Ultracold rubidium atoms in periodic potentials

by

Robert Saers
Detta verk skyddas enligt lagen om upphovsrätt (URL 1960:729).


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Abstract

This thesis includes both experimental and theoretical investigations, presented in a series of eight papers.

The experimental part ranges from the construction procedures of an apparatus for Bose-Einstein condensates, to full scale experiments using three different set-ups for ultracold atoms in optical lattices.

As one of the main themes of the thesis, an experimental apparatus for production of Bose-Einstein Condensates is under construction. A magneto-optically trapped sample, hosting more than 200 million $^{87}$Rb atoms, have successfully been loaded into a magnetic trap with high transfer rate. The lifetime of the sample in the magnetic trap is in the range of 9s, and the atoms have been shown to respond to evaporative cooling. The experiment is ready for optimization of the magnetic trap loading, and evaporative cooling parameters, which are the final steps for reaching Bose-Einstein condensation. The set-up is designed to host experiments including variable geometry optical lattices, and includes the possibility to align laser beams with high angular precision for this purpose.

The breakdown of Bloch waves in a Bose-Einstein condensate is studied, attributed to the effect of energetic and dynamical instability. This experimental study is performed using a Bose-Einstein condensate in a moving one-dimensional optical lattice at LENS, Florence Italy. The optical lattice parameters, and the thermal distribution of the atomic sample required to trigger the instabilities, are detected, and compared with a theoretical model developed in parallel with the experiments. In close connection with these one-dimensional lattice studies, an experimental survey to characterize regimes of superradiant Rayleigh scattering and Bragg scattering is presented.

Tunneling properties of repulsively bound atom pairs in double well potentials are characterized in an experiment at Johannes Gutenberg University, Mainz Germany. A three-dimensional optical lattice, producing an array of double wells with tunable properties is let to interact with a Bose-Einstein condensate. Pairs of ultracold atoms are produced on one side in the double wells, and their tunneling behavior, dependent on potential barrier and repulsion properties, is studied.

A theoretical study of the crossover between one- and two-dimensional systems has been performed. The simulations were made for a two-dimensional array of atoms, where the behavior for different tunneling probabilities and atom-atom repulsion strengths was studied. Scaling relations for systems of variable sizes have been examined in detail, and numerical values for the involved variables have been found.
List of papers:

This thesis is based on the following papers:

**I** Observation of Dynamical Instability for a Bose-Einstein Condensate in a Moving 1D Optical Lattice
L. Fallani, L. De Sarlo, J. E. Lye, M. Modugno, R. Saers, C. Fort and M. Inguscio

**II** Unstable regimes for a Bose-Einstein condensate in an optical lattice
L. De Sarlo, L. Fallani, J. E. Lye, M. Modugno, R. Saers, C. Fort and M. Inguscio

**III** Dynamics of Bloch Matter Waves and Its Breakdown: a Bose-Einstein Condensate in a Moving 1D Optical Lattice

**IV** From superradiant Rayleigh scattering to Bragg scattering
L. De Sarlo, R. Saers, S. Bartalini, F. S. Cataliotti, L. Fallani, C. Fort, I. Herrera and M. Inguscio

**V** A set-up for flexible geometry optical lattices
R. Saers, M. Rehn, T. Scheler, M. Zelán, and A. Kastberg

**VI** Direct observation of second-order atom tunnelling
S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller and I. Bloch
Nature 448, 1029 (2008)

**VII** Transition from a Two-Dimensional Superfluid to a One-Dimensional Mott Insulator
S. Bergkvist, A. Rosengren, R. Saers, E. Lundh, M. Rehn and A. Kastberg

**VIII** One-dimensional phase transitions in a two-dimensional optical lattice
M. Rehn, S. Bergkvist, A. Rosengren, R. Saers, M. Zelán, E. Lundh, and A. Kastberg
Comments to my contribution to the work in the thesis and the included papers

The design and composition of the experimental apparatus at Umeå University, was initiated when the group was based in Stockholm. In collaboration with other students, the apparatus has been rebuilt and redesigned continuously. This work have been shared within the laboratory, and the main responsible persons for the laboratory work have been me, Magnus Rehn, Martin Zelán, and earlier in Stockholm, Kristian Stöchkel.

- Papers I, II and III. These papers present the work on the non-linear effects; energetic and dynamical instability. I have participated in the group work setting up the experiment, the measurements, and also in the discussion with collaborating theoreticians. Paper III reviews the results of papers I and II. It also includes measurements in the linear regime, to which I have made a small contribution.

- Paper IV. For the measurements on superradiant Rayleigh scattering, my main contribution has been to take part in the verification of the experimental techniques, as presented in this paper. I have also made minor experimental contributions to the other work on the subject, presented in related publications by the same group.

- Paper V. I have contributed to this paper by playing an essential role in the building of the experimental set-up. I have also been the main responsible in the experimental implementation of the optical lattices, the measurements included in this paper and the analysis of the acquired data. The models used to analyse the experimental results are to a large portion implemented by me.

- Paper VI. For the work on correlated tunneling of atom pairs in double well potentials, I have participated throughout the measurements in the laboratory. My work was concentrated to acquiring and evaluating data, maintaining and improving the alignment of the set-up, and discussions relating the experimental procedures.

- Paper VII and VIII. In this theoretical project I have taken a large active role, from the initial idea, to the current papers. I have contributed with simulations of realistic experimental parameters, connecting Quantum Monte Carlo results by Sara Bergkvist in paper VII, to an experimental set-up. I have computed the expected signals that can be compared to future experimental data. In paper VIII, I have participated extensively in the evaluation of the Monte Carlo data, including the finite size scaling.
Acknowledgment

There are so many people that stood by my side during the work of this thesis, that any attempt to name all of you will fail.

Most of all, I thank my supervisor, professor Anders Kastberg. You made it all possible, you have supported me, and given me challenging tasks to dig into. By your side, my assistant supervisor, Svante Jonsell, has played an important role by balancing the laboratory parts of my work, with a firm theoretical background.

Before going to Umeå, Anders sent me to the city of Florence in Italy for a year. During this year I had the pleasure to work with a group of lovely people, a memorable time. I worked in one of the laboratories of the visionary professor M. Inguscio; with Chiara, Leonardo, a-Luigi, Jacopo, Jessica, Francesco, Michele, and all of you others who wandered in and out of that laboratory door. I found myself accompanied by talented and pleasant people. Your open-heartedness will always inspire me in life.

There are so many other people I want to thank from Florence, in addition to the people in the laboratory. Most important are Riccardo×2, Silvia, Gloria, Franceschino, Antonino, and others in the great house in Sesto Fiorentino, where you adopted me, and became my Italian family. Then there are all the friends and colleagues from the other laboratories, where especially Herwig, Laura, Giacomo, Paola, Alessandra, and Valentina should not be forgotten.

Going back to Sweden, Umeå invited me, dressed in New Years white. The first to meet up with me was Magnus, who invited me to the laboratory work, as well as to the social life in Umeå. We started working on unpacking and remounting equipment in the rubidium lab. Soon we got great help from Meena, coming from Bangalore to help us building electronics, and asking the most wonderful questions about snow. For the initial work, Kristian was very helpful in quickly answering questions, and even coming up here in order to help us save time.

Then came Markus, with everlasting energy and creativity, making good progress in the lab, and becoming a good friend. There was also Fred, who worked hard to build a new laser. It was a pleasure to see you develop with the lab, and I had a great time working with you. Two new master students followed; Thomas who came to work on our first lattice experiments, and Martin our future hope in the lab, doing great progress then, and now as a PhD student - keep up the good work! In the last semester, I have had the pleasure to work
with Samuel, who brought many good ideas into the lab.

It has been great having a sister lab to bandy alignment ideas with, or just to share a beer or two. Thank you Peder, Stefan, and Henning, along with your master students, especially Johan and Joakim.

For many small experimental solutions, and the possibility to share and borrow equipment, a special thank to Martin, Leif, Lars, Lars-Erik, Tomas, Lena, Ove, Magnus, and not to forget Erik, who I wish could still be here with us.

Working hard to solve experimental problems, it has been great to share an office, or at least a department, with a bunch of cheerful theorists. I have already mentioned Svante, but there has also been Claude, Emil, Alberto, Mats, Andrei, Peter, and a whole group of master students. Great working with you all, and I hope Martin keeps the tradition of having a special mirror for you in the lab.

