum_l \left[ e^{i\phi(-1)^l} a^\dagger_r b_{r+e_l} + h.c. \right], \quad (2.10)$$

where $J = \sqrt{J_0^2 + (\chi_1 \chi_2/\hbar \Omega)^2}$ and $\phi = \tan^{-1}(\chi_1 \chi_2/\hbar \Omega J_0)$.

### 2.3.1 Finite Momentum Superfluid

Adding the well known on-site interaction term to Eq. (2.10), we recover the full generalized Bose-Hubbard Hamiltonian. It is given by

$$H = -J \sum_{r \in A, l=1,4} \left[ e^{i\phi(-1)^l} a^\dagger_r b_{r+e_l} + h.c. \right] + \frac{U}{2} \sum_{r \in A \otimes B} n_r (n_r - 1). \quad (2.11)$$

This Hamiltonian describes ultracold bosonic atoms trapped in a a two dimensional optical lattice subjected to staggered rotation. We now compute the corresponding dispersion relation.

To obtain the single particle spectrum, we first perform a Fourier-transformation of the kinetic part of $H$ in the two sublattices $A$ and $B$, according to

$$a_{r \in A} = \sqrt{\frac{2}{N}} \sum_k a_k e^{-i k r}, \quad b_{r \in B} = \sqrt{\frac{2}{N}} \sum_k b_k e^{-i k r}, \quad (2.12)$$
where $N/2$ denotes the number of sites in each of the two sublattices and where we take $b_k^\dagger (b_k)$ to create (annihilate) an atom in the $B$-sublattice with momentum $k$ while $a_k^\dagger$ and $a_k$ create and annihilate atoms in the $A$-sublattice. The noninteracting Hamiltonian now reads

$$H_0^{\text{eff}} = -J \sum_{k,l} e^{i\phi(-1)^l} a_k^\dagger b_k e^{-i\kappa_{el}} + \text{h.c.},$$

where we used that

$$\delta_{k_1, k_2} = \frac{2}{N} \sum_{r} e^{ir(k_1 - k_2)}.$$

Performing the summation over $l$ we find

$$H_0^{\text{eff}} = -2J \sum_{k} a_k^\dagger b_k \left[ e^{-i\phi} \cos(d_l k_\pm) + e^{i\phi} \cos(d_l k_\mp) \right] + \text{h.c.},$$

where $k_\pm = (k_x \pm k_y)/2$ and $d_l = \lambda/\sqrt{2}$. To diagonalize the Hamiltonian, we perform a variable substitution according to

$$a_k = (\alpha_k - \beta_k) \frac{|\epsilon_k|}{\sqrt{2}}, \quad b_k = \frac{1}{\sqrt{2}} (\alpha_k + \beta_k),$$

with

$$\epsilon_k = -2J \left[ e^{-i\phi} \cos(d_l k_\pm) + e^{i\phi} \cos(d_l k_\mp) \right],$$

(2.14)

so that we find the energy values

$$\pm |\epsilon_k| = \pm 2J \sqrt{\cos^2 (d_l k_\pm) + \cos^2(d_l k_\mp) + 2 \cos (2\phi) \cos(d_l k_\pm) \cos(d_l k_\mp)}.$$

(2.16)

The energy spectrum consists of two bands, as it can be seen in Figure 2.7. We see that for $\phi < \pi/4$, the minimum of $\epsilon_k$ is at the origin, for $\phi > \pi/4$ it is at the edges of the Brillouin-zone. For $\phi \neq 0$ we have two inequivalent Dirac-cones emerging at $(k_+, k_-) = (0, \pi)$ and $(k_+, k_-) = (\pi, 0)$. Those Dirac cones are anisotropic, except at $\phi = \pi/4$, where isotropy is recovered (see Figure 2.7.c). At $\phi = \pi/2$ the Dirac-cones evolve into two Dirac-lines along $(k_+, k_-) = (0, k_-)$ respectively $(k_+, k_-) = (k_+, 0)$.

We now seek to compute the energy spectra of the superfluid phases for a system of interacting atoms. We start with the generalized Bose-Hubbard Hamiltonian, Eq. (2.11), apply a Fourier transformation, and then perform the same substitution that we used when calculating the energy spectrum for the noninteracting case [Eq. (2.13)]. We know that the kinetic part of $H$ is given by Eq. (2.15), so we only need to apply the
procedure described to the potential term of the generalized Bose-Hubbard model, which yields

\[ V = \frac{U}{4N} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2,k_3+k_4} \left[ \frac{|\epsilon_{k_1}| |\epsilon_{k_2}| |\epsilon_{k_3}| |\epsilon_{k_4}|}{\epsilon_{k_1}^* \epsilon_{k_2}^* \epsilon_{k_3} \epsilon_{k_4}^*} (\alpha_{k_1}^\dagger - \beta_{k_1}^\dagger)(\alpha_{k_2}^\dagger - \beta_{k_2}^\dagger) \times \right. \\
\left. \times (\alpha_{k_3} - \beta_{k_3})(\alpha_{k_4} - \beta_{k_4}) + (\alpha_{k_1}^\dagger + \beta_{k_1})(\alpha_{k_2}^\dagger + \beta_{k_2})(\alpha_{k_3} + \beta_{k_3})(\alpha_{k_4} + \beta_{k_4}) \right], \]

and we note that the first term in the sum originates from atoms in the A-sublattice and the second term from those in the B-sublattice. Here, \( N \) denotes the total number of lattice sites, of which half are situated in the A and the other half in the B-sublattice.

We are considering the full Hamiltonian \( H \) in the grand canonical ensemble and apply a fluctuation expansion for the condensation mode according to

\[ \beta_k \rightarrow \sqrt{N_0} \delta_{k,k_0} + \beta_k, \quad \beta_k^\dagger \rightarrow \sqrt{N_0} \delta_{k,k_0} + \beta_k^\dagger, \]

where \( N_0 \) denotes the condensate number corresponding to the number of Bose-Einstein condensed atoms and \( k_0 \) the momentum of the condensed phase, which was found to be either \( k_0 = 0 \) for the uniform superfluid or \( k_0 = \pi \) for the staggered vortex phase. In this way, we can expand the Hamiltonian in powers of the creation and annihilation operators according to

\[ H = H^{(0)} + H^{(1)} + H^{(2)} + \ldots, \]

where

\[ H^{(0)} = \frac{n_0 U N_0}{2}, \]

where the condensate fraction \( n_0 = N_0/N \) was introduced. \( H^{(1)} \) must be equal to zero, yielding an equation for the chemical potential \( \mu \),

\[ \mu = -|\epsilon_{k_0}| + U n_0. \]
For $H^{(2)}$ we find the expression

$$H^{(2)} = \sum_k (|\epsilon_k| - \mu)\alpha_k^\dagger \alpha_k + \sum_k (-|\epsilon_k| - \mu)\beta_k^\dagger \beta_k$$

$$+ \frac{U}{4N} \sum_k N_0 \left[ \alpha_k^\dagger \alpha_k^\dagger + \beta_k^\dagger \beta_k + h.c. \right] \left[ 1 + \frac{|\epsilon_k||\epsilon_{-k}||\epsilon_{k_0}|^2}{\epsilon_k \epsilon_{-k} \epsilon_{k_0}^* \epsilon_{k_0}^*} \right]$$

$$+ \frac{U}{4N} \sum_k N_0 \left[ \alpha_{-k}^\dagger \beta_{-k}^\dagger + \beta_{-k}^\dagger \alpha_{-k}^\dagger + h.c. \right] \left[ 1 - \frac{|\epsilon_k||\epsilon_{-k}||\epsilon_{k_0}|^2}{\epsilon_k \epsilon_{-k} \epsilon_{k_0}^* \epsilon_{k_0}^*} \right]$$

$$+ \frac{2U}{N} \sum_k N_0 \left[ \alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k \right]$$

where we used that, [see Def. of $\epsilon_k$ in Eq. (2.14)], $\epsilon_k = \epsilon_{-k}$. It proves convenient at this point to introduce the abbreviations

$$A_{k,k_0} = 1 + \frac{|\epsilon_k||\epsilon_{-k}||\epsilon_{k_0}|^2}{\epsilon_k \epsilon_{-k} \epsilon_{k_0}^* \epsilon_{k_0}^*},$$

$$B_{k,k_0} = 1 - \frac{|\epsilon_k||\epsilon_{-k}||\epsilon_{k_0}|^2}{\epsilon_k \epsilon_{-k} \epsilon_{k_0}^* \epsilon_{k_0}^*}.$$

Now we can write the Hamiltonian up to second order in the fields as

$$H^{(2)} = \sum_k (-|\epsilon_k| - \mu + 2U\alpha_k)\alpha_k^\dagger + \sum_k (|\epsilon_k| - \mu + 2U\alpha_k)\beta_k^\dagger \beta_k$$

$$+ \frac{U}{4N} \sum_k N_0 \left[ \alpha_k^\dagger \alpha_k^\dagger + \beta_k^\dagger \beta_k \right] A_{k,k_0} + h.c.$$

$$+ \frac{U}{4N} \sum_k N_0 \left[ \alpha_{-k}^\dagger \beta_{-k}^\dagger + \beta_{-k}^\dagger \alpha_{-k}^\dagger \right] B_{k,k_0} + h.c.. \quad (2.17)$$

We are now ready to write down the corresponding action $S[\Psi, \Psi^\dagger]$ to calculate the energy eigenvalues of the system,

$$S[\Psi, \Psi^\dagger] = -\frac{n_0UN_0}{2} - \frac{\hbar}{2} \sum_k \left( \Psi_k^\dagger \Psi_{-k} \right) \frac{1}{G_k} \left( \begin{array} \Psi_k \\ \Psi_{-k} \end{array} \right),$$

where the inverse Green’s function $G_k^{-1}$ is given by

$$-\hbar G_k^{-1} = \begin{pmatrix} \Delta E_k^+ - i\hbar \omega_m & \frac{1}{2} n_0 U A_{k,k_0}^* \\ \frac{1}{2} n_0 U A_{k,k_0}^* & \Delta E_k^+ + i\hbar \omega_m \end{pmatrix},$$

$$\begin{pmatrix} 0 & \frac{1}{2} n_0 U B_{k,k_0}^* \\ \frac{1}{2} n_0 U B_{k,k_0}^* & 0 \end{pmatrix},$$

$$\begin{pmatrix} \Delta E_{-k}^- - i\hbar \omega_m & \frac{1}{2} n_0 U A_{k,k_0}^* \\ \frac{1}{2} n_0 U A_{k,k_0}^* & \Delta E_{-k}^- + i\hbar \omega_m \end{pmatrix},$$

where $\Delta E_k^\pm = U n_0 + |\epsilon_{k_0}| \pm |\epsilon_k|$. This yields the dispersion relation

$$\hbar \omega_{k,k_0}^\pm = \sqrt{|\epsilon_k|^2 + |\epsilon_{k_0}|^2 + 2n_0 U|\epsilon_{k_0}| \pm 2n_0 U|\epsilon_k| \sqrt{G_{k,k_0}^{-1}},} \quad (2.18)$$
with $G_{k,k_0} = \cos^2(\phi_k) + 2|\epsilon_{k_0}|/2n_0U + 1/n_0U$.