Keeping track of all the practical things, there have always been Karin, Margaretha, Ann-Charlott, Lilian, Katarina, and Jörgen to turn to.

At KTH in Stockholm, I’ve had the pleasure to work with Sara and Anders. Thank you Sara, for quickly understanding the ideas, and devoting yourself to our small project.

Working in Mainz gave me the pleasure to collaborate with the group of the creative professor I. Bloch, where I spent many joyful nights in the lab with Stefan, Patrick, Simon, Michael and Artur. Thank you for this opportunity, and beware of the meadows!

Besides work, there are both friends and family to thank. Being the best of both, I would like to thank my girlfriend Emma for being there, no matter how good or bad a day I have had. Without your devotion and love, I would have missed so much happiness in life.

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Chapter 1

Introduction

In the early twentieth century, the wave nature of matter was a young and quickly growing field of physics. During this era, a Bengali physicist, S. N. Bose, active at Dacca University in today’s Bangladesh, sent a study to the famous physicist A. Einstein. In this study, S. N. Bose derives Planck’s radiation law from a statistical physics point of view, excluding the use of the classical radiation field. This caught the eyes of A. Einstein, who submitted the manuscript, after translating it from English to German. He also appended a comment including; “nach meiner Meinung einen wichtigen Fortschritt” - “according to my opinion an important advance”, to the paper, convincing the editorial board to accept the manuscript for publication [1].

A. Einstein also informed S. N. Bose about his intentions to submit the translated manuscript by sending him a postcard, also stating that the work is a ”beautiful step forward”. This postcard granted S. N. Bose a visa to travel to Germany, and the favorable response on his paper rewarded him a two year study leave for this European journey, where he could meet up with all the masters of the era.

Shortly after S. N. Bose’s paper, A. Einstein extended and generalized this theory to include atoms [2]. His paper concluded that for higher temperatures, the statistical properties of a gas using the quantum theory, are the same as for the earlier known classical theory, in accordance with the correspondence theory. He also noted, that for low temperatures, the classic and quantum theories deviated from each other, and that a macroscopic population of a state can be achieved, later referred to as a Bose-Einstein condensate.

Even though Bose-Einstein condensation was predicted in the early days of quantum physics, it would take many years until it was finally realized in a gas. The first experimental evidences were achieved in 1995, and E. A. Cornell, W. Ketterle and C. E. Wieman were awarded with the Nobel prize in physics in 2001 for their contributions [3, 4].

Coming from the field of atomic physics, the experimental research of Bose-Einstein condensates has grown quickly. The narrow momentum spread, and the quantum wave nature of the experimental sample, opened the door to a
neighboring and already prospering field, being optical lattices [5, 6]. Introducing these periodic structures, created by interference of laser beams, bridged the gap between Bose-Einstein condensates and solid state physics, quickly leading to a large quantity of experiments and theoretical work [7].

The work presented in this thesis summarizes experimental and theoretical work performed within several research groups. Several experimental investigations of non-linear effects for Bose-Einstein condensates in one-dimensional optical lattices have been undertaken at LENS (European Laboratory for Nonlinear Spectroscopy), Florence, Italy. Other experimental work, investigating tunneling properties of atoms in double well potentials were performed at Johannes Gutenberg University, Mainz, Germany. The main focus has been to construct and prepare an experimental apparatus locally at Umeå University. The status of this experimental apparatus has largely improved over the years, even though a Bose-Einstein condensate is not yet produced. In parallel with the experimental work, theoretical studies of low dimensional crossovers for cold atoms in optical lattices have been undertaken, in close collaboration with the Royal Institute of Technology, Stockholm, Sweden.

Common throughout the work of this thesis is the direct manipulation of the wave function of a Bose-Einstein condensate. Optical lattices have been used to impose periodic potentials where the potential strength can be varied from small perturbations, to deep wells where atoms become localized. The geometry of these potentials can easily be varied, a feature used in several of the projects. It has also motivated the implementation of high precision alignment methods.

The thesis starts with two theoretical chapters, 2 and 3, treating the subject of Bose-Einstein condensation and optical lattices respectively. These chapters, especially the one about optical lattices, give introductions to the deeper, and more specialized studies, presented in chapters 5, 6 and 7, where the first two are experimental investigations and the latter is theoretical.

The three experimental set-ups, and a selection of alignment procedures are presented in chapter 4. This chapter is meant as a technical background for the experimental achievements, helping the reader to fully appreciate the realizability of the rest of the thesis.
Chapter 2

Theory

2.1 Bose-Einstein Condensation

Nature divides particles into two groups, bosons and fermions. The nucleons and electrons are fermions, but atoms and molecules are composite particles and can be either bosonic or fermionic. For an atom it is the nuclear and electronic composition that decides the nature of the complete atom. Combining an even number of fermions results in a bosonic particle, while an uneven gives a fermionic particle. A neutral atom has an equal number of protons and electrons. Therefore the bosonic or fermionic nature of an atom is decided by the number of neutrons [8]. The experimental and theoretical work in this thesis is concentrated to the bosonic isotope of rubidium, $^{87}$Rb, having 37 electrons and protons, and 50 neutrons.

A difference between bosons and fermions is manifested when occupation probabilities of any energy state become large. Several bosons may occupy the same energy state, whereas only one fermion is allowed in a single state. This difference makes it possible for bosons to form a macroscopic occupation of an energy state; the formation of a Bose-Einstein Condensate (BEC).

In an experiment, the creation of a BEC is achieved by increasing the phase space density of a gas to a value close to unity. The phase space density, $\rho_{ph}$ is defined as the number of particles contained in a box with the volume of the thermal de Broglie wavelength cubed:

$$\rho_{ph} = n_{atom} \lambda_{dB}^3 = n_{atom} \left( \frac{2\pi \hbar^2}{mk_B T} \right)^{3/2}, \quad (2.1)$$

with the particle density $n_{atom}$, particle mass $m$, temperature $T$, and the constants $\hbar = h/2\pi$, with $h$ being Planck’s constant, and $k_B$ Boltzmann’s constant.

The transition to BEC occurs when $\rho_{ph} = 2.612 [9]$, which can be achieved by cooling a gas to temperatures in the range of a nanokelvin, keeping the density low in order to maintain the conditions of a weakly interacting gas. When the atoms are cooled, the spatial extents of their wave packets increase. At the
transition point, the wave packets have become large enough to overlap, and the indistinguishability of the particles becomes important. The BEC is created as a gigantic matter wave of atoms having a macroscopic occupation of the ground state [9], as will be seen in more detail later in this section.

### 2.1.1 Statistical properties for macroscopic occupation

Many properties of a BEC can be derived from statistical physics. Starting off with the non-interacting, and untrapped atomic sample will give a good approximation for the critical temperature and the number of condensed atoms, which holds even for a gas of interacting atoms. Within a few derivations, the basic requirements for a macroscopic occupation of the ground state can be obtained.

Starting in the grand canonical ensemble\(^1\), the partition function, \(\Xi\), is the Boltzmann weighted sum of all possible microscopic states of a system.

\[
\Xi = \sum_{\nu} e^{-\beta(E_{\nu} - \mu N_{\nu})},
\]

where \(\beta = 1/k_B T\) is the inverse thermal energy, \(\nu\) is the index of a state of the system with occupation \((N_1, N_2, ...\) of the single particle states, giving a total number of particles \(N_\nu = \sum_j N_j\). Each single particle state \(j\) has the energy \(\epsilon_j\) adding up to a total energy \(E_\nu = \sum_j \epsilon_j N_j\) of the system state \(\nu\). The chemical potential \(\mu\) regulates the exchange of particles between the grand system and the reservoir, and it can be seen as the cost of adding one particle to the state. If the number of particles would be fixed, the partition function would reduce to the case of the canonical ensemble\(^2\). The partition function can also be rewritten using the occupation number \(N_j\),

\[
\Xi = \prod_j \left\{ \sum_{N_j=0}^{\infty} e^{-\beta(\epsilon_j - \mu)N_j} \right\} = \prod_j \left\{ \sum_{N_j=0}^{\infty} \left( e^{-\beta(\epsilon_j - \mu)} \right)^{N_j} \right\} = \prod_j \frac{1}{1 - e^{-\beta(\epsilon_j - \mu)}}.
\]

The Bose distribution function, being the average occupation number of particles \(\langle N_j \rangle\) of the state \(j\), can thus be calculated as

\[
f^0(\epsilon_j) = \langle N_j \rangle = \sum_{\nu} N_j \exp\{-\beta(\epsilon_j - \mu)\} = \frac{\partial \Xi}{\partial(-\beta \epsilon_j)} = \frac{\partial \ln \Xi}{\partial(-\beta \epsilon_j)} = \frac{1}{e^{\beta(\epsilon_j - \mu)} - 1}.\]

To reach a macroscopic occupation of the ground state, \(N_0\) should diverge. This occurs when the chemical potential reaches the same value as the lowest energy level, which is normally very close to zero. In a BEC, the chemical potential is thus close to zero, while for non condensed systems, the occupation number is non-macroscopic, and thus the chemical potential is negative.