We note that $n_0$ and $U$ only display as the product $n_0U$ in this equation. A plot of the energy spectrum for different values of $\phi \in [0, \pi/2]$ for $n_0U = 1$ can be seen in Figure 2.8. It consists of two branches, denoted here by $\omega_{k,k_0}^\pm$. The two branches are always connected at the four Dirac points $(k_+,k_-) = (0,\pm\pi), (\pm\pi,0)$, because at these points $|\epsilon_k| = 0$. Assuming that the condensation still takes place at $k_0 = 0$ for $\phi < \pi/4$ and at $k_0 = \pi$ for $\phi > \pi/4$, the $\omega_{k,k_0}^\pm$ spectrum seems to display qualitatively similar behavior as in the noninteracting case. Approaching $\phi = \pi/2$ the two spectra seem to join each other in two Dirac lines defined by $(k_+,k_-) = (0,k_-), (k_+,0)$. Just like in the noninteracting case, the minimum of the spectrum is always located at the point $k = (0,0)$ for $k_0 = 0, \phi \leq \pi/4$ and at $k = (\pi,\pi)$ for $k_0 = \pi$ with $\phi \geq \pi/4$. Inspecting the border between the uniform superfluid and the staggered vortex superfluid phase, we realize that the change in the energy spectrum is not smooth this time. Figure 2.9 illustrates this point. It shows the lower branch of the spectrum for $n_0U/J = 1, \phi = \pi/4$ for the two cases where the condensation of the atoms is either assumed to happen at $k = 0$ or $k = \pi$. Both spectra have their minima at the correct momentum values, but they do not agree, in contrast to the single particle spectrum. A Taylor-expansion in $n_0U/J$ at $\phi = \pi/4$ and $(k_x,k_y) = (\pm\pi,\pm\pi)$ suggests that the energy value $\Delta \omega$ of the lower branch of the spectrum at this point can be estimated to be $\Delta \omega \approx 2n_0U$ for $n_0U \ll J$. It turns out that the energy spectra for $k_0 = 0$ stays real in an interval $\phi \in (0,\phi_{\text{crit}})$, where $\phi_{\text{crit}} > \pi/4$ is given as a function of $n_0U$ and $J$. The larger $n_0U$ gets, the larger $\phi_{\text{crit}}$. The two local minima of the spectrum at $k = 0,\pi$ have equal height at $\phi = \phi_{\text{crit}}$. For $\phi > \phi_{\text{crit}}$ we recover a spectrum that has imaginary parts. For sufficiently large values of $n_0U/J$ the value of $\phi_{\text{crit}}$ can be found almost anywhere in the interval $(\pi/4,\pi/2)$. 

Figure 2.8: Plot of $\omega_{k,k_0}^\pm$ for $Un_0/J = 1$ and (a) $\phi = 0 (k_0 = 0)$, (b) $\phi = \pi/8 (k_0 = 0)$, (c) $\phi = \pi/4 (k_0 = 0)$, (d) $\phi = 3\pi/8 (k_0 = \pi)$, (e) $\phi = 7\pi/16 (k_0 = \pi)$ and (f) $\phi = \pi/2 (k_0 = \pi)$. 
The situation is reversed if we assume the condensation point to be located at \( k_0 = \pi \). We recover a critical value of \( \phi \) at \( \pi/2 - \phi_{\text{crit}} \), at equal distance to \( \pi/4 \) as \( \phi_{\text{crit}} \), where the two local minima of the energy spectrum have equal height, like before. A lower value of \( \phi \) also recovers an imaginary spectrum.

Plots of the energy spectra at the critical values of \( \phi \) for the different values of \( k_0 \) can be seen in Figure 2.10. We see that also in these pictures, there is no smooth transition between the energy spectra recovered for \( k_0 = 0 \) and \( k_0 = \pi \). This sudden change in the excitation spectrum as \( \phi = \pi/4 \) is crossed is not a problem though, since the transition between uniform superfluid and finite-momentum superfluid is a first order phase transition.
Figure 2.10: Plot of $\frac{\hbar\omega}{4J}$ for $Un_0/J = 1$ and (a) $\phi = \phi_{\text{crit}} \approx 3\pi/10$, $k_0 = 0$, (b) $\phi \approx 3\pi/10$, $k_0 = \pi$, (c) $\phi = \pi/2 - \phi_{\text{crit}} \approx \pi/5$, $k_0 = \pi$, (d) $\phi \approx \pi/5$, $k_0 = 0$. 
Chapter 3

Molecule Formation in Optical Lattices

In this section we will review ways to create diatomic molecules in optical lattices. A molecule is here defined as a stable bound state of two atoms moving through the lattice in such a way that it can effectively be described as one entity. The first way to create molecules discussed here was found by Dennis Dickerscheid et. al. in 2005 (see Ref. [6]) utilizing Feshbach resonances and thereby an external magnetic field. The second way was first described by Winkler et. al. (Ref. [14]) and does not require adding new ingredients like an external field but can be simply understood in terms of energy conservation in the Bose-Hubbard model.

3.1 Feshbach Resonances in Optical Lattices

Consider a scattering process of two fermionic alkali atoms with spin degrees of freedom. The spin of the valence electrons of those atoms will couple to form either a singlet or a triplet. Since the complete wave function of a fermionic system has to be antisymmetric, the singlet potential may be deeper than the triplet potential for small interatomic distances, since the singlet is an antisymmetric state. In this case, the spatial part of the wave function must be symmetric, so that atoms are in principle allowed to approach each other very closely, while the symmetric triplet state leads to an antisymmetric spatial part of the wave function.

Therefore, we treat the problem as a two-channel scattering problem, where the potential is deeper for one channel than for the other one. We call the channel with the deeper potential the open and the other one the closed channel.

In practical situations it is possible that the two channels are coupled through an exchange interaction that can change the scattering channel from open to closed or the other way around. This can be archived utilizing the hyperfine interaction, where the spin $S$ of the electron couples to the spin of the nucleus $I$ through a potential

$$V_{hf} \propto I \cdot S.$$ 

If the two atoms approach each other in the open channel with a scattering energy of the size of the energy of a bound-state in the closed channel, this leads to resonance and
the formation of a (virtual) molecular state, indicated by a divergence of the scattering length associated with the problem.

The basic idea behind the concept of Feshbach resonances is to find a way to control the energy difference between the two channels in a way that allows us to witness molecule formation in a controlled environment. This can be realized by utilizing the Zeeman shift that the energy levels of the system undergo as we apply an external magnetic field.

This idea has been applied in the context of optical lattices in Ref. [10] and I will repeat here the discussion given there. We suppose that we are dealing with a deep optical lattice and that we can approximate the optical potential on each lattice site as that of a harmonic oscillator with energy splitting $\hbar \omega$. The Schrödinger equation corresponding to the scattering of two atoms in the relative coordinate reads

$$
P = \left( \begin{array}{cc}
H_0 + V_{aa} & V_{am} \\
V_{am} & \delta_B
\end{array} \right) \left( \begin{array}{c}
|\Psi_a\rangle \\
|\Psi_m\rangle
\end{array} \right) = E \left( \begin{array}{c}
|\Psi_a\rangle \\
|\Psi_m\rangle
\end{array} \right),
$$

(3.1)

where $H_0 = -\hbar^2 \nabla^2 / m + m \omega^2 r^2 / 4$ is the noninteracting Hamiltonian for the atomic motion, $V_{aa}$ denotes the atom-atom interaction, $V_{am}$ the atom-molecule coupling and $\delta_B$ the bare detuning between the two channels, corresponding to the energy difference between them resulting from the external magnetic field. We can rewrite the matricial Eq. (3.1) as two equations,

$$
\begin{align}
(E - H_0 - V_{aa}) |\Psi_a\rangle &= V_{am} |\Psi_m\rangle, \\
(E - \delta_B) |\Psi_m\rangle &= V_{am} |\Psi_a\rangle,
\end{align}
$$

which can be combined to yield

$$
E - \delta_B = \langle \Psi_m | V_{am} \frac{1}{E - H_0 - V_{aa}} V_{am} | \Psi_m \rangle.
$$

For most atoms we find $V_{aa} \ll \hbar \omega$, therefore we assume that we are allowed to neglect the atom-atom interaction in the following. Call the eigenstates of $H_0 |\phi_n\rangle$, so that $H_0 |\phi_n\rangle = (2n + 3/2) \hbar \omega$ in three dimensions. By inserting a complete set of these states, we find

$$
\sum_n \frac{\langle \Psi_m | V_{am} | \phi_n \rangle^2}{E - E_n} = E - \delta_B.
$$

We now apply a pseudo potential approximation $\langle r | V_{am} | \Psi_m \rangle = \sqrt{2} g \delta(r)$, with $g \propto \sqrt{a_{bg} \Delta B \Delta \mu / m}$, where we introduce the so-called background scattering length $a_{bg}$, the width of the resonance $\Delta B$, and the difference in magnetic moments of the relevant Feshbach resonance $\Delta \mu$. Inserting two complete sets of position states we find (see Ref. [10])

$$
\begin{align}
E - \delta_B &= 2g^2 \sum_n \frac{\phi_n^*(0) \phi_n(0)}{E - E_m} \\
&= g^2 \left[ \frac{G(E)}{\sqrt{2} \pi \hbar^3 \hbar \omega} - \lim_{r \to 0} \frac{m}{2 \pi \hbar^2 r} \right],
\end{align}
$$

25
where \( G(E) = \Gamma(-E/2\hbar\omega+3/4)/\Gamma(-E/2\hbar\omega+1/4) \). The right hand side of this equation can be interpreted as the self energy of the molecules. We assume that we can absorb the divergent term included in it into the detuning \( \delta \) because it is energy-independent. Hence, we may write

\[
E = g^2 \frac{G(E)}{\sqrt{2\pi l^3\hbar\omega}} + \delta_B,
\]

a plot of which can be seen in Figure 3.1. We see in the figure that there are lots of molecular states, corresponding to the modified energy levels of the harmonic oscillator. For negative detuning, the energy of the lowest molecular state lies below the ground state of the harmonic oscillator, thus it becomes favorable for the atomic pair to occupy this state. We now only consider the two lowest molecular states and change them to the states \(|\Psi_\downarrow\rangle, |\Psi_\uparrow\rangle\) by utilizing the wave function renormalization factors \( Z_\downarrow, Z_\uparrow \), that are given in terms of the molecular selfenergy \( h\Sigma_m(E) \) by \( Z_\sigma = 1/(1 - \partial\Sigma_m(E)/\partial E) \), so that \( Z_\downarrow \) is related to the lowest energy level of \( h\Sigma_m(E) \) and \( Z_\uparrow \) to the second lowest. A plot of these renormalization factors as a function of the detuning \( \delta \) can be seen in Figure 3.1b. With this, a generalized Bose-Hubbard Hamiltonian for atoms and two species of molecules can be found,

\[
H = -J^a \sum_{r,l=1..4} a_\uparrow^\dagger a_{r+l} - J^m \sum_{r,\sigma,l=1..4} c_{\sigma,r+l}^\dagger c_{r,l} + \sum_r (\epsilon^a - \mu) a_\uparrow^\dagger a_r
+ \sum_{r,\sigma} (\epsilon^m - 2\mu) c_{\sigma,r}^\dagger c_{r,\sigma} + g \sum_{i,\sigma} \sqrt{Z_\sigma}^\gamma [c_{i,\sigma}^\dagger a_i a_i + h.c.] + \frac{U}{2} \sum_r a_r^\dagger a_r^\dagger a_r a_r, \tag{3.2}
\]

where \( \epsilon^a \) denotes the single-particle ground state of the harmonic oscillator potential and the \( \epsilon^m \) the shifted oscillator states for the two kinds of molecules. Here, \( a_\uparrow^\dagger, a_r \) are the atomic creation and annihilation operators and \( c_{\sigma,r}^\dagger, c_{r,\sigma} \) the corresponding operators for molecules in the \( \sigma \) state.

Looking at the Hamiltonian (3.2), we see that it obeys \( U(1) \) phase invariance

\[
a_k \to e^{i\phi_k} a_k, \\
c_{k,\sigma} \to e^{i\phi_k} c_{k,\sigma},
\]
as long as $\phi_c = 2\phi_a$. Now, imagine we know that the system contains an atomic condensate, $a_{k=0} \rightarrow \sqrt{N_0^a}$. This fixes the phase $\phi_a$ and therefore the phase $\phi_c = 2\phi_a$ is obtained. This suggests that if we have an atomic condensate, we must also find a molecular condensate.

If, on the other hand, we assume the existence of a molecular condensate, we have that $c_{k=0,\sigma} \rightarrow \sqrt{N_0^{c\sigma}}$, which fixes the phase $\phi_c$. For the atomic phase we obtain $\phi_a = \phi_c/2 + n\pi$, where $n$ is some integer. This suggests that the existence of a molecular Bose-Einstein condensate does not necessarily imply the existence of an atomic condensate.

Indeed, the Hamiltonian (3.2) can realize two different phases, a phase with only a molecular condensate and a phase that contains both a molecular and an atomic condensate.

### 3.2 Two Particle Scattering

Consider two repulsively interacting atoms on the same lattice site in the Bose-Hubbard model,

$$H = -J \sum_{<i,j>} a_i^\dagger a_j + \frac{U}{2} \sum n_i(n_i-1).$$

We recall that if one of the atoms hops to a nearest neighboring site, an amount of energy $J$ will be gained through the hopping term in the model. But if the particle number on the site where the atom is hopping to is unequal to one, there will also be energy paid through the interaction term.

Consider the case where two atoms are sitting on the same lattice site. Let one of them hop to a site where no other atoms are placed, then an amount of energy $J + U$ will be gained. This process is illustrated in Figure 3.2. This leads us to the following idea: Is it possible that for very high repulsive on-site interaction energy $U$, it can be difficult for pairs of atoms on the same lattice site to break up due to conservation of energy? This indeed turns out to be the case, as shown in Refs. [15] and [14]. The rest of this paragraph repeats the argumentation laid out there to elaborate the idea just explained utilizing two-particle scattering theory.

We label the coordinates of the two particles under consideration $x_1$ and $x_2$ and write
down the corresponding Schrödinger equation \( H \Psi = E \Psi \) in the lattice,

\[
[-J(\Delta_{x_1} + \Delta_{x_2}) + U\delta_{x_1,x_2}]\Psi(x_1, x_2) = E\Psi(x_1, x_2).
\]

Here, the action of the discrete displacement operator \( \Delta_{x_1} \) on \( \Psi(x_1, x_2) \) is given by

\[
\Delta_{x_1}\Psi(x_1, x_2) \equiv \sum_{l=1}^{d} [\Psi(x_1 + e_l, x_2) + \Psi(x_1 - e_l, x_2) - 2\Psi(x_1, x_2)].
\]

The displacement operator \( \Delta_{x_1} \) on \( \Psi(x_1, x_2) \) plays a role very similar to a discrete Laplacian here. We note that we introduced a constant energy offset of \( 4Jd \) through the last term, that is there to allow the displacement operator in the lattice to have the traditional form of a discrete Laplacian (this corresponds to an offset of \( 2J \) per particle and spatial dimension). Now, we change to relative coordinates \( r = x_1 - x_2, 2R = x_1 + x_2 \), so that \( R \) lives in a lattice with only half the lattice constant \( d_l/2 \) of the original lattice. We separate the wave function according to

\[
\Psi(x_1, x_2) = e^{iKR}\Psi_K(r),
\]

therefore the Schrödinger equation now reads

\[
[-J\Delta_{\mathbf{r}}^K + E_K + U\delta_{\mathbf{r},0}]\Psi_K(r) = E\Psi_K(r),
\]

where

\[
\Delta_{\mathbf{r}}^K\Psi_K(r) = \sum_{i=1}^{d}[\Psi(r + e_i) + \Psi(r - e_i) - 2\Psi(r)] [e^{iKe_i/2} + e^{-iKe_i/2}],
\]

and

\[
E_K = J\sum_{i} \left\{ 4 - 2 \left[ e^{iKe_i/2} + e^{-iKe_i/2} \right] \right\}.
\]

Hence, we find

\[
E_K = 4J\sum_{i} \left[ 1 - \cos \left( \frac{Ke_i}{2} \right) \right],
\]

\[
\Delta_{\mathbf{r}}^K\Psi_K(r) = 4\sum_{i=1}^{d} [\cos(ke_i) - 1] \cos \left( \frac{Ke_i}{2} \right) \Psi_K(r).
\]

We try to solve the Schrödinger equation via the Green’s function of the relative motion without interaction \( (U = 0) \),

\[
[E - J\Delta_{\mathbf{r}}^K]G_K(E, r) = \delta_{\mathbf{r},0}.
\]

This can be done by Fourier-transformation,

\[
G(E, r) = \frac{1}{(2\pi)^d} \int dk G(E, k)e^{ikr},
\]

28
with
\[ G_K(E, k) = \frac{1}{E - \epsilon_K(k) + i\eta}, \]
where \( \epsilon_K(k) \) is given by
\[ \epsilon_K(k) = -4J \sum_{i=1}^{d} \left[ \cos(k e_i) - 1 \right] \cos \left( \frac{K e_i}{2} \right). \]

As explained above, we are interested in bound-state solutions of the scattering problem. Our starting point is the Lippmann-Schwinger equation
\[ \Psi_E(r) = e^{ikr} + \sum_{r'} G_K(E, r - r') U \delta_{r,0} \Psi_E(r'). \]
This can be solved by resummation, to yield
\[ \Psi_E(r) = e^{ikr} - 8\pi J f_E(K) G_K(E, r), \]
where the scattering amplitude \( f_E(K) \) is given by
\[ f_E(K) = -\frac{1}{4\pi} \frac{U/2J}{1 - G_K(E, 0) U}. \]
This has a pole at \( U = 1/G_K(E, 0) \), corresponding to a bound molecular state of energy \( E \). Since
\[ \frac{1}{U} = G_K(E, r = 0) \]
\[ = \frac{1}{(2\pi)^d} \int_{-\pi/d}^{\pi/d} \frac{1}{E - 4J \sum_{i=1}^{d} \cos \frac{K e_i}{2} (1 - \cos k_i d_i)}, \]
we know that only two of the three variables \( U, J \) and \( E \) are independent for the two-particle bound state for a given center-of-mass momentum \( K \). A plot of the energy values of the bound state and scattering state energies in one dimension can be seen in Figure 3.3. The figure shows that the bound state energy lies above the continuum of the scattering-state energies.

It is interesting to note that in three dimensions there is a minimal value of \( U/J \) that is required to form bound states (see Refs. [15] and [14] for a more comprehensive discussion). In Figure 3.4 we see plots of \( U \) as a function of \( E \) for the bound states in one, two and three dimensions. It is known that there is no minimal value of \( U \) required for the formation of bound states in one dimension, as confirmed by the figure. To determine the critical value of \( U \) for bound state formation in three dimensions, we note that (see Ref. [16])
\[ \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \frac{1}{dK} \sum_{i=1,3} \frac{1}{(1 - \cos k_i d_i)} \approx 0.505, \]
Figure 3.3: Plot of the energy spectrum for two particles in one dimension as a function of their center-of-mass momentum $K$. The red line denotes the bound-state energy, the grey area the continuum for scattering states. The plot was made for $U/J = 5$.

Figure 3.4: Plot of $U/J$ as a function of $E/J$ for the bound states in (a) one dimension, (b) two dimensions and (c) three dimensions. Plots taken for $K = 0$. 
From this it can be deduced that the critical interaction strength in three dimensions is $U_{\text{crit}}^d = 3 \approx 8J$, which agrees with our guess from Figure 3.4. In two dimensions, we find that $\lim_{E \to 0} U = 0$, suggesting no minimal value of $U$, therefore $U_{\text{crit}}^d = 0$. Figure 3.4b seems to contradict this, but further numerical investigation yields that indeed $U \to 0$ for $E \to 0$ independent of the value of $K$. It must be noted however, that $U$ decreases so rapidly as $E \to 0$, that it is not clear whether our result is of any practical use. Therefore, the question of a critical value of $U$ that is required for the formation of bound states in two dimensions remains open.

Now we want to investigate the wave function of the bound states. Assume $U > 0$ and write the Schrödinger equation associated with the relative motion as

$$[E - J \Delta^K_r]G(K, r) = \frac{1}{G(K, E, 0)} \delta_{r,0}G(K, r).$$

This is solved by

$$\Psi_{\text{BS}}^K(r) = G(K, E, r),$$

$$U = \frac{1}{G(K, E, 0)},$$

which yields the bound-state wave function

$$\Psi(E, r) = \frac{1}{(2\pi)^d} \int d^d k \frac{e^{i k r}}{E - \epsilon_K(k) + i \eta}.$$

I plotted the (non normalized) $|\Psi(r)|^2$ in Figure 3.5 for interaction strengths of $U/J = 3$ and $U/J = 25$. We see that indeed the probability of finding the pair of atoms with a mutual distance $r$ decreases rapidly over only a few lattice sites, even for not too strong interactions. We also see that a greater interaction strength corresponds to more tightly bound states, as expected. It is also noticeable that the wave functions valleys and mountains coincide more and more with the lattice potential as the two-particle interaction strength is driven up.

### 3.2.1 Scattering in the Generalized Bose-Hubbard model

We proceed to work out the two-particle scattering theory for the generalized Bose-Hubbard Hamiltonian 2.11. Like before, we consider the scattering of two atoms at positions $r_1$ and $r_2$. The corresponding Schrödinger equation reads

$$\begin{pmatrix}
U \delta_{r_1, r_2} & \Delta_{r_2} & \Delta_{r_1} & 0 \\
\Delta_{r_2}^* & U \delta_{r_1, r_2} & 0 & \Delta_{r_1} \\
\Delta_{r_1}^* & 0 & U \delta_{r_1, r_2} & \Delta_{r_2} \\
0 & \Delta_{r_1}^* & \Delta_{r_2}^* & U \delta_{r_1, r_2}
\end{pmatrix} \Psi = E \Psi,$$

with $\Psi^\dagger = (\Psi_{AL(r_1, r_2)}, \Psi_{AB(r_1, r_2)}, \Psi_{AL(r_1, r_2)}, \Psi_{BB(r_1, r_2)}).$ Here, we define the displacement operator as

$$\Delta_r(r) = -Je^{i \phi} [f(r + e_x) + f(r - e_x)] - Je^{-i \phi} [f(r + e_y) + f(r - e_y)],$$
Figure 3.5: Plot of $|\Psi(r)|^2$ in two dimensions for a center-of-mass momentum $K = (0, 0)$ for (a) $U/J = 3$ and (b) $U/J = 25$
with \( \mathbf{e}_x \) and \( \mathbf{e}_y \) the unit vectors of length \( d_l \) in the \( x-\) and \( y-\)directions, connecting sites in the \( A \) and \( B \) sublattices. By using a unitary matrix \( \hat{S} \), we can perform a rotation of Eq. (3.3), to express it in terms of the center-of-mass and relative coordinates \( \mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2 \) and \( \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \), like we did in the case of the conventional Bose-Hubbard model. Again, we use plane wave states \( \hat{S}\bar{\Psi}(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{KR}e^{ikr}}\bar{\Psi}_{K,k} \), to rewrite the non-interacting Schrödinger equation, which may then be diagonalized using another matrix \( \hat{S}' \), to yield

\[
\begin{pmatrix}
E^1 & 0 & 0 & 0 \\
0 & E^2 & 0 & 0 \\
0 & 0 & E^3 & 0 \\
0 & 0 & 0 & E^4
\end{pmatrix}
\begin{pmatrix}
\Phi^1_{0,K,k}(\mathbf{R}, \mathbf{r}) \\
\Phi^2_{0,K,k}(\mathbf{R}, \mathbf{r}) \\
\Phi^3_{0,K,k}(\mathbf{R}, \mathbf{r}) \\
\Phi^4_{0,K,k}(\mathbf{R}, \mathbf{r})
\end{pmatrix} = 0,
\] (3.4)