\(^1\)A large number of particles in equilibrium with a reservoir, with respect to both particle number and energy.

\(^2\)Energy, but no particle exchange with the reservoir.
2.1.2 Transition temperature and condensed fraction

A BEC can only be created in a small range of parameters. The creation of the BEC is a phase transition, where the macroscopic change of the temperature, will affect microscopic parameters such as occupation number and specific heat.

Density of states for a harmonic oscillator

To calculate statistical properties of a BEC, the density of states is needed and can be computed for various confining potentials following the path used below for harmonic potentials [10]. The three-dimensional harmonic oscillator potential for an atom with mass \( m \) takes the form

\[
V_{\text{ho}}(r) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2),
\]

(2.5)

where the state \( \nu \) excited to \( \nu_{\text{ho}x}, \nu_{\text{ho}y}, \nu_{\text{ho}z} \) have the eigenenergy given by

\[
\epsilon_{\nu}(\nu_{\text{ho}x}, \nu_{\text{ho}y}, \nu_{\text{ho}z}) = \left( \nu_{\text{ho}x} + \frac{1}{2} \right) \hbar \omega_x + \left( \nu_{\text{ho}y} + \frac{1}{2} \right) \hbar \omega_y + \left( \nu_{\text{ho}z} + \frac{1}{2} \right) \hbar \omega_z.
\]

(2.6)

Using this relation one can calculate the number of states with energies lower than \( \epsilon; \)

\[
G(\epsilon) = \frac{1}{\hbar^3 \omega_{\text{ho}}^3} \int_0^\epsilon d\epsilon_x \int_0^{\epsilon-\epsilon_x} d\epsilon_y \int_0^{\epsilon-\epsilon_x-\epsilon_y} d\epsilon_z = \frac{1}{6\hbar^3 \omega_{\text{ho}}^3} \epsilon^3,
\]

(2.7)

where \( \omega_{\text{ho}} = (\omega_x \omega_y \omega_z)^{1/3} \) is the geometric average of the harmonic oscillator angular frequencies. From equation 2.7 the density of states can be derived as

\[
g(\epsilon) = \frac{dG(\epsilon)}{d\epsilon} = \frac{1}{2\hbar^3 \omega_{\text{ho}}^3} \epsilon^2 = C_\alpha \epsilon^{\alpha-1},
\]

(2.8)

where \( \alpha = 3 \) for a three-dimensional harmonic oscillator potential, and the constant \( C_\alpha \) depends only on the trapping parameters.

Transition temperature \( T_c \)

The transition temperature to a BEC is the maximal temperature, for which a macroscopic occupation of the lowest energy state appears. At this temperature the chemical potential will be close to zero, which is a requirement to reach this macroscopic occupation, as equation 2.4 diverges for \( \mu = \epsilon_0 \).

To calculate \( T_c \), the limit when \( \mu = 0 \) and all particles are in the excited state is taken;

\[
N = N_{\text{exc}}(\mu = 0) = \int_0^\infty d\epsilon g(\epsilon) f_0(\epsilon) = \\
= \int_0^\infty d\epsilon \frac{\epsilon^2}{2\hbar^3 \omega_{\text{ho}}^3} \exp\left\{ \frac{1}{k_B T} (\epsilon_\nu - 0) \right\} - 1 = \\
= \frac{(k_B T_c)^3}{2\hbar^3 \omega_{\text{ho}}^3} \int_0^\infty d\tilde{\epsilon} \frac{\tilde{\epsilon}^2}{\tilde{\epsilon}^2 - 1} = \frac{(k_B T_c)^3}{2\hbar^3 \omega_{\text{ho}}^3} \Gamma(3) \zeta(3),
\]

(2.9)
Table 2.1: The gamma function $\Gamma(\alpha)$ and the Riemann zeta function $\zeta(\alpha)$ [10].

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\Gamma(\alpha)$</th>
<th>$\zeta(\alpha)$</th>
<th>Type of trapping confinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>$\infty$</td>
<td>1D harmonic oscillator</td>
</tr>
<tr>
<td>1.5</td>
<td>$\sqrt{\pi}/2$</td>
<td>2.612</td>
<td>3D box</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>$\pi^2/6$</td>
<td>2D harmonic-oscillator</td>
</tr>
<tr>
<td>2.5</td>
<td>$3\sqrt{\pi}/4$</td>
<td>1.341</td>
<td>2D harmonic-oscillator</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>1.202</td>
<td>3D harmonic-oscillator</td>
</tr>
<tr>
<td>3.5</td>
<td>$15\sqrt{\pi}/8$</td>
<td>1.127</td>
<td>3D harmonic-oscillator</td>
</tr>
</tbody>
</table>

where $\gamma(\alpha)$ is the Gamma function, $\zeta(\alpha)$ is the Riemann Zeta function, both shown in table 2.1 and $\bar{\epsilon} = \epsilon/k_B T_c$. Thus;

$$k_B T_c = \frac{\hbar \omega_{ho}}{\zeta(3)^{1/3}} N^{1/3}. \quad (2.10)$$

**The number of non-condensed atoms as a function of temperature**

At the temperature $T_c$, a BEC starts forming, but there is still a large fraction of thermally excited atoms left. Using the same procedure as in equation 2.9, but taking the temperature as a variable between 0 and $T_c$, the number of excited atoms as a function of $T$ can be calculated

$$N_{exc}(\mu = 0, T < T_c) = \int_0^\infty d\epsilon g(\epsilon) f^0(\epsilon) = \frac{(k_B T)^3}{2\hbar^3 \omega_{ho}^3} \Gamma(3) \zeta(3) = N \left( \frac{T}{T_c} \right)^3, \quad (2.11)$$

with a pure BEC at absolute zero, and a fully thermal cloud above $T_c$.

**Ground state of non-interacting atom cloud**

For an atomic cloud trapped in a harmonic potential, as the one in equation 2.6, the ground state for each atom is a Gaussian of the form

$$\varphi_0(\mathbf{r}) = \left( \frac{m \omega_{ho}}{\pi \hbar} \right)^{3/4} \exp \left[ -\frac{m}{2\hbar} \left( \omega_x x^2 + \omega_y y^2 + \omega_z z^2 \right) \right]. \quad (2.12)$$

For a cloud of $N$ non-interacting atoms, the ground state wave function is then given by

$$\phi(\mathbf{r}_1, ..., \mathbf{r}_N) = \prod_i \varphi_0(\mathbf{r}_i), \quad (2.13)$$

having the density $n(\mathbf{r}) = N|\varphi(\mathbf{r})|^2$, and a cloud size given by the harmonic oscillator length

$$a_{ho} = \left( \frac{\hbar}{m \omega_{ho}} \right)^{1/2}. \quad (2.14)$$
2.1.3 BEC of interacting atoms

When atom-atom interactions are included for \( N \) bosons in an external potential, here being the harmonic potential from equation 2.5, the Hamiltonian is in second quantization given by \[9\]:

\[
\hat{H} = \int \! d\mathbf{r} \, \hat{\Psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ho}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \int \! d\mathbf{r} d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') V_{\text{int}}(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}), \tag{2.15}
\]

where \( V_{\text{int}}(\mathbf{r} - \mathbf{r}') \) is the atom-atom effective interaction. For a cold and dilute gas, such as the ones used for creating a BEC, the interaction term is dominated by the s-wave scattering, \( a_s \), and can be written as

\[
V_{\text{int}}(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}') = \frac{4\pi\hbar^2 a_s}{m} \delta(\mathbf{r} - \mathbf{r}'), \tag{2.16}
\]

where \( g \) is called the coupling constant \[9\].

When the condensed fraction becomes large, the time dependent field operator is composed mainly by the ground state and can be written as

\[
\hat{\Psi}(\mathbf{r}, t) = \left\langle \sqrt{N_0} \Psi_0(\mathbf{r}) \right\rangle + \delta \hat{\Psi}(\mathbf{r}, t), \tag{2.17}
\]

where \( N_0 \) is the number of atoms in the ground state \( \Psi_0(\mathbf{r}, t) \), and \( \delta \hat{\Psi}(\mathbf{r}, t) \) is treated as a small perturbation. The first term on the right hand side of equation 2.17 is the expectation value of the field operator and is referred to as the condensate wave function. It is a classical field having the meaning of an order parameter in statistical physics. Generally this function is defined as

\[
\psi(\mathbf{r}, t) \equiv \left\langle \hat{\Psi}(\mathbf{r}, t) \right\rangle. \tag{2.18}
\]

This wave function is a complex wave with an inherent phase. This wave can be used as a source for many experiments such as wave interference.

Solving the time dependent Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r}, t) = \left[ \hat{\Psi}(\mathbf{r}, t), \hat{H} \right], \tag{2.19}
\]

can now be done using the condensate wave function of equation 2.18 and the s-wave scattering potential 2.16, yielding the Gross-Pitaevskii (GP) equation \[9\];

\[
i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{ho}(\mathbf{r}) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t), \tag{2.20}
\]

commonly used to solve theoretical problems for the BEC in the mean-field limit.

Neglecting the perturbative term in equation 2.17 is only strictly valid for absolute zero temperature, but is a good approximation for many problems at temperatures in the range of normal experiments.
Ground state properties for a BEC of interacting atoms

When calculating the ground state properties of the GP equation 2.20, the kinetic term $-\hbar^2 \nabla^2 / 2m$, can be neglected in the center of the cloud, where the non-linear interaction term is dominant. The kinetic term will only play an important role at a thin layer near the edge of the condensate. This approximation is referred to as the Thomas-Fermi approximation (TF) \cite{9}. In computing the density profile of the condensate wave function in this limit, the ansatz

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-i\mu t/\hbar}, \quad (2.21)$$

for the GP equation 2.20, gives the non-linear Schrödinger equation

$$\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{ho}(\mathbf{r}) + g|\psi(\mathbf{r})|^2 \right) \psi(\mathbf{r}) = \mu \psi(\mathbf{r}). \quad (2.22)$$

In the TF approximation, the density is therefore given by an inverted parabola

$$n_{\psi(\mathbf{r})} = \psi(\mathbf{r})^2 = \begin{cases} g^{-1} (\mu - V_{ho}(\mathbf{r})) , & \text{for } \mu > V_{ho}(\mathbf{r}), \\ 0 , & \text{outside}. \end{cases} \quad (2.23)$$

By normalizing the density with the number of atoms, the chemical potential is given by

$$\mu = \frac{\hbar \omega_{ho}}{2} \left( \frac{15Na_s}{a_{ho}} \right)^{2/5}, \quad (2.24)$$

from where one can obtain the radius of a condensate by taking

$$\mu = V_{ho}(R_{\psi(\mathbf{r})}) = m\omega_{ho}^2 R_{\psi(\mathbf{r})}^2/2. \quad (2.25)$$

The last step is an approximation for a spherical condensate with the radius $R_{\psi(\mathbf{r})}$ that can be expressed by

$$R = a_{ho} \left( \frac{15Na_s}{a_{ho}} \right)^{1/5}, \quad (2.26)$$

which is a macroscopic radius, typically of the order of 100 $\mu$m.

2.2 Theory of laser cooling

Laser cooling is used as a first step in experiments achieving BEC and the first successful experiments with laser cooled atoms were awarded the Nobel price in physics in 1997 \cite{11, 12, 13}. In this section a brief introduction is made to the field, while for a deeper understanding reference is made to \cite{14}.
2.2.1 Light Pressure on Atoms

A two-level atom absorbing a photon will get a momentum kick in the same direction as the photon was propagating. The atom will be excited, and will eventually spontaneously emit a photon in a random direction, giving the atom a recoil in the opposite direction of the photon emission. If the atom absorbs many photons from a light beam, always reemitting in random directions, the average effect will be one momentum kick per absorption and reemission cycle. The recoils from the emissions averages to zero as the number of events approaches infinity [14]. The average force on an atom affected by an absorption-spontaneous emission cycle can be written as

\[ \langle F_{sp} \rangle = \frac{\hbar k s_0 \gamma}{1 + s_0 + (2\Delta/\gamma)^2}, \]  

(2.27)

where \( \hbar k \) is the momentum carried by each photon, \( k \) is the angular wave vector of the light, \( \gamma \) is the linewidth of the transition, \( s_0 \equiv I/(\pihc\gamma/3\lambda^3) \) is the saturation parameter for the relevant radiative transition and for the irradiance \( I \). Here, \( c \) is the speed of light and \( \lambda \) is the atomic transition wavelength. The force also depends on the angular detuning \( \Delta = \omega_L - \omega_A \), where \( \omega_{L,A} \) are the angular frequencies of the laser and of the atomic transition respectively. If the laser frequency is off-resonant, or if the atom is moving with respect to the beam, equation 2.27 can be modified to take into account the Doppler shift. An atom moving slowly towards a red detuned laser beam will have its transition shifted closer to resonance by the Doppler effect, leading to the equation:

\[ \langle F \rangle = \langle F_0 \rangle - \zeta_d \frac{k}{|k|} v. \]  

(2.28)

The average force will thus have one part that is the same as for the atom at rest, and another where the force is proportional to the atomic velocity \( v = |v| \). Using red detuned beams, the velocity sensitive force will act as a damping on the system, where the damping coefficient can be written as:

\[ \zeta_d = -\hbar |k|^2 \frac{4s_0(\Delta/\gamma)}{(1 + s_0 + (2\Delta/\gamma)^2)^2}. \]  

(2.29)

An atom moving towards the beam will thus feel a retardation force.

2.2.2 Laser Cooling and Trapping

To cool atoms in three-dimensional space, a set of six laser beams, all red detuned from the atomic transition, is used. The beams are pairwise counter propagating, and each pair is orthogonal to the others, forming a velocity reduction in all directions for all velocities within the capture range of the cooling configuration [14]. The atoms tend to move around as in a high viscosity medium, an optical molasses [15].

The optical molasses will only cool atoms, but not trap them. To achieve trapping, the forces used need to be position dependent, pushing the atoms
towards a trap center. Such a position dependent force is produced in a magnetooptical trap (MOT) [14]. In a MOT, the transition used is typically of the type \( J_g \rightarrow J_e = J_g + 1 \), where \( J_g,e \) are the angular momenta of the ground and excited states respectively. The center of the MOT will be situated at the magnetic zero point of a linearly increasing magnetic field. In one dimension, this field can be expressed as \( B = B(z) = Az \), where \( z \) is the position and \( A \) is the field gradient.

All energy levels, except \( M_J = 0 \) will be Zeeman shifted, resulting in a position dependent potential energy.

Figure 2.1: A model of a one-dimensional MOT. For velocities towards, or positions to, the right (left), \( \sigma^- \) (\( \sigma^+ \)) light will be more resonant. Choosing this polarisation from right (left) will slow down the atoms and push them to the trap center. The MOT can be modelled as an over-damped spring with forces as in equation 2.32. The picture is taken from [16].

The MOT uses red detuned light, like optical molasses. Since the magnetic field induces a Zeeman shift, the atoms will be sensitive to the light polarization. Atoms at positive \( z \) will have the Zeeman levels \( M_J < 0 \) tuned closer to resonance and from this direction \( \sigma^- \) polarized light should be used to push the atoms back towards the center of the trap. At negative \( z \), positive \( M_J \) will be tuned closer to resonance and consequently \( \sigma^+ \) polarized light should be used. In figure 2.1, an example with \( J_g = 0 \) can be seen. Because of the position dependent force and the red detuning, the MOT efficiently traps and cools the atoms. It is not very sensitive to polarization purity, beam irradiance or magnetic field imperfections. The MOT is a good start for cooling the atoms to the microkelvin range, with relatively high densities. The density is however limited by radiation pressure from photons spontaneously emitted from atoms and then reabsorbed by others.