with \( E^i = E - \lambda^{(i)}_{K,k}, \) \( i = 1, 2, 3, 4 \), the eigenvalues of the non-interacting Hamiltonian, and the eigenvector \( \bar{\Phi}^i_{0,K,k} = \hat{S}'\bar{\Psi}_{K,k} \). Working with the new basis \( \bar{\Phi}^i_{0,K,k} \), the interaction part of the Hamiltonian remains diagonal since \( \hat{S}'\hat{U}\hat{S}^t = \hat{U} = U \). The full problem then has the same structure as Eq. (3.4), we simply have to replace \( E^i \) with \( E - \lambda^{(i)}_{K,k} - U \) and \( \Phi^i_{0,K,k}(\mathbf{R}, \mathbf{r}) \) with \( \Phi^i_{K,k}(\mathbf{R}, \mathbf{r}) \). Thus, the corresponding Lippman-Schwinger equation takes the form

\[
|\bar{\Phi}_{K,k}\rangle = |\bar{\Phi}^0_{0,K,k}\rangle + G_0(E_{K,k})\hat{U}|\Phi_{K,k}\rangle,
\]

where \( G_0(E_{K,k}) \) is the Green’s function matrix of the non-interacting problem and

\[
\begin{pmatrix}
\Phi^1_{K,k}(\mathbf{r}) \\
\Phi^2_{K,k}(\mathbf{r}) \\
\Phi^3_{K,k}(\mathbf{r}) \\
\Phi^4_{K,k}(\mathbf{r})
\end{pmatrix} = \begin{pmatrix}
\Phi^1_{0,K,k}(\mathbf{r}) \\
\Phi^2_{0,K,k}(\mathbf{r}) \\
\Phi^3_{0,K,k}(\mathbf{r}) \\
\Phi^4_{0,K,k}(\mathbf{r})
\end{pmatrix} + \begin{pmatrix}
f^1 \\
f^2 \\
f^3 \\
f^4
\end{pmatrix},
\]

with

\[
f^j = \frac{UG^{(j)}(E_{K,k}, \mathbf{r})}{1 - UG^{(j)}(E_{K,k}, 0)},
\] (3.5)

where the Green’s function \( G^{(j)}(E_{K,k}, \mathbf{r}) \) is given by

\[
G^{(j)}(E_{K,k}, \mathbf{r}) = \frac{1}{(2\pi)^2} \int d\mathbf{k}' \frac{e^{i\mathbf{k}'\cdot \mathbf{r}}}{E^{(j)}_{K,k} - \lambda^{(j)}_{K,k} + i\epsilon}.
\]

A boundstate with energy \( E_B \) is then found at the pole of Eq. 3.5, given by

\[
\frac{1}{U} = G^{(j)}(E_B, 0).
\]

We have thus found four different scattering continua and four different bound states for the problem.
Chapter 4

Bogoliubov Theory for Atoms and Molecules

We now proceed to determine the energy spectrum of the Bose-Hubbard Hamiltonian for a system consisting of atoms and molecules described by Eq. (3.2) utilizing a Bogoliubov approach. First, we assume that the system contains a nonzero amount of Bose-Einstein condensed molecules and later, that the system contains an atomic as well as a molecular condensate. We will then use a similar ansatz to describe the condensation of atoms and molecules in the generalized Bose-Hubbard model. We will explore the possibility of oscillations between the molecular and the atomic condensate number, meaning that the two condensates periodically transform into one another with progressing time. Specifically, we will find oscillations between atomic and molecular condensates of distinct momenta.

4.1 Condensation of Molecules

We can apply a Fourier-transformation to the grand canonical Hamiltonian 3.2 to arrive at

\[
H = \sum_k (\epsilon^a_k - \mu) a^\dagger_k a_k + \sum_{k,\sigma} (\epsilon^m_{k,\sigma} - 2\mu) c^\dagger_{k,\sigma} c_{k,\sigma} \\
+ \frac{g}{\sqrt{N}} \sum_{k_1,k_2,k_3,\sigma} \sqrt{Z_{\sigma}} \delta_{k_1,k_2+k_3} \left( c^\dagger_{k_1,\sigma} a_{k_2} a_{k_3} + h.c. \right) \\
+ \frac{U}{2N} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2,k_3+k_4} a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4},
\]  

(4.1)

where

\[
\epsilon^a_k = -2J^a \sum_{i=1}^d \cos(d_i k_i) + \epsilon^a,
\]

\[
\epsilon^m_{k,\sigma} = -2J^m \sum_{i=1}^d \cos(d_i k_i) + \epsilon^m_{\sigma}.
\]
First, we consider the case with a condensate of molecules in the ↓-channel, but no condensate of atoms or molecules in the ↑-channel, following the treatment in [6]. We expand the molecular operators around their condensation point,

\[ c_{k,\sigma} \rightarrow \sqrt{N^m_0} \delta_{k,0} \delta_{\sigma,\downarrow} + c_{k,\sigma}, \]

with \( N^m_0 \) the molecular condensate number in the ↓-channel. Further, we neglect any contributions to the Hamiltonian that are higher than second order in the fields, so that the atomic on-site interaction in the Hamiltonian (4.1) will not be considered in what follows. The remaining terms of the Hamiltonian yield

\[
\sum_k (\epsilon^a_k - \mu) a^\dagger_k a_k + \sum_{k,\sigma} (\epsilon^m_{k,\sigma} - 2\mu) c^\dagger_{k,\sigma} c_{k,\sigma} \rightarrow \epsilon^a_0 - 2\mu) N^m_0 + (\epsilon^m_0 - 2\mu) \sqrt{N^m_0} \left( c^\dagger_{0,\downarrow} + c_{0,\downarrow} \right) + \sum_k \sum_{k,\sigma} \left( \epsilon^m_{k,\sigma} - 2\mu \right) c^\dagger_{k,\sigma} c_{k,\sigma},
\]

\[
g \sqrt{\frac{N}{N^m_0}} \sum_{k_1,k_2,k_3,\sigma} \sqrt{Z_\downarrow} \delta_{k_1,k_2+k_3} \left( c^\dagger_{k_1,\sigma} a_{k_2} a_{k_3} + h.c. \right) \rightarrow g \sum_k \sqrt{n^m_0} \sqrt{Z_\downarrow} (a_k a_{-k} + h.c.).
\]

Here, \( n^m_0 = N^m_0 / N \) denotes the molecular condensate fraction in the ↓-channel. We want the terms of first order in the fields to vanish. This fixes the chemical potential,

\[ 2\mu = \epsilon^m_{0,\downarrow}. \]

The Hamiltonian now reads

\[
H = N^m_0 (\epsilon^m_{0,\downarrow} - 2\mu) + \sum_k (\epsilon^a_k - \mu) a^\dagger_k a_k + \sum_{k,\sigma} (\epsilon^m_{k,\sigma} - 2\mu) c^\dagger_{k,\sigma} c_{k,\sigma} + g \sqrt{n^m_0} \sum_k \sqrt{Z_\downarrow} (a_k a_{-k} + h.c.).
\]

In this approximation, the inverse Greens functions for the atoms and molecules read

\[
-hG^{-1}_a = \begin{pmatrix} -i \hbar \omega_n + \epsilon^a_k - \epsilon^m_{0,\downarrow} / 2 & 2g \sqrt{n^m_0} \sqrt{Z_\downarrow} \\ 2g \sqrt{n^m_0} \sqrt{Z_\downarrow} & +i \hbar \omega_n + \epsilon^a_k - \epsilon^m_{0,\downarrow} / 2 \end{pmatrix},
\]

and

\[
-hG^{-1}_\sigma = \begin{pmatrix} -i \hbar \omega_n + \epsilon^m_{k,\sigma} - \epsilon^m_{0,\downarrow} & 0 \\ 0 & +i \hbar \omega_n + \epsilon^m_{k,\sigma} - \epsilon^m_{0,\downarrow} \end{pmatrix},
\]

so that we find the energy eigenvalues for the atoms and molecules

\[
\hbar \omega_k = \sqrt{\left( \epsilon^a_k - \epsilon^m_{0,\downarrow} / 2 \right)^2 - 4g^2 Z_\downarrow n^m_0},
\]

\[
\hbar \omega_{\sigma,k} = \epsilon^m_{k,\sigma} - \epsilon^m_{0,\downarrow}.
\]
4.2 Condensation of Atoms and Molecules

Now we consider the Hamiltonian (4.1) again. This time, we neglect the terms that correspond to molecules in the \( \uparrow \)-channel, which can be archived by using a suitable detuning \( \delta_B \) (see Figure 3.1). Since there is only one kind of molecules, we drop the \( \downarrow \)-index in what follows and absorb the value of \( Z_1 \) into the definition of \( g \), so that \( g \rightarrow g/\sqrt{Z_1} \). We expand the atoms as well as the molecules according to

\[
a_k \rightarrow \sqrt{N_0^a} \delta_{k,0} + a_k, \quad c_k \rightarrow \sqrt{N_0^m} \delta_{k,0} + c_k.
\]

The terms of the Hamiltonian (4.1) are, up to second order in the fields, now given by

\[
\sum_k (\epsilon_k^a - \mu) a_k^\dagger a_k \rightarrow (\epsilon_0^a - \mu) N_0^a + (\epsilon_0^a - \mu) \sqrt{N_0^a} a_0^\dagger a_0 + \sum_k (\epsilon_k^a - \mu) a_k^\dagger a_k,
\]

\[
\sum_k (\epsilon_k^m - 2\mu) c_k^\dagger c_k \rightarrow (\epsilon_0^m - 2\mu) N_0^m + (\epsilon_0^m - 2\mu) \sqrt{N_0^m} c_0^\dagger c_0 + \sum_k (\epsilon_k^m - 2\mu) c_k^\dagger c_k,
\]

\[
\frac{g}{\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} \left( c_{k_1}^\dagger a_{k_2} a_{k_3} + h.c. \right) \rightarrow 2g \sum_k \sqrt{n_0^m} N_0^a
\]

\[
+ 2g \sum_k \sqrt{n_0^m} \sqrt{N_0^a} \left( a_0 + a_0^\dagger \right) + g \sum_k \sqrt{N_0^a} \left( e_k^\dagger + c_0 \right)
\]

\[
+ g \sum_k \sqrt{n_0^m} \left( a_k a_{-k} + a_{k}^\dagger a_{-k}^\dagger \right) + 2g \sum_k \sqrt{n_0^m} \left( e_k a_k + c_k a_k^\dagger \right),
\]

\[
\frac{U}{2N} \sum_{k_1,k_2,k_3,k_4} \delta_{k_1+k_2+k_3+k_4} \left( a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \right) \rightarrow \frac{U}{2} \frac{(N_0^a)^2}{N} + \frac{U}{N} (N_0^a)^{3/2} \left( a_0 + a_0^\dagger \right)
\]

\[
+ \frac{U}{2} n_0^m \sum_k \left( a_k a_{-k} + a_k^\dagger a_{-k}^\dagger + 4a_k^\dagger a_k \right),
\]

where \( N_0^a \) denotes the atomic condensate number, \( n_0^a = N_0^a/N \) the condensate fraction and \( n_0^m, n_0^a \) the corresponding quantities for the molecules in the \( \downarrow \)-channel. The terms of first order in the fields vanish, yielding two coupled equations for the chemical potential, given by

\[
\epsilon_0^a - \mu + U n_0^a + 2g \sqrt{n_0^m} = 0,
\]

\[
\epsilon_0^m - 2\mu + g \frac{n_0^m}{\sqrt{n_0^m}} = 0.
\]

This gives us a relation between the condensate densities of the atoms and molecules, given by

\[
n_0^a = \frac{\epsilon_0^m - \epsilon_0^a - 2g \sqrt{n_0^m}}{U - \frac{g}{2 \sqrt{n_0^m}}}, \quad (4.2)
\]

which can be reversed to read

\[
\sqrt{n_0^m} = \frac{\epsilon_0^m/2 - \epsilon_0^a - U n_0^a}{4g} + \sqrt{\left( \frac{\epsilon_0^m/2 - \epsilon_0^a - U n_0^a}{4g} \right)^2 + \frac{n_0^m}{4}}. \quad (4.3)
\]