The forces acting on the atoms in the molasses, and in the MOT can, in the low irradiance limit, be derived from equation 2.27 by including both a velocity and position dependent detuning. The forces from the two beams in the one-dimensional case are given by \( \mathbf{F} = \mathbf{F}_+ + \mathbf{F}_- \), where

\[
\mathbf{F}_\pm = \pm \frac{\hbar k \gamma}{2} \frac{s_0}{1 + s_0 + (2\Delta_\pm / \gamma)^2},
\]  

(2.30)
and the effective angular detuning is given by:

$$\Delta_\pm = \Delta \mp k \cdot v \pm \mu' B(z)/\hbar. \quad (2.31)$$

Here $$\mu' = (g_e M_{J_e} - g_g M_{J_g}) \mu_B$$ is the effective magnetic moment for the transition used, $$g_e, g_g$$ is the excited and ground state fine structure Landé g-factors, $$M_{J_e, g}$$ are the $$M_J$$ magnetic quantum numbers for the involved states, and $$\mu_B$$ is the Bohr magneton. In figure 2.2, equation 2.30 is visualized for different velocities in the center of the trap in (a), and for different positions, with zero velocity in (b).

![Figure 2.2: A visualization of the forces in equation 2.30 acting on an atom. In (a) the atomic velocity is varied for an atom positioned in the center of the trap. In (b) the velocity is zero, but the atomic position is varied. Equation 2.30 is evaluated for $^{87}\text{Rb}$, the magnetic gradient $5 \cdot 10^{-4} \text{T/m}$, and $$s_0 = 2$$. The detuning from the cooling transition (see section 4.5.1) is $$\gamma$$ for the blue solid lines and $$3\gamma$$ for the red dashed line.](image)

For small detunings and velocities equation 2.27 can be approximated with

$$F = -\zeta_d v - \kappa r, \quad (2.32)$$

with $$\zeta_d$$ as in equation 2.29, $$r$$ being the position and

$$\kappa = \frac{\mu' A}{\hbar k} \zeta_d. \quad (2.33)$$

In this limit a MOT can be seen as an overdamped harmonic oscillator [14].
2.3 Magnetic Trapping

The working principle of the MOT includes spontaneous emission of photons, and is limited in temperature by the velocity spread created by the random direction of the photon recoils. To reach lower temperatures, pure magnetic traps can be used. These traps are very shallow and therefore only atoms with very low energy can be confined. The potential energy in a magnetic trap depends on the Zeeman energy,

$$V_B(r) = -\mu_m B(r),$$  \hspace{1cm} (2.34)

where $C_B$ is a constant, $\mu_m$ is the state dependent magnetic moment \cite{17} and $B(r)$ is the magnetic field strength at the position $r$. Atomic states with positive magnetic moment have potential minima at magnetic maxima and are called high-field seekers. The states with negative magnetic moment are driven towards lower magnetic field and are called low-field seekers. A magnetic maximum in three dimensions cannot be created in a region where there are no electric currents and therefore only atomic states with $\mu_m B < 0$ can be trapped in 3D \cite{10}. There are several types of traps used in different experiments; some of these are presented here.

2.3.1 The Quadrupole Trap

A quadrupole trap has a linearly increasing magnetic field in all directions, with a zero point in the center. The trap can be created with two magnetic coils in an anti-Helmholtz configuration \cite{18}. In the case of axial symmetry around the $z$ axis, and a magnetic field gradient of $A$, the field is given by

$$B = A(x + y - 2z),$$ \hspace{1cm} (2.35)

with a magnitude of $B = A(x^2 + y^2 + 4z^2)^{1/2}$ at the position $(x, y, z)$. A trap needs to follow certain constrains in order to be able to trap atoms. The atoms must be able to follow the magnetic field adiabatically not to change its energy state while moving around in the trap \cite{10}. This condition is fulfilled if

$$\omega_{La} \gg \frac{|dB/dt|}{B},$$ \hspace{1cm} (2.36)

where $\omega_{La} = \mu_B B/\hbar$ is the Larmor precession frequency. This condition is not fullfilled close to the center of the trap, where the field is zero, and effectively the trap has a hole at this point. This hole can cause the atoms to change to another Zeeman level through a Majorana spin flip and therefore go from a low-field to a high-field seeking state and consequently be ejected from the trap \cite{10, 14}. This hole makes this trap a bad choice for cooling atoms down to low energies.

Several techniques have been used to tap this hole. One is to tightly focus a blue detuned, *i.e.*, repelling, laser beam on the bottom of the hole \cite{19}. Another way to cope with the problem is to add an oscillating magnetic field, the Time-averaged Orbiting Potential (TOP) Trap \cite{20}. The oscillating field move the zero point magnetic field around in space, preventing the atoms to reach it.
2.3.2 The Ioffe-Pritchard trap

The most commonly used magnetic trap, avoiding the Majorana flips in the region of a potential minimum, is the Ioffe-Pritchard trap (IP trap) [21, 22]. The magnetic field component in an IP trap will never reach zero, which is accomplished by using a quadratic trap, with an offset, $B_0$, in the center. The magnetic field of such a trap is given by:

$$
B = B_0 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + B' \begin{pmatrix} x \\ -y \\ 0 \end{pmatrix} + B'' \begin{pmatrix} -xz \\ -yz \\ z^2 - \frac{1}{2}(x^2 + y^2) \end{pmatrix}.
$$

(2.37)

The potential created by an IP trap has two important regimes. For temperatures $k_B T > \mu m B_0$, the trap is essentially linear in the radial direction, and harmonic in the axial direction;

$$
V_{B\perp} = \mu m B' r_\perp, \\
V_{Bz} = \frac{\mu m B''}{2} z^2.
$$

(2.38)

When the temperature is lowered, the atoms will sense the effective potential in the center of the trap, which is a cylindrically symmetric harmonic trap;

$$
V_B(r_\perp, z) = \frac{\mu m}{2} \left( B_0 + B'' r_\perp^2 + B'' z^2 \right),
$$

(2.39)

where the effective radial curvatures depend on the parameters of equation 2.37,

$$
B''_\perp = \frac{B'^2}{B_0} \approx \frac{B'^2}{B_0},
$$

(2.40)

with the approximation being valid for small bias fields $B_0$.

The trapping strength can be related to the harmonic potential trapping angular frequencies in equation 2.6 by:

$$
\omega_x = \omega_y = \sqrt{\frac{\mu m B''}{m B_0}}, \\
\omega_z = \sqrt{\frac{\mu m B''}{m}},
$$

(2.41)

which are experimentally tunable, as will be further explained in chapter 4. The variety of magnetic traps sorted under the name of IP traps is substantial, which opens the possibility for experiments requiring different kinds of optical access [21].

Magnetic traps provide flexible ways of trapping neutral atoms, but there is no inherent cooling process in the trap. Adding cooling into the magnetic trap is most commonly made by evaporation [23].
2.4 Evaporative cooling

Since it is not possible to reach the desired phase space density

\[ \rho_{ph} \geq 2.612, \]  

(2.42)

with a MOT, and with the absence of inherent cooling mechanisms in a pure magnetic trap, evaporative cooling is often used to further cool and compress the atomic cloud. Evaporative cooling is, in a simple picture, the same thing as happens in nature when water evaporates from the ocean, or when hot steam is blown away from a coffee cup, leaving the liquid colder. In evaporative cooling, the trap walls are lowered, letting the hottest atoms escape the trap and thereby lowering the average energy.

To efficiently lower the temperature, and increasing the phase space density, care has to be taken in how the magnetic trap is designed, how fast the potential walls are lowered, and how high the collision rate is with background gases. Background gas collisions cause losses because of heating of the trapped sample due to the large difference in energy of trapped and untrapped atoms.

Evaporative cooling will be a competition between two effects; the rethermalization of the gas, caused by elastic collisions between the trapped atoms, and the rate of cropping the high velocity tail of hot atoms in the Maxwell-Boltzmann distribution at lower and lower energy.

The evaporation is realized by coupling trapped and untrapped energy levels with a radio frequency wave (RF wave). In the dressed state picture, the effective trap will in two dimensions have the shape of an egg cup (see figure 2.3) [14]. The dressed state picture is a description of the system where the atomic states and the radiation field are combined. The energy offset is here set so that the trapped state is left unchanged. The energy of the untrapped state will have the potential energy of an untrapped atom plus the energy of one emitted radio frequency photon. This photon is created in the stimulated emission when the atom reaches the point \( x_{crit} \) in figure 2.3. Since the photon energy is included, there will be no discontinuity at the critical point.

2.4.1 Theoretical model for evaporative cooling

Several models exist for evaporative cooling, and some of them are presented in [10, 14, 24, 25]. Evaporative cooling is in practice often performed by continuously tuning a radio frequency in the MHz range, in order to force the warmest atoms to leave, while the remaining atoms simultaneously collide to re-equilibrate a thermal distribution. The theoretical models however, divide the problem into discrete steps, where the RF is initially on, removing the hot atoms, followed by a re-equilibrating phase, where the potential barriers are infinitely deep. When equilibrium is reached, another RF step is performed, again followed by an equilibration, etc.

As the shape of the magnetic trap potential will vary with temperature, as seen in equation 2.38 and 2.39, a model for evaporative cooling needs to be generalized for different potentials. For a three-dimensional potential, the influence
Figure 2.3: During evaporative cooling a trapped and an untrapped energy level are connected. In (a) the different energy levels for the trapped and the untrapped state, and the frequency coupling them are shown. The trapped level is the upper parabola, with a potential minimum and the untrapped level is the lower parabola with a potential maximum. The two arrows mark the transitions from the trapped to the untrapped system. Particles reaching the points ±x_{crit} will be transferred to the untrapped system and lost from the system. In (b) the dressed state picture, including the radiation energy E_{ph} in the Hamiltonian, shows the egg cup shaped effective potential, where the energy consists of a the potential energy of a trapped atom for |x| < x_{crit}, and the same energy for an untrapped atom plus the photon energy from stimulated emission for |x| > x_{crit}. The dressed state picture gives the effective potential seen by the atoms.

of the potential can be characterized by the parameter [14]

$$\xi_{ev} = \frac{1}{s_x} + \frac{1}{s_y} + \frac{1}{s_z},$$  \hspace{1cm} (2.43)

where s_x, s_y and s_z are the power exponents in a power law potential. (s_x = s_y = s_z = 2 in a purely harmonic trap, and s_x = s_y = s_\| = 1 and s_z = 2 in the combined linear and harmonic trap for a warm cloud trapped in an IP trap.)

The reduction of temperature per lost atom gives a measure of the efficiency of evaporative cooling. Therefore two parameters are defined;

$$\nu_{ev} \equiv \frac{N'}{N},$$  \hspace{1cm} (2.44)
as the fractional number of atoms remaining in the trap after an evaporation step and
\[
\gamma_{ev} \equiv \frac{\ln(T'/T)}{\ln(N'/N)},
\]
being the change in temperature scaled by the loss in atom number. From \(\xi_{ev}\), \(\nu_{ev}\) and \(\gamma_{ev}\) the change of other properties of the trapped cloud, due to evaporation, can be computed. The atom number and the temperature scaling can be rewritten as \(N' = N\nu_{ev}\) and \(T' = T\nu_{ev}^{\gamma_{ev}}\). From [26], it is known that the volume that a sample occupies in a power law potential scales as \(\tilde{V} \propto T^{\xi_{ev}}\), and thus \(\tilde{V}' = \tilde{V}\nu_{ev}^{\gamma_{ev}\xi_{ev}}\).

The aim of evaporative cooling is to increase the phase space density in equation 2.1. After one step of evaporation, using the above relations, \(\rho_{ph}\) will scale as
\[
\rho'_{ph} = \rho_{ph}\nu_{ev}^{1-\gamma_{ev}(\xi_{ev}+3/2)}.
\]
From the definition 2.44, it can be seen that \(0 \leq \nu_{ev} \leq 1\), and thus to achieve an increase in phase space density due to evaporative cooling, the exponent needs to be negative, which lead to
\[
\xi_{ev} > \frac{1}{\gamma_{ev}} - \frac{3}{2}.
\]
To prevent the evaporative cooling from slowing down, the elastic collision rate should also increase for each step. Since the velocity of the atoms scale as \(v_{rel} \propto \sqrt{T}\), and the cross section for the relevant collisions is constant, the collision rate will scale as
\[
P'_{coll} = P_{coll}\nu^{1-\gamma_{ev}(\xi_{ev}-1/2)},
\]
leading to a much more strict constraint on the trap
\[
\xi_{ev} > \frac{1}{\gamma_{ev}} + \frac{1}{2}.
\]
In the magnetic trap, the relation 2.49 is best fulfilled in the beginning, where the linear terms dominate the potential, leading to \(\xi_{ev} = 3\). If the collision rate is sufficiently high at the start of the evaporation process, and \(\gamma_{ev}\) is correctly tuned, evaporation can be successful.

A numerical calculation of the dependence between \(\gamma_{ev}\) and the chosen RF cut has been performed in [25]. To achieve a complete picture, the collisions with the background gas should also be included. In reference [10], the background collisions are included in the model by swapping
\[
\gamma_{ev} \rightarrow \frac{\tau_{trap}}{\tau_{trap} + \tau_{ev}}\gamma_{ev},
\]
where \(\tau_{trap}\) is the trap lifetime and \(\tau_{ev}\) is the evaporation speed. For a trap with a lifetime in the range of the evaporation speed, the removal of atoms by background collisions, will reduce the efficiency of the process, as they do not
alter the temperature of the sample. If the lifetime is infinite, this re-scaling will be one, and all atoms removed will have an energy above the average of the sample. The evaporation speed can be optimized, by relating it to the collision rate in the trap. For practical purposes, the evaporation process should be as slow as the trap lifetime permits, leading to a maximal decrease in energy for each removed atom.
Chapter 3

Optical Lattices

The concept of optical lattices plays a central role in all the work included in this thesis. As the research field of cold atoms has grown bigger with the years, optical lattices have proven to be a useful tool for both laboratory work and theoretical simulations. In all the papers included in this thesis, optical lattices have been used either in simulations or as a test-bench for a physical system in the laboratory.

In this chapter, a general introduction to the optical lattice models for this thesis is made. For a more extensive reading, reference is made to review papers in the field, i.e. [6, 7, 27, 28, 29].

3.1 Light induced potentials

Optical lattices are periodic potentials created by the interference between two or more laser beams. The light interacts with the atoms through dissipative and conservative forces. In the conservative case, the photon absorption probability is low, and the atoms mainly experience the dipole potential created by the irradiance pattern $I(r)$ from the laser beams. In the semiclassical approach, the local potential depth is given by [30]:

$$V_{\text{dip}}(r) = -\frac{1}{2} \langle \mathbf{p}_{\text{dip}} \cdot \mathbf{E} \rangle = -\frac{1}{2\varepsilon_0 c} \text{Re}(\alpha) I(r),$$

(3.1)

where $\mathbf{p}_{\text{dip}} = \alpha \mathbf{E}$ is the induced dipole moment, $\mathbf{E}$ the electric field vector, $\varepsilon$ the vacuum permittivity, $c$ the speed of light, and $\alpha$ is the complex polarizability of the atom with the real part given by

$$\text{Re}(\alpha) = 6\pi\varepsilon_0 c^3 \frac{\gamma}{\omega_A^2 - \omega_L^2} \frac{\omega_L^2 - \omega_A^2}{\omega_A^2 (\omega_A^2 - \omega_L^2)^2 + (\frac{\omega_L^2}{\omega_A^2} \gamma)^2}.$$  

(3.2)

Here $\omega_{A,L}$ are the angular frequencies of the atomic resonance and of the laser light.
If there are several fine structure resonances with transitions in the vicinity of the laser frequency, the light induced potential will have contributions from all these atomic resonances. At large detunings, $\Delta/\Delta_{FS} \gg 1$, where $\Delta_{FS}$ is the fine structure splitting, equation 3.1 can be approximated by [30]:

$$V_{\text{dip}}(r) = \frac{3\pi c^2 \gamma}{2\omega_\lambda^3 \Delta} \left( 1 + \frac{1}{3} P(r) g_F M_F \frac{\Delta_{FS}}{\Delta} \right) I(r),$$  \tag{3.3}$$

where $\Delta$ in the approximation, is the average angular detuning of the laser from the fine structure resonances. $P(r)$ is a function of the local polarization, being 0 for linear polarized light and $\pm 1$ for circular, $\sigma^\pm$ light [30]. $g_F$ is the hyperfine Landé g-factor, and $M_F$ is the projection of the total atomic angular momentum [8].