36
The Hamiltonian now reads up to second order in the fields
\[
H = N_0^m (\epsilon_0^m - 2\mu) + N_0^a \left( \epsilon_0^a - \mu + \frac{Un_0^a}{2} \right) + 2g\sqrt{n_0^m} N_0^a \\
+ \sum_k (\epsilon_k^a - \mu + 2Un_0^a) a_k^+ a_k + \sum_k \left( \frac{Un_0^a}{2} + g\sqrt{n_0^m} \right) a_k a_{-k} \\
+ \sum_k \left( \frac{Un_0^a}{2} + g\sqrt{n_0^m} \right) a_k^+ a_{-k} + \sum_k (\epsilon_k^m - 2\mu) c_k^+ c_k + \sum_k (2g\sqrt{n_0^m}) c_k^+ a_k \\
+ \sum_k (2g\sqrt{n_0^m}) a_k^+ c_k.
\]

We write the corresponding action up to second order in the fields as
\[
S[\Psi, \Psi^\dagger] = -H^{(0)} - \frac{\hbar}{2} \sum_{k, \omega} \Psi_k^\dagger G_k^{-1} \Psi_k,
\]
with
\[
H^{(0)} = N_0^m (\epsilon_0^m - 2\mu) + N_0^a \left( \epsilon_0^a - \mu + \frac{Un_0^a}{2} \right) + 2g\sqrt{n_0^m} N_0^a,
\]
and where \(G_k^{-1}\) denotes the inverse Green’s function of the system, given by
\[
-\hbar G_k^{-1} = \begin{pmatrix}
\Delta E^a + i\omega & Un_0^a + 2g\sqrt{n_0^m} & 2g\sqrt{n_0^m} & 0 \\
Un_0^a + 2g\sqrt{n_0^m} & 2g\sqrt{n_0^m} & 0 & \Delta E^m + i\omega \\
2g\sqrt{n_0^m} & 0 & \Delta E^m - i\omega & 0 \\
0 & 2g\sqrt{n_0^m} & 0 & \Delta E^m - i\omega
\end{pmatrix}.
\]

Here, we introduced the abbreviations
\[
\Delta E^a = \epsilon_k^a - \mu + 2Un_0^a, \\
\Delta E^m = \epsilon_k^m - 2\mu.
\]

We rotate back \(i\omega \rightarrow \hbar \omega\) to determine the energy spectrum of the system. Even though this can be done in an analytical fashion, the resulting expressions are quite long and we only look at some numerical results.

A plot of the atomic and molecular condensate density and the energy spectrum for \(\epsilon^m = 0, J^a/\hbar \omega = 0.11, J^m/\hbar \omega = 0.08, U/\hbar \omega = 0.1, g/\hbar \omega = 0.5\) can be seen in Figure 4.1a. The excitation spectrum consists of two branches, the upper one of which is gapped, while the energy value at zero momentum is always equal to zero for the lower branch. A feature of this model is, that it only works reliable for \(g \gg U\). If \(U\) gets larger, the energy spectrum will diverge at some point, see Figure 4.2. This does not surprise us, since the Dickerscheid model was derived for negligible atom-atom interaction. This feature is also reflected in the existence of a pole in Eq. (4.2) for nonzero \(U\).

From now on, we set \(U = 0\) and consider only two dimensional systems, since the results for two and three dimensions agree qualitatively. In Figure 4.1c and d we see plots of the energy spectrum and the relation between atomic and molecular condensate...
Figure 4.1: (a) Plot of the excitation spectrum for a two dimensional system with molecular condensate number $n_0^m = 0.2$ for $\epsilon^m = 0, J^a/\hbar\omega = 0.11, J^m/\hbar\omega = 0.08, U/\hbar\omega = 0.1, g/\hbar\omega = 0.5$ and (b) the corresponding plot of the condensate densities for atoms and molecules for the same system parameters as in (a). (c) Plot of the excitation spectrum for a two dimensional system with molecular condensate number $n_0^m = 0.2$ for $\epsilon^m = 0, J^a/\hbar\omega = 0.11, J^m/\hbar\omega = 0.08, U = 0, g/\hbar\omega = 0.1$ and (d) the corresponding plot of the condensate densities for atoms and molecules for the same system parameters as in (c).
fractions for such a system. The energy spectrum does not look qualitatively different to the \(U \neq 0\) case. The main difference is that the mode at zero momentum does not appear as linear as it was before, since we chose a value for \(g\) this time that is much smaller than before. This, in addition to the elimination of on-site atom-atom interaction, lessens the effect of the broken symmetry that is responsible for the linear Goldstone mode.

In Figure 4.2 we see a plot of the energy values at zero momentum versus \(g\). The frequency corresponding to the nonzero energy value at zero momentum is called the Josephson frequency. It describes out of phase fluctuations between atoms and molecules with a very long wavelength.

### 4.3 Condensation of Atoms and Molecules in the Generalized Bose-Hubbard Model

We proceed to compute the excitation spectrum of a system that contains atoms and molecules consisting of two atoms like in the previous paragraph, but this time by setting up the optical potential in such a way that it gives rise to an atom-molecule Hamiltonian based on the generalized Bose-Hubbard model, given by Eq. (2.11). Assume we can write the Hamiltonian as

\[
H = H_a + H_m + H_{\text{int}},
\]

with

\[
H_a = -J^a \sum_{r \in A, l=1..4} \left[ e^{i\phi^a_l} a_r^\dagger b_{r+l} + h.c. \right] + \frac{U}{2} \sum_{r \in A \oplus B} n_r^a (n_r^a - 1) + \sum_{r \in A \oplus B} (\epsilon^a - \mu) n_r^a,
\]

\[
H_m = -J^m \sum_{r \in A, l=1..4} \left[ e^{i\phi^m_l} c_r^\dagger d_{r+l} + h.c. \right] + \sum_{r \in A \oplus B} (\epsilon^m - 2\mu) n_r^m,
\]

\[
H_{\text{int}} = g \sum_{r \in A} [a_r^\dagger a_r + h.c.] + g \sum_{i \in B} [d_i^\dagger d_i + h.c.],
\]

39
where $a_r \,(c_r)$ annihilates an atom (molecule) at lattice site $r \in A$ while the corresponding creation operations in $A$ are executed by $a^\dagger_r$ and $c^\dagger_r$. In the $B$ sublattice, those operations are applied through the operators $b_r, b^\dagger_r$ for atoms and $d_r, d^\dagger_r$ for molecules. Here $H_a$ and $H_m$ are the single-species Hamiltonians for atoms and molecules, while the process of molecule formation and break-up are described by $H_{\text{int}}$. The atomic and molecular hopping parameters $J^a$ and $J^m$ can be positive or negative in this model, a fact that we will utilize later on in this paragraph.

Again, we want to expand the Hamiltonian in powers of the fluctuations of the fields. We already did this for the $H_a$ part (see Eq. 2.17). The calculations to be done for the $H_m$ part are obviously the same, so only $H_{\text{int}}$ remains to be treated. Apply a Fourier-transformation to it, to arrive at

$$H_{\text{int}} = g \sqrt{\frac{2}{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} \left[ c^\dagger_{k_1} a_{k_2} a_{k_3} + d^\dagger_{k_1} b_{k_2} b_{k_3} \right] + \text{h.c.},$$

where $a^\dagger_k \,(a_k)$ creates (annihilates) an atom with momentum $k$ in the $A$ sublattice, $b^\dagger_k \,(b_k)$ creates (annihilates) a similar atom in the $B$ sublattice, $c^\dagger_k \,(c_k)$ creates (annihilates) a molecule with momentum $k$ in the $A$ sublattice, while $d^\dagger_k$ and $d_k$ perform the corresponding operations in the $B$ sublattice. Now we apply the transformation

$$\alpha_k = \frac{1}{\sqrt{2}} \left( \frac{\epsilon^a_k}{|\epsilon^a_k|} a_k + b_k \right), \quad \beta_k = \frac{1}{\sqrt{2}} \left( \frac{\epsilon^a_k}{|\epsilon^a_k|} a_k + b_k \right),$$

$$\gamma_k = \frac{1}{\sqrt{2}} \left( \frac{\epsilon^m_k}{|\epsilon^m_k|} c_k + d_k \right), \quad \sigma_k = \frac{1}{\sqrt{2}} \left( -\frac{\epsilon^m_k}{|\epsilon^m_k|} c_k + d_k \right),$$

so that $H_{\text{int}}$ now reads

$$H_{\text{int}} = \frac{g}{2\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} \left[ \frac{|\epsilon^m_k||\epsilon^a_k||\epsilon^a_k|}{\epsilon^a_k \epsilon^a_k \epsilon^a_k} \left( \gamma^\dagger_{k_1} - \sigma^\dagger_{k_1} \right) (\alpha_k - \beta_k) (\alpha_k - \beta_k) \right.$$

$$+ \left( \gamma^\dagger_{k_1} + \sigma^\dagger_{k_1} \right) (\alpha_k + \beta_k) (\alpha_k + \beta_k) \left. \right] + \text{h.c.}$$

$$= \frac{g}{2\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} \left\{ D_{k_1,k_2,k_3} \left[ \gamma^\dagger_{k_1} \alpha_k a_k + \gamma^\dagger_{k_1} \beta_k a_k + 2\sigma^\dagger_{k_1} \alpha_k \beta_k \right] + C_{k_1,k_2,k_3} \left[ 2\gamma^\dagger_{k_1} \beta_k a_k + 2\sigma^\dagger_{k_1} \alpha_k a_k + 2\sigma^\dagger_{k_1} \beta_k a_k \right] \right\} + \text{h.c.}$$

Here, we introduced the abbreviations

$$C_{k_1,k_2,k_3} = 1 - \frac{|\epsilon^m_k||\epsilon^a_k||\epsilon^a_k|}{\epsilon^a_k \epsilon^a_k \epsilon^a_k},$$

$$D_{k_1,k_2,k_3} = 1 + \frac{|\epsilon^m_k||\epsilon^a_k||\epsilon^a_k|}{\epsilon^a_k \epsilon^a_k \epsilon^a_k}.$$