The combined irradiance from $N$ interfering laser beams, with polarizations along the $e_i$ axes, is given by

$$I(r) = 2\varepsilon_0 c \langle |E(r)|^2 \rangle =$$

$$= 2\varepsilon_0 c \sum_i N E_i^2 +$$

$$+ 2\varepsilon_0 c \sum_{i\neq j} E_i E_j (e_i \cdot e_j^*) \exp\{i [(k_i - k_j) \cdot r + \phi_i - \phi_j] \},$$

where the first term only off-sets the over-all potential, and the second term gives an interference pattern depending on the difference between the angular wave vectors $k_i$, and between the phases $\phi_i$. Changing the phases will only translate the interference pattern in space, as long as none of the differences between the wave vectors can be described as a superposition of the other differences. The interference pattern has a structure in space, having many properties in common with crystals in solid state physics, and is therefore referred to as an optical lattice. The periodicity of the optical lattice is set by the angular wave vectors, and the scalar product of the polarizations, $e_i \cdot e_j^*$ change the local properties (basis of primitive cell) of the lattice [28].

### 3.1.1 Real and reciprocal lattice vectors

The description of a lattice, as normally applied in solid state physics, is done both in real space and reciprocal space [31, 32], where the reciprocal lattice is a Fourier transform into momentum space, of the real lattice. For most applications the reciprocal space is convenient, but for visualizing the structure of the lattice, real space images are used. The connection between real and reciprocal lattice vectors is made by the relations

$$b_i \cdot a_j = 2\pi \delta_{ij},$$  \tag{3.5}$$

where $a_j$ is any of the real lattice vectors, and $b_i$ is any of the reciprocal lattice vectors. For three-dimensional lattices, going from real to reciprocal lattice
vectors can be done by the relation

\[ b_i = 2\pi \frac{a_j \times a_k}{a_i \cdot (a_j \times a_k)}, \quad (3.6) \]

with \( i, j, k \) cyclic. The same relation will also work in transforming reciprocal lattices into real.

A periodic structure, formed, e.g., by an optical lattice, is invariant under the space translation \( \mathbf{R} = \nu_i a_i \), where \( \nu_i \) are integer numbers. For a two-dimensional case, constructed by three laser beams with angular wave vectors \( k_1, k_2 \) and \( k_3 \), the real lattice vectors \( a_1 \) and \( a_2 \) are given by the relations

\[
(k_1 - k_2) \cdot a_1 = 2\pi, \quad (k_1 - k_3) \cdot a_1 = 0, \\
(k_1 - k_2) \cdot a_2 = 0, \quad (k_1 - k_3) \cdot a_2 = 2\pi.
\]

(3.7)

The equations 3.5 and 3.7 states that the reciprocal lattice vectors are given by \( b_1 = (k_1 - k_2) \) and \( b_2 = (k_1 - k_3) \) [28]. The same type of relations can be found for lattices of higher dimensions. Further extrapolating the relation above, a reciprocal lattice from a set of \( N \) laser beams is therefore given by the \( N - 1 \) different \( \Delta k_{ij} = k_i - k_j \). With \( N \) laser beams, with linear independent \( \Delta k_{ij} \), one can therefore construct an \( N - 1 \) dimensional optical lattice. When an optical lattice is constructed from a set of laser beams, only those having wave vectors that cannot be constructed from any other combination of wave vectors of the constituent laser beams, will contribute to the dimensionality. Introducing more than three beams in a plane will give an optical lattices that has an over-determined basis. As a consequence, it will be phase sensitive and/or contain more than one spatial frequency component in the topography. The same thing can happen in one dimension and three dimensions, when introducing extra beams.

In the following, the theory for some special cases, such as running wave optical lattices, 3D cubic optical lattices and double well potentials will be discussed more in detail. The theoretical studies can also be divided into distinct regimes by the potential barriers between the lattice wells. The atoms are, for low potential barriers in relation to the excitation energy of the atom, delocalized over several wells, whereas for high potential barriers, the atoms can be localized and inter-well movements are described by tunneling properties through the potential barriers.

### 3.2 Theoretical treatment of cold atoms in periodic potentials

The general Schrödinger equation for particles in a potential \( V(\mathbf{r}) \) can be written as

\[
\hat{H} \Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \Psi = E_{\text{eig}} \Psi, \quad (3.8)
\]
where $\hat{\mathcal{H}}$ is the Hamiltonian, and $\Psi$ is the particle wave function corresponding to the eigenenergy $E_{\text{eig}}$. This equation is valid for both periodic and non-periodic potentials. In this chapter equation 3.8 will be studied more in detail for the periodic case, where many simplifications can be done. The terminology and ideas for this model come from standard solid state physics texts [31, 32].

3.2.1 Bloch’s theorem and periodic potentials

Periodic potentials obey $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$, and according to Bloch’s theorem, the eigenfunctions of the Schrödinger equation for periodic potentials in a Bravais lattice can be written as [31]

$$\Psi_{nq}(\mathbf{r}) = e^{i\mathbf{q} \cdot \mathbf{r}/\hbar} u_{nq}(\mathbf{r}),$$  \hspace{1cm} (3.9)

where $e^{i\mathbf{q} \cdot \mathbf{r}/\hbar}$ is a plane wave, $\mathbf{q}$ is a vector, often related to as the quasimomentum, and $u_{nq}(\mathbf{r})$ is a periodic function with the same periodicity as the potential $V(\mathbf{r})$. The eigenfunctions $\Psi_{nq}(\mathbf{r})$ are often referred to as Bloch functions.

Inserting the ansatz of equation 3.9 into the Hamiltonian 3.8 gives

$$e^{i\mathbf{q} \cdot \mathbf{r}/\hbar} \left( \frac{1}{2m} (-i\hbar \nabla + \mathbf{q})^2 + V(\mathbf{r}) \right) u_{nq} = E_{\text{eig}} e^{i\mathbf{q} \cdot \mathbf{r}/\hbar} u_{nq}. \hspace{1cm} (3.10)$$

The equation above is a rewritten version of the original Schrödinger equation. In the rewritten form, a set of equations for $u_{nq}$ is obtained by dropping the running wave factor $e^{i\mathbf{q} \cdot \mathbf{r}/\hbar}$;

$$\left( \frac{1}{2m} (-i\hbar \nabla + \mathbf{q})^2 + V(\mathbf{r}) \right) u_{nq} = E_{\text{eig}} u_{nq}, \hspace{1cm} (3.11)$$

and the analysis is thus simplified from the full three-dimensional Hamiltonian to a set of eigenvalue problems for the periodic functions $u_{nq}$.

The solutions to equation 3.11 can in cases where it is possible to write the potential as $V(x, y, z) = V(x) + V(y) + V(z)$, be achieved by splitting the problem into three one-dimensional problems. In these cases, the potential $V(z)$ and the periodic part of the wavefunction $u_{nq}(z)$ are expanded in the same basis;

$$V(z) = \sum_b V_b e^{i2bkz} \hspace{1cm} (3.12)$$

and

$$u_{nq}(z) = \sum_d c_d^{nq} e^{i2dkz}, \hspace{1cm} (3.13)$$

where the discrete Fourier sums run over all frequencies $2bk$ and $2dk$. The quasimomentum $\mathbf{q} = q_z$ is in the one-dimensional case the corresponding element of the vector $\mathbf{q} = (q_x, q_y, q_z)$, where the index is dropped.

Inserting the expansions 3.12 and 3.13 into the Schrödinger equation 3.11 leads to the set of equations:
\[
\sum_d \frac{(2hd + q)^2}{2m} c_d^{nq} e^{i2dkz} + \sum_d \sum_b V_b e^{i2(b+d)kz} c_d^{nq} = E_{\text{eig}}(n, q) \sum_d c_d^{nq} e^{i2dkz}.
\]

(3.14)

In a typical one-dimensional experiment, the periodic potential from an optical lattice is given by

\[
V(z) = -V_{1D} \cos^2(kz) = -\frac{1}{4} V_{1D} \left( e^{i2kz} + e^{-i2kz} + 2 \right),
\]

(3.15)

which leaves three terms in equation 3.12; \( V_{-1} = V_1 = -\frac{1}{4} V_{1D} \) and \( V_0 = -\frac{1}{2} V_{1D} \). The last term, \( V_0 \) only shifts the potential in height, and does not affect the overall result, and can therefore be left out.