Now we apply a mean-field approximation to the Hamiltonian by substituting

$$\beta_k \to \sqrt{N_0^a \delta_{k_1,k_1}^a} + \beta_k, \quad \sigma_k \to \sqrt{N_0^m \delta_{k_1,k_1}^m} + \sigma_k.$$
where the atoms (respectively molecules) condense at momentum $k_0^a \in (0, \pi)$, $k_0^m \in (0, \pi)$. This substitution changes the terms in the Hamiltonian according to

$$
\frac{g}{2\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} D_{k_1,k_2,k_3} \gamma_{k_1} \alpha_{k_2} \alpha_{k_3} \to 0,
$$

$$
\frac{g}{2\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} D_{k_1,k_2,k_3} \gamma_{k_1} \beta_{k_2} \beta_{k_3} \to \frac{gN_0^a}{2\sqrt{N}} D_{k_0^a,k_0^a,k_0^a} \gamma_{2k_0^a}^\dagger
$$

$$
+ \frac{2g\sqrt{N_0^a}}{2\sqrt{N}} \sum_k D_{k,k_0^a,k-k_0^a} \gamma_{k,k-k_0^a}^\dagger \beta_{k-k_0^a},
$$

$$
\frac{g}{\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} D_{k_1,k_2,k_3} \sigma_{k_1} \alpha_{k_2} \beta_{k_3} \to \frac{g}{\sqrt{N}} \sqrt{N_0^a \sqrt{N_0^m}} D_{k_0^a,k_0^a,k_0^m-k_0^a} \alpha_{k_0^m-k_0^a}
$$

$$
+ \frac{g}{\sqrt{N}} \sqrt{N_0^a} \sum_k D_{k,k_0^a,k} \sigma_{k}^\dagger \alpha_{k-k_0^a} + \frac{g}{\sqrt{N}} \sqrt{N_0^m} \sum_k D_{k_0^m,k,k_0^m-k} \alpha_k \beta_{k_0^m-k},
$$

$$
\frac{g}{\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} C_{k_1,k_2,k_3} \gamma_{k_1} \alpha_{k_2} \beta_{k_3} \to \frac{g}{\sqrt{N}} \sqrt{N_0^a \sqrt{N_0^m}} C_{k_0^a,k_0^a,k_0^m-k_0^a} \gamma_{k_0^m-k_0^a}
$$

$$
+ \frac{g}{\sqrt{N}} \sqrt{N_0^a} \sum_k C_{k,k_0^a,k-k_0^a} \gamma_{k} \beta_{k-k_0^a} + \frac{g}{\sqrt{N}} \sqrt{N_0^m} \sum_k C_{k_0^m,k,k_0^m-k} \beta_{k_0^m-k},
$$

$$
\frac{g}{2\sqrt{N}} \sum_{k_1,k_2,k_3} \delta_{k_1,k_2+k_3} C_{k_1,k_2,k_3} \sigma_{k_1} \alpha_{k_2} \beta_{k_3} \to \frac{g}{2\sqrt{N}} \sqrt{N_0^a \sqrt{N_0^m}} C_{k_0^a,k_0^a,k_0^m-k_0^a} \sigma_{2k_0^a}
$$

$$
+ \frac{2g}{2\sqrt{N}} \sqrt{N_0^a \sqrt{N_0^m}} C_{k_0^a,k_0^a,k_0^m-k_0^a} \sigma_{2k_0^a}^\dagger
$$

$$
+ \frac{2g}{2\sqrt{N}} \sqrt{N_0^a} \sum_k C_{k,k_0^a,k-k_0^a} \sigma_{k} \beta_{k-k_0^a} + \frac{g}{2\sqrt{N}} \sqrt{N_0^m} \sum_k C_{k_0^m,k,k_0^m-k} \beta_{k_0^m-k},
$$

We can expand the Hamiltonian up to second order in the fields,

$$
H_{\text{int}} = H_{\text{int}}^{(0)} + H_{\text{int}}^{(1)} + H_{\text{int}}^{(2)} + \ldots,
$$

to find

$$
H_{\text{int}}^{(0)} = \frac{g}{2\sqrt{N}} N_0^a \sqrt{N_0^m} C_{k_0^a,k_0^a,k_0^a} \delta_{2k_0^a,k_0^a},
$$

$$
H_{\text{int}}^{(1)} = \frac{g}{2\sqrt{N}} N_0^a \left[ C_{2k_0^a,k_0^a,k_0^a} \sigma_{2k_0^a}^\dagger + D_{2k_0^a,k_0^a,k_0^a} \gamma_{2k_0^a}^\dagger \right] + \text{h.c.}
$$

$$
+ \frac{g}{2\sqrt{N}} \sqrt{N_0^a \sqrt{N_0^m}} \left[ 2\alpha_{k_0^p-k_0^a} D_{k_0^p,k_0^p,k_0^p-k_0^a} + 2\beta_{k_0^p-k_0^a} C_{k_0^p,k_0^p,k_0^p-k_0^a} \right] + \text{h.c.},
$$

$$
H_{\text{int}}^{(2)} = \frac{g}{2\sqrt{N}} \sum_k \sqrt{N_0^m} \left[ C_{k_0^m,k_0^m-k} \left( \alpha_{k_0^a(k_0^m-k)} + \beta_{k_0^a(k_0^m-k)} \right) + 2D_{k_0^m,k_0^m-k,k} \alpha_{k_0^a(k_0^m-k)} \right]
$$

$$
+ \frac{g}{2\sqrt{N}} \sum_k \sqrt{N_0^m} \left[ C_{k,k_0^a,k-k_0^a} \left( 2\gamma_{k_0^a(k-k_0^a)}^\dagger + 2\sigma_{k}^\dagger \beta_{k-k_0^a} \right) + D_{k,k_0^a,k-k_0^a} \left( 2\gamma_{k_0^a(k-k_0^a)} + 2\sigma_{k}^\dagger \alpha_{k-k_0^a} \right) \right] + \text{h.c.},
$$

41
The first order in the fluctuations yield zero,

\[ D_{2k_0^0, k_0^0, k_0^0} = 0, \]
\[ D_{k_0^0, k_0^0, k_0^m - k_0^a} = 0, \]
\[ \sqrt{N_0^a} (-|\epsilon_{k_0^0}^a| - \mu + \epsilon^a + U^a n_0^a) + g \frac{\sqrt{N_0^a}}{\sqrt{N_0}} C_{k_0^0, k_0^0, k_0^m} \delta_{k_0^m, 2k_0^a} = 0, \]
\[ \sqrt{N_0^m} (-|\epsilon_{k_0^m}^m| - 2\mu + \epsilon^m) + \frac{g N_0^a}{2 \sqrt{N}} C_{k_0^m, k_0^0, k_0^m} \delta_{k_0^m, 2k_0^a} = 0. \]

From \( \epsilon^{a,m}(k) = -2J^{a,m} \left[ e^{-i\phi^{a,m}} \cos(d k_-) + e^{i\phi^{a,m}} \cos(d k_+) \right] \), we can determine the relevant values for the \( C_{k_1, k_2, k_3, \pm, \pm} \) and \( D_{k_1, k_2, k_3, \pm, \pm} \) in the following table (here, the first \( \pm \) is related to the sign of the atomic hopping parameter \( J^a = \pm |J^a| \), the second one to that of the molecules),

<table>
<thead>
<tr>
<th>( k_0^a )</th>
<th>( k_0^m )</th>
<th>( C_{k_0^0, k_0^0, k_0^m - k_0^a, k_0^0} )</th>
<th>( D_{k_0^0, k_0^m, k_0^m - k_0^a, k_0^0} )</th>
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We realize that the values of the \( C_{k_1, k_2, k_3, \pm, \pm}, D_{k_1, k_2, k_3, \pm, \pm} \) only depend on the condensation modes \( k_0^0, k_0^m \) and the sign of \( J^m \) but not the sign of \( J^a \). The kinetic and interaction parts of the Hamiltonian stay unchanged and are still given by Eq. 2.17. Thus, we find two equations for the chemical potential which will only be correlated if molecules condense in the zero mode and atoms in the \( \pi \)-mode for \( J^m < 0 \) or if atoms and molecules both condense in the zero mode for \( J^m > 0 \). Those equations impose a constraint on the system,

\[ \mu - \epsilon^a = -|\epsilon_{k_0}^a| + U n_0^a + 2g \sqrt{n_0^m}, \]
\[ 2\mu - \epsilon^m = -|\epsilon_{k_0}^m| + g \frac{n_0^a}{\sqrt{n_0^m}}. \]
This implies that not all the observables can be freely chosen. Again, we find a relation between the atomic and molecular condensate numbers,

\[
\sqrt{n_0^m} = -\frac{\Delta \epsilon_0 + U n_0^a}{4g} + \sqrt{\left(\frac{\Delta \epsilon_0 + U n_0^a}{4g}\right)^2 + n_0^a/4},
\] (4.6)

where we introduced the abbreviation

\[
\Delta \epsilon_0 = -|\epsilon_{k_0}^a| + \frac{|\epsilon_{k_0}^m|}{2} + \epsilon^a - \epsilon^m.
\]

We note that Eq. 4.6 has the same structure as the corresponding Eq. 4.3 for the conventional Bose-Hubbard model. Now, we are ready to write down the corresponding action \( S_{k_0^a,k_0^m} \),

\[
S[\Psi, \Psi^\dagger]_{k_0^a,k_0^m} = -\frac{n_0 U N_0}{2} - \frac{\hbar}{2} \sum_{k,\omega} \Psi_k^\dagger G^{-1}_{k,\omega} \Psi_k,
\]

where the fields in \( \Psi_k \) depend on the condensation modes \( k_0^a \) of the atoms and \( k_0^m \) of the molecules. They are given by

\[
\Psi_k^\dagger = \begin{pmatrix} \alpha_k^\dagger & \alpha_k^\dagger \beta_k^\dagger & \gamma_k^\dagger \kappa_0^a & \gamma_k^\dagger \kappa_0^m \sigma_k^\dagger + \kappa_0^m \end{pmatrix},
\]

and the matrix representing the respective inverse Green’s function becomes

\[
G^{-1}_k = \begin{pmatrix} C_{aa,k}^{-1} & C_{am,k}^{-1} \\ C_{ma,k}^{-1} & C_{mm,k}^{-1} \end{pmatrix}.
\]

The submatrices are given by

\[
-hC^{-1}_{aa,k} = -hC^{-1}_{aa,k,0} - \hbar g \sqrt{n_0^m} \begin{pmatrix} 0 & C_{0,k,-k}^* & 0 & D_{0,k,-k}^* \\ C_{0,k,-k} & 0 & D_{0,k,-k} & 0 \\ 0 & D_{0,k,-k}^* & 0 & C_{0,k,-k}^* \\ D_{0,k,-k} & 0 & C_{0,k,-k} & 0 \end{pmatrix},
\]

where \( G^{-1}_{aa,k,0} \) denotes the inverse Green’s functions of the atomic problem without atom-molecule coupling,

\[
-hG^{-1}_{aa,k,0} = \begin{pmatrix} \Delta E_{k,a}^+ - i \hbar \omega_n & \frac{1}{2} n_0^a U A_{k,k_0}^a & 0 & \frac{1}{2} n_0^a U B_{k,k_0}^a \\ \frac{1}{2} n_0^a U A_{k,k_0}^a & \Delta E_{k,a}^+ + i \hbar \omega_n & 0 & 0 \\ 0 & 0 & \Delta E_{k,a}^- - i \hbar \omega_n & \frac{1}{2} n_0^a U A_{k,k_0}^a \\ \frac{1}{2} n_0^a U B_{k,k_0}^a & 0 & \frac{1}{2} n_0^a U A_{k,k_0}^a & \Delta E_{k,a}^- + i \hbar \omega_n \end{pmatrix}.
\]

Here, we used the abbreviations

\[
\Delta E_{k,a}^+ = |\epsilon_k^a| - \mu + \epsilon^a + 2n_0^a U,
\]

\[
\Delta E_{k,a}^- = -|\epsilon_k^a| - \mu + \epsilon^a + 2n_0^a U.
\]
We also find that

$$-\hbar G^{-1}_{m,n,k} = \begin{pmatrix} \Delta E^+_{k,m} - i\hbar \omega_n & 0 & 0 \\ 0 & \Delta E^+_{k,m} + i\hbar \omega_n & 0 \\ 0 & 0 & \Delta E^-_{k,m} - i\hbar \omega_n \\ 0 & 0 & \Delta E^-_{k,m} + i\hbar \omega_n \end{pmatrix},$$

with the abbreviations

$$\Delta E^+_{k,m} = |\epsilon^m_k| - 2\mu + \epsilon^m,$$

$$\Delta E^-_{k,m} = -|\epsilon^m_k| - 2\mu + \epsilon^m.$$

The two remaining matrices are given by

$$-\hbar G^{-1}_{a,n,k} = -\hbar g \sqrt{n_0} \begin{pmatrix} C_{k+k_0^n,k,k_0^m}^* & 0 & D_{k+k_0^n,k,k_0^m}^* \\ 0 & C_{-k-k_0^n,-k,-k_0^m} & 0 \\ D_{k+k_0^n,k,k_0^m} & 0 & D_{-k-k_0^n,-k,-k_0^m} \end{pmatrix},$$

$$-\hbar G^{-1}_{m,a,k} = -\hbar g \sqrt{n_0} \begin{pmatrix} C_{k+k_0^n,k,k_0^m} & 0 & D_{k+k_0^n,k,k_0^m} \\ 0 & C_{-k-k_0^n,-k,-k_0^m}^* & 0 \\ D_{k+k_0^n,k,k_0^m}^* & 0 & D_{-k-k_0^n,-k,-k_0^m}^* \end{pmatrix}.$$

In Figure 4.3 we see two plots of the energy spectra corresponding to $(k_0^n, k_0^m) = (0,0), (\pi,0)$. We see that each of the spectra consists of four bands, further denoted by $\epsilon_1^k, \epsilon_2^k, \epsilon_3^k,$ and $\epsilon_4^k$ down from the highest to the lowest, that are grouped in pairs of two. We see that the two upper bands are gapped in both cases. Comparing the plots with our previous results, we interpret the two highest bands $\epsilon_1^k$ and $\epsilon_2^k$ as corresponding to out-of-phase fluctuations between atoms and molecules and the two lowest bands $\epsilon_3^k$ and $\epsilon_4^k$ as corresponding to in-phase fluctuations between the two species. Further, there are two bands of each kind because we can also have the fluctuations in the sublattices $A$ and $B$ either in phase (corresponding to $\epsilon_2^k$ and $\epsilon_4^k$) or out of phase (corresponding to $\epsilon_1^k$ and $\epsilon_3^k$). Of special interest is the dependence of the Josephson frequencies on the atom-molecule coupling $g$, since this parameter can be tuned in experiments, for example through an external magnetic field as discussed in chapter 3. Figure 4.4 shows this dependence. The Josephson frequency corresponding to in-phase fluctuations in the two sublattices $A$ and $B$ is of the same size as that obtained from the conventional Bose-Hubbard model for $g \to 0$, but for larger values of $g$ they behave differently, since in the conventional model the Josephson frequency was rising linear with $g$, a behavior that can only be witnessed here for $g/\hbar \omega \gg 1$, compare Figure 4.2b.
Figure 4.3: Plots of the excitation spectrum for $J^a/h\omega = 0.11$, $J^m/h\omega = 0.08$, $U = 0$, $g/h\omega = 0.1$, $\epsilon^a/h\omega = 1$, $\epsilon^m = 0$. (a) Plot of the excitation spectrum for $\phi^a = \pi/3$, $\phi^m = \pi/5$, corresponding to $(k^a_0, k^m_0) = (\pi, 0)$. (b) Plot of the excitation spectrum for $\phi^a = \phi^m = \pi/5$, which corresponds to $(k^a_0, k^m_0) = (0, 0)$.

Figure 4.4: Plots of the two upper parts of the excitation spectrum at $k = 0$, $\epsilon^3_0$, $\epsilon^4_0$, corresponding to the Josephson frequencies for in-phase ($\epsilon^3_0$) and out-of-phase ($\epsilon^4_0$) oscillation of the two sublattices A and B. (a) Plot for the $(k^a_0, k^m_0) = (\pi, 0)$ case (with $\phi^a = \pi/3$, $\phi^m = \pi/5$). (b) Plot for the $(k^a_0, k^m_0) = (0, 0)$ case (with $\phi^a = \phi^m = \pi/5$). Both plots were computed for $J^a/h\omega = 0.11$, $J^m/h\omega = 0.08$, $U = 0$, $g/h\omega = 0.1$, $\epsilon^a/h\omega = 1$ and $\epsilon^m = 0$. 45
Chapter 5

Conclusion

In this thesis, we explored the possibility of molecule formation and coherent oscillations between atomic and molecular Bose-Einstein condensates in optical lattices. We developed the theory for the conventional Bose-Hubbard model as well as for a generalized model, which incorporates a staggered flux that leads to the existence of a finite-momentum superfluid phase.

The first central result of this thesis was the proof that there exist four different molecular levels in the generalized Bose-Hubbard model for ultracold atoms. This was derived by using two-particle scattering theory in the lattice.

We then used Bogoliubov theory to determine the energy spectra of these systems with atomic and molecular Bose-Einstein condensates. Hereby, we found that the energy spectrum extracted from the conventional Bose-Hubbard model consisted of two bands that corresponded to in-phase and out-of-phase fluctuations in the condensate densities of the two species. For the generalized version of the theory that includes a staggered flux, we found four bands in the excitation spectrum, corresponding to in-phase and out-of-phase density fluctuations not only between atomic and molecular condensates, but also between the condensates in the two distinct sublattices $A$ and $B$ that the model incorporates. We found that the generalized atom-molecule theory only works if Bose-Einstein condensation for atoms and molecules takes place either in a uniform, zero-momentum superfluid phase for both species, with a molecular hopping parameter that satisfies $J^m > 0$ or for molecules condensed in a zero- and atoms in a finite-momentum superfluid phase for $J^m < 0$.

The second central result of this thesis was the extraction of the Josephson frequency, corresponding to long wavelength fluctuations between atomic and molecular condensates. We were able to determine the dependence of the Josephson frequency on the atom-molecule coupling parameter $g$, which mediates the formation of molecules out of two atoms as well as the reverse process, the decay of a molecule into two atoms. We extracted the Josephson frequency first for the conventional Bose-Hubbard model, then for the generalized model, in the latter case for zero-momentum condensates of both atoms and molecules, as well as for a zero-momentum molecular and a finite-momentum atomic condensate. This is important for experiments, since the value of $g$ can be tuned, for example through the utilization of Feshbach resonances. We found a dependence of the Josephson frequency on $g$ that is rising linear in the conventional Bose-Hubbard model, while the dependence in the generalized model was more complicated, but still
linear for large values of $g$. We found that the Josephson frequency for in-phase oscillations between $A$ and $B$ sublattices in the generalized model agrees with the Josephson frequency of the conventional model for small $g$. 
Acknowledgements

My gratitude goes out to my supervisors, Cristiane de Morais Smith and Lih-King Lim. They always had open ears and helpful advice for all of my problems, and their dedication to research has been a constant source of inspiration. I want to especially thank Cristiane for always finding the right words when stuff went wrong, for the Christmas dinner at her home and the fact that, through her influence, I am now using at least three times as many commas as before when writing texts. I am grateful to Lih-King, who had the idea for this thesis in the first place, for finding all that time to guide me through the jungle of cold matter physics while having all the stress of completing his own PHD at the same time.

I also want to thank the Studienstiftung des deutschen Volkes that provided me with invaluable monetary and moral support through a scholarship in the last years.

I say thank you to my fellow master students for the great times I had with them in the student room and outside.

A special thanks goes to my parents, who always helped and supported me wherever they could.
Appendix A

Bloch States and Band Structure

We will now calculate the energy eigenvalues of particles that are moving in one dimension in the potential

\[ V(x) = V_0 \sin \left( \frac{2\pi x}{d_l} \right). \]

According to Bloch’s theorem, we can write the wave functions of particles moving in a periodic potential as a product of so called Bloch functions \( u_{kn}(x) \) and a plane wave envelope function \( e^{ikx} \),

\[ \Psi_{k,n}(x) = u_{k,n}(x)e^{ikx}, \]

where \( k \) is the wavenumber and \( n \) a band index. The Bloch functions have the same periodicity as the lattice, so that \( u_{kn}(x) = u_{kn}(x + d_l) \), where \( d_l \) denotes the lattice constant. From now on, we drop the band index and utilize as an ansatz for the Bloch functions

\[ u_k(x) = \sum_m a_m e^{\frac{2\pi mx}{d_l}}, \]

with \( m \) taking integer values. The corresponding Schrödinger equation is

\[ \left[ -\frac{\hbar^2}{2m_0} \nabla^2 + V(x) - E \right] \psi_k(x) = 0. \]

Let us perform a Fourier-transformation of \( V(x) \) and \( \psi_k(x) \) according to

\[ V(x) = \sum_m V_m e^{\frac{2\pi mx}{d_l}}, \]

\[ \psi_k(x) = \sum_m a_m e^{i(k + \frac{2\pi m}{d_l})x}, \]

so that we find

\[ V(x)\psi_k(x) = \sum_{m,l} V_m e^{\frac{2\pi mx}{d_l}} a_l e^{i(k + \frac{2\pi l}{d_l})x}, \]
and the Schrödinger equation becomes

\[
\sum_l \frac{\hbar^2}{2m_0} \left( k + \frac{2\pi l}{d_l} \right)^2 a_l e^{i \left( k + \frac{2\pi l}{d_l} \right) x} + \sum_{m,l} V_m a_l e^{i \left( k + \frac{2\pi (l+m)}{d_l} \right) x} - E \sum_l a_l e^{i \left( k + \frac{2\pi l}{d_l} \right) x} = 0.
\]

Each Fourier-component should vanish separately, hence

\[
\frac{\hbar^2}{2m_0} \left( k + \frac{2\pi l}{d_l} \right)^2 a_l + \sum_m V_m a_{l-m} - E a_l = 0. \tag{A.1}
\]

The Fourier transform of the potential is given by

\[
V_m = \frac{1}{2\pi} \sum_x V_0 \sin \left( \frac{2\pi x}{d_l} \right) e^{-i \frac{2\pi m x}{d_l}} = \frac{V_0}{2\pi} \sum_x \left[ e^{-ix(m-1)\frac{2\pi}{d_l}} - e^{-ix(m+1)\frac{2\pi}{d_l}} \right]
\]

so that Eq. A.1 becomes

\[
\frac{\hbar^2}{2m_0} \left( k + \frac{2\pi l}{d_l} \right)^2 a_l + \frac{V_0}{2i} [a_{l-1} - a_{l+1}] - E a_l = 0.
\]

To determine the possible energy spectrum, we have to calculate the eigenvalues of the matrix (for the moment we only consider the coefficients \( a_l \) for \( l = +1, 0, -1 \))

\[
\begin{pmatrix}
(k + 2\pi/d_l)^2 & V_0/2i & 0 \\
-V_0/2i & k^2 + V_0/2i & 0 \\
0 & -V_0/2i & (k - 2\pi/d_l)^2
\end{pmatrix}.
\]

In this simple approximation, the energy eigenvalues are given as the solutions of the cubic equation

\[
aE^3 + bE^2 + cE + d = 0,
\]

with

\[
a = -1,
b = + \left( k + \frac{2\pi}{d_l} \right)^2 + k^2 + \left( k - \frac{2\pi}{d_l} \right)^2,
c = - \left( k + \frac{2\pi}{d_l} \right)^2 k^2 - \left( k + \frac{2\pi}{d_l} \right)^2 \left( k - \frac{2\pi}{d_l} \right)^2 - k^2 \left( k - \frac{2\pi}{d_l} \right)^2 + \frac{V_0^2}{2},
d = \left( k - \frac{2\pi}{d_l} \right)^2 k^2 \left( k + \frac{2\pi}{d_l} \right)^2 - \frac{V_0^2}{4} \left[ \left( k + \frac{2\pi}{d_l} \right)^2 + \left( k - \frac{2\pi}{d_l} \right)^2 \right].
\]
Define the parameters $A_+$ and $A_-$ as

$$A_{\pm} = \left( \frac{2b^3 - 9abc + 27a^2d \pm \sqrt{(2b^3 - 9abc + 27a^2d)^2 - 4(b^2 - 3ac)^3}}{2} \right)^{\frac{1}{3}},$$

so that the three energy eigenvalues are now given by

$$E_1 = -\frac{b}{3a} - \frac{1}{3a}A_+ - \frac{1}{3a}A_-,$$

$$E_2 = -\frac{b}{3a} + \frac{1 + i\sqrt{3}}{6a}A_+ + \frac{1 - i\sqrt{3}}{6a}A_-,$$

$$E_3 = -\frac{b}{3a} + \frac{1 - i\sqrt{3}}{6a}A_+ + \frac{1 + i\sqrt{3}}{6a}A_-.$$

The energy eigenvalues are plotted in Figure A.1. We see here that a variation of $V_0$ has a larger impact on the band structure on the edges of the first Brillouin zone than in the center. A larger potential widens the band gap, which only occurs for a nonzero potential.

In this approximation, the band gap at the edge of the Brillouin zone can be determined by subtracting $E_2$ from $E_3$ at the edge of the zone, given by $k = \pi/d_l$. The result is

$$\Delta E = -\frac{i\sqrt{3}}{3a}A_+ + \frac{i\sqrt{3}}{3a}A_-.$$

We see that the band gap is very small but nonzero if we turn the potential off. This is due to the fact that we recurred to an approximation. I plotted $\Delta E$ as a function of the potential in Figure A.2. The connection between them is almost linear, as we might have expected from looking at the calculation. I also plotted the band structure for the case where we consider five of the $a_m'$s instead of three in Figure A.3.
Figure A.1: Band spectrum in the first Brillouin-zone in units of $d_l = \hbar^2/2m_0 = 1$ for (a) $V_0 = 0$, (b) $V_0 = 6$, and (c) $V_0 = 12$. In (d) the $V_0 = 6$ and $V_0 = 12$ plots are shown together.

Figure A.2: Plot of $\Delta E$ as a function of the potential in units of $d_l = \hbar^2/2m = 1$. 
Figure A.3: Band spectrum in units of $d_t = \hbar^2/2m = 1$ for $V_0 = 10$ plotted (a) from $k = -3\pi$ to $k = +3\pi$ and (b) in the first Brillouin zone from $k = -\pi$ to $k = \pi$
Appendix B

Wannier Functions and Periodic Potentials

We consider a lattice of $N$ sites, where each lattice site is labeled by a vector $\mathbf{r}$. The lattice potential is given by $V(\mathbf{x})$ and we have $V(\mathbf{x}) = V(\mathbf{x} + \mathbf{r}_n)$ where $\mathbf{r}_n$ is a vector pointing from one lattice site to another. Let the solution of the single particle Schrödinger equation be denoted by $\Psi_{kn}(\mathbf{x})$, with energy eigenvalues $\epsilon_{kn}$. Now, we introduce Wannier functions $W_m(\mathbf{x} - \mathbf{r}_n)$ that describe a particle localized around a position $\mathbf{r}_n$ in the band indexed by $m$. They are determined through the relation

$$\Psi_{km}(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_n e^{i\mathbf{k}\mathbf{r}_n} W_m(\mathbf{x} - \mathbf{r}_n).$$

Inversely, we see that the Wannier functions are given by

$$W_m(\mathbf{x} - \mathbf{r}_n) = \frac{1}{\sqrt{N}} \sum_n e^{-i\mathbf{k}\mathbf{r}_n} \Psi_{km}(\mathbf{x}).$$

If we assume the wavefunctions to be normalized and proportional to the number of particles $N$ in the system,

$$\int d\mathbf{x} \Psi_{km}(\mathbf{x}) \Psi_{k'm'}(\mathbf{x}) = N \delta_{kk'} \delta_{mm'},$$

we obtain for the normalization of the Wannier functions

$$\int d\mathbf{x} W_m^*(\mathbf{x} - \mathbf{r}_n)W_{m'}(\mathbf{x} - \mathbf{r}_{n'}) = \delta_{nn'} \delta_{mm'},$$

which also demonstrates neatly that the Wannier functions are indeed attached to particular lattice sites and that different bands do not overlap with each other.

Let us consider the free-particle case $V(\mathbf{x}) = 0$, for which $\Psi_{kn}(\mathbf{x}) = A_n \exp(i\mathbf{k}\mathbf{x})$, where $A_n$ is a normalization constant. We then get

$$W_m(\mathbf{x} - \mathbf{r}_n) = \sqrt{N} A_m \delta(\mathbf{x} - \mathbf{r}_n).$$
Now we consider bosons in a periodic lattice potential and approximate their interactions as pairwise additive. The corresponding second-quantized Hamiltonian can be written as

\[
H = \int \! \! dx \Psi^\dagger(x) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(x) \right] \Psi(x) \\
+ \int \! \! dx \int \! \! dx' \Psi^\dagger(x) \Psi^\dagger(x') \frac{V_{\text{int}}(x - x')}{2} \Psi(x') \Psi(x),
\]

with \(\Psi(x)\) and \(\Psi^\dagger(x')\) the bosonic annihilation and creation operators, respectively, and \(V_{\text{int}}(x - x')\) the interaction potential. Now, we introduce operators \(a_{nm}, a^\dagger_{nm}\) that create or annihilate an atom in the Wannier state \(W_m(x - r_n)\), so that it will be found at lattice site \(r_n\) in the band indexed by \(m\). We choose as an ansatz

\[
\Psi(x) = \sum_{n,i} a_{ni} W_n(x - x_i), \\
\Psi^\dagger(x) = \sum_{n,i} a^\dagger_{ni} W_n^*(x - x_i),
\]

which immediately leads us to

\[
H = \sum_{i,j,k,l} a^\dagger_{ik} J_{ij,kl} a_{jl} + \sum_{i,j,k,l,m,n,o,p} a^\dagger_{im} a^\dagger_{jn} U_{ijkl,mnop} a_{ko} a_{lp},
\]

where we defined the hopping parameter \(J_{ij,nm}\) and the on-site interaction parameter \(U_{ijkl,mnop}\) in the new basis as

\[
J_{ij,kl} = \int \! \! dx W^*_k(x - x_i) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(x) \right] W_l(x - x_j), \\
U_{ijkl,mnop} = \int \! \! dx dx' W^*_m(x - x_i) W^*_n(x' - x_j) \frac{V_{\text{int}}(x - x')}{2} W_o(x - x_k) W_p(x - x_l). \quad (B.1)
\]

For given potential the quantities \(J_{ij,nm}\) and \(U_{ijkl,mnop}\) can be evaluated in an analytical or numerical fashion. This way we can treat bosons in a periodical potential as sitting on sites of a lattice.
Appendix C

Approximate Values for Hopping and Interaction Parameters

We want to find an approximation for the magnitude of the interaction strength $U$ and the hopping parameter $J$ for atom-atom and molecule-molecule interaction. For atoms, these parameters are given in terms of the Wannier states $W_m(x - x_j)$ by Eq. B.1. For deep lattice potentials we expect the atoms to be localized around the bottom of the potential at each lattice site. As an ansatz we approximate the Wannier-states as the ground states of harmonic oscillators,

$$\Psi_0(x) = \prod_{i=1}^d \left( \frac{1}{\pi} \right)^{\frac{d}{4}} e^{-\frac{x^2}{4}} = \prod_{i=1}^d \Psi_i(x_i),$$

where we rescaled the original value of $x$ in terms of the oscillator length $l = \sqrt{\hbar/m\omega}$ according to

$$x_{i,\text{rescaled}} = x_{i,\text{old}} l,$$

so that now we have to evaluate

$$J = \int d\mathbf{x} \Psi(x) \frac{h\omega}{2} \left[ -\nabla^2 + x^2 \right] \Psi(x - \frac{\lambda}{2} e_x),$$

$$U = T \int d\mathbf{x} |\Psi(x)|^4,$$

where we assumed that we can approximate the lattice potential as harmonic oscillators according to

$$V(x) = \sum_{i=1}^d V_0 \sin^2(kx_i) \approx \sum_{i=1}^d V_0(kx_i)^2 = \sum_{i=1}^d \frac{m\omega^2}{2} x_i^2,$$

(where $k = 2\pi/\lambda$), that the strength of the on-site interaction can be approximated by $T = 4\pi h^2 a/m$, with the scattering length $a$, and that it is sufficient to consider nearest-neighbor hopping. For the kinetic energy part of $J$, we have to consider

$$\nabla^2 \Psi(x - x^j) = \left[ -d + \sum_{i=1}^d (x_i - x^j)^2 \right] \Psi(x - x^j),$$
so that the expression for $J$ now reads

$$J = \int dx \Psi(x) \frac{\hbar \omega}{2} \left[ d - (x_1 - \lambda/2)^2 - x_2^2 - \ldots - x_d^2 + x_1^2 + x_2^2 + \ldots + x_d^2 \right] \Psi(x - \frac{\lambda}{2} e_1)

= \int dx \Psi(x) \frac{\hbar \omega}{2} \left[ d - \frac{\lambda^2}{4} + \lambda x_1 \right] \Psi(x - \frac{\lambda}{2} e_1)

= \frac{\hbar \omega}{2} e^{\lambda^2/16}

Solving the resulting Gaussian integrals and switching back to non-dimensionless units we find

$$J = d \sqrt{V_0 E_R} \exp \left( -\frac{\pi^2}{4} \sqrt{\frac{V_0}{E_R}} \right)

U = \frac{4\pi \hbar^2}{m} \frac{1}{(2\pi)^{d/2}} \frac{a}{l},

where we introduced the recoil energy

$$E_R = \frac{(2\pi \hbar)^2}{2m} \frac{1}{\lambda^2},

which an atom initially at rest picks up after absorbing one photon from the lattice laser.
Appendix D

Time-Ordered Two-Particle Correlation Functions

The definition of the path integral is

\[ K(x_f, t_f, x_i, t_i) = \langle x_f, t_f \mid x_i, t_i \rangle = N \int Dxe^{iS[x(t)}/\hbar, \]

and the expectation values of observables are defined as

\[ \langle A(x_f, t_f, x_i, t_i) \rangle = \langle x_f, t_f \mid A \mid x_i, t_i \rangle = N \int DXe^{iS[x}/\hbar. \]

The time-dependence of an operator is given by

\[ a_i(t) = e^{iHt/\hbar}a_i e^{-iHt/\hbar}, \]

so we can write the time dependent two-particle correlation function \( \langle a_i(t)a_{i'}(t') \rangle_{S(0)} \) as

\[ \langle a_i(t)a_{i'}(t') \rangle_{S(0)} = \langle g|e^{iHt'/\hbar}a_{i'} e^{-iHt'/\hbar}e^{iHt'/\hbar}a_i e^{-iHt'/\hbar}|g \rangle = \sqrt{g + 1} e^{-ie_{i'}t'/\hbar} \langle g|e^{iHt'/\hbar}a_{i'} e^{-iH(t-t')/\hbar} | g + 1 \rangle = (g + 1) e^{-ie_{i'}t'/\hbar} e^{-ie_{i'+1}(t-t')/\hbar} e^{iE_0 t'/\hbar} = (g + 1) e^{-i(E_{i'+1} - E_0)(t-t')/\hbar}, \]

where \( |g \rangle \) denotes the unperturbed ground state. Proceeding in the same way we find

\[ \langle a_{i'}(t')a_i(t) \rangle_{S(0)} = \langle g|e^{iHt'/\hbar}a_i e^{-iHt'/\hbar}e^{iHt'/\hbar}a_{i'} e^{-iHt'/\hbar}|g \rangle = ge^{-iE_0 t'/\hbar} e^{iE_{i'-1}(t-t')/\hbar} e^{iE_0 t'/\hbar} = ge^{i(E_{i'-1} - E_0)(t-t')/\hbar}. \]

By performing a Wick rotation \( t \to -i\tau \) we find

\[ \langle a_i(\tau)a_{i'}(\tau') \rangle_{S(0)} = (g + 1) e^{-(E_{i'+1} - E_0)(\tau-\tau')/\hbar}, \]
\[ \langle a_{i'}(\tau')a_i(\tau) \rangle_{S(0)} = ge^{i(E_{i'-1} - E_0)(\tau-\tau')/\hbar}. \]
And so we find the time ordered two particle correlation function

\[ \langle T[a_i(\tau)a_{i'}^\dagger(\tau')] \rangle_{S^{(0)}} = \Theta(\tau - \tau')(g + 1)e^{-(E_{g+1}^0 - E_g^0)(\tau - \tau')/\hbar} \]

\[ + \Theta(\tau' - \tau)ge^{(E_{g-1}^0 - E_g^0)(\tau - \tau')/\hbar}. \]
Bibliography