### 3.2.2 Band structure

Solutions to equation 3.14 can be found by solving the eigenvalue problem for \( c_d^{nq} \) in matrix form, where the elements \( [(2hd + q)^2]/2m \) are the diagonal elements of a \((2l + 1)\)-dimensional matrix, and \( V_{-1} \) and \( V_1 \) are the off-diagonal elements, leading to the deformation of a free particle potential. The size of the matrix, and therefore the precision of the calculation, is set by choosing \( l \) such that the off-diagonal elements can be treated as perturbations. The \( n \) lowest eigenvalues of this problem give the \( n \) lowest band energies for the quasimomenta \( q \) used in the calculation. The corresponding \( n \) eigenfunctions give the periodic functions for the Bloch functions in equation 3.13 and 3.9.

Reducing the optical lattice potential, one will eventually reach a case were the physical system is that of a free particle, \( i.e., V_{1D} = 0 \). The corresponding eigenvalues, are represented by a parabola \( E_{\text{eig}} \propto q^2 \), where the quasimomentum \( q \) is equal to the real momentum in this case. As the potential \( V_{1D} \) is increased, the energy eigenvalues will split into regions, separated by forbidden band gaps. In figure 3.1 the two situations, \( V_{1D} = 0 \) and \( V_{1D} = 3E_{\text{rec}} \), are illustrated, where \( E_{\text{rec}} \) is the recoil energy of the atom from photon absorption or emission. Because of the periodicity of the running wave factor \( e^{iq \cdot r/h} \), the energy levels can be represented either in an extended zone scheme, where the momentum can take any number, or in the repeated zone scheme where states with momentum higher than \( \hbar k \) are shifted into the first Brillouin zone\(^1\), represented in higher energy band. This is illustrated by the thick solid line in figure 3.1. In the presence of an optical lattice, the momentum and quasimomentum will therefore no longer be the same. The free particle parabola \( (V_{1D} = 0) \) is represented with a dashed blue line in the figure. For large momentum, and far from the Brillouin zone edges, the energy levels of the cases with and without lattice come closer together. If the lattice is tuned higher, the bandgaps at the Brillouin zone edges will increase, and the bands will be increasingly flat.

From solid state physics, it is also known that the group velocity of a wave packet in a periodic potential can be written as \([31, 32]\)

\(^1\)The first Brillouin zone is limited to \(|q| < \hbar k\), the second to \( \hbar k < |q| < 2\hbar k \), etc.
Figure 3.1: Band structure energies for a free atom (blue dashed line) and an atom in a one-dimensional optical lattice with $V_{1D} = 3E_{\text{rec}}$ (red solid lines). For the latter case, the energy levels can be displayed in the repeated zone scheme (thick red lines), where all energy bands are plotted in the first Brillouin zone where $|q| < \hbar k$.

$$v_B(n, q) = \frac{\partial E_{\text{eig}}(n, q)}{\partial q}, \quad (3.16)$$

where the subscript B refers to the Bloch velocity. By adding a small force to the system, small enough not to perturb the band structure, one could accelerate the particle in the potential, changing its quasimomentum, without interband excitations;

$$\frac{\partial q}{\partial t} = F_{\text{ext}}, \quad (3.17)$$

where $F_{\text{ext}}$ is a small external force. This relation would be equal to Newton’s second law by changing $F_{\text{ext}}$ to the total force and the quasimomentum into real momentum. However, in the band structure picture, all forces from the lattice are already included in the model.

By combining equation 3.16 and 3.17 one gets the acceleration $a_B$ of a wave packet in a periodic potential, caused by an external force;

$$a_B = \frac{\partial v_B(n, q)}{\partial t} = \frac{\partial^2 E_{\text{eig}}(n, q)}{\partial q^2} \frac{\partial q}{\partial t} = \frac{F_{\text{ext}}}{m^*(n, q)}, \quad (3.18)$$
where $m^*(n, q)$ is called the effective mass, depends on the curvature of the energy band:

$$m^*(n, q) = \left[ \frac{\partial^2 E_{\text{eig}}(n, q)}{\partial q^2} \right]^{-1}.$$  

(3.19)

Looking again at figure 3.1, there are distinct regions where the energy bands have maxima (negative curvature) and minima (positive curvature). This will affect the response to an external force in a non-intuitive way, where a negative effective mass will cause a wave packet movement opposing an external force.

### 3.3 BEC in one-dimensional optical lattices

The combination of an optical lattice and a BEC has been investigated in several experiments. The solution to the GP equation 2.20, takes the form of a gigantic matter wave of the form given in equation 2.21. The matter wave will typically spread out over several hundreds of lattice sites for a shallow lattice, and it has a momentum spread that is much smaller than the width of the first Brillouin zone. These properties make it possible to load a well-defined energy state in the band structure of an optical lattice. Since the BEC is also a macroscopic population of a single quantum state, it can be used as a probe for the quantum mechanical interactions between the lattice and a particle, with a signal to noise ratio much larger than for experiments using single-particle probes.

There are several ways to address different quasimomentum states of an energy band. The most straightforward method is to use a system where the BEC is moving in the optical lattice reference frame. The BEC can be loaded into an energy state $E_{\text{eig}}(n, q)$, where $n$ and $q$ are selected by the initial relative velocities of the BEC and lattice.

#### 3.3.1 Non-interacting BEC and band structure

The non-linear interaction term, $g|\psi(r, t)|^2$, in equation 2.20 enriches the physics of a BEC in optical lattices. However, if desired it is possible to avoid this effect in several ways. If a BEC is expanded, by removing the confining potential before the lattice is ramped up, the density will be much lower, and the interaction energy is converted to kinetic energy during the expansion. The coherence properties of such a cloud are preserved, and it can be used as a probe for band structure experiments. In reference [33], an expanding BEC was loaded into different quasimomentum states of a moving optical lattice, investigating the band structure and effective mass properties.

#### 3.3.2 Instabilities due to interactions

If the density of the BEC is high enough to make the non-linear term of the GP equation important, the simple picture from the Bloch theory has to be extended. Two types of non-linear effects are investigated in this thesis, both related to the instabilities of the BEC, which cause it to break down by heating followed by
the loss of condensed atoms. The first effect is energetic instability, caused by
the existence of an energy saddle point in configuration space, while the second
effect, dynamical instability is due to the exponential growth of other states by
perturbation of the BEC wave function. The two effects have been studied using
several different theoretical models, where references [34, 35, 36] are strongly re-
lated to the theory and experiments included in this thesis. Energetic instability
is also called Landau instability in the literature, whereas dynamical instability
is synonymous to modulational instability. An experimental investigation of this
is included in chapter 5 and in papers I, II and III.

**Energetic instability**

Looking back at equation 2.22, for a more general case, the harmonic oscillator
potential can be changed to a more general form \( V_{\text{tot}}(r) = V_{\text{ho}} + V(z) \), including
possible confinement and a one-dimensional optical lattice potential along \( z \).
Restricting the model to one dimension also for the confinement, the equation
can be rewritten as:

\[
\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{tot}}(z) + g|\psi(z)|^2 \right) \psi(z) = \mu \psi(z).
\]

(3.20)

In such a system, a state is energetically stable if the energy,

\[
E_{\psi_0(z)} = \int d^3 z \left\{ \psi_0^*(z) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{tot}}(z) - \mu \right) \psi_0(z) + \frac{g}{2} |\psi_0(z)|^4 \right\},
\]

(3.21)

has a local minimum for the state \( \psi_0(z) \). If the energy can be lowered by small
changes \( \delta \psi(z) \) to the wave function, \( i.e.\), having a saddle point for the energy in
\( \psi(z) \) space, the system has an energetic instability.

The onset of energetic instability can thus be calculated by expanding equation 3.21 to quadratic terms, for a perturbed state of the ground state;

\[
\psi(z) = \psi_0(z) + \delta \psi(z),
\]

(3.22)

leading to an energy of the perturbed state being

\[
E_{\psi(z)} = E_{\psi_0(z)} + \delta E_{\delta \psi(z)}.
\]

(3.23)

The energy change, \( \delta E_{\delta \psi(z)} \), due to the perturbation, \( \delta \psi(z) \), expanded to quadratic
form reads;

\[
\delta E_{\delta \psi(z)} = \int d^3 z \left\{ \delta \psi^*(z) \hat{H}_M \delta \psi(z) + \frac{g}{2} \left( \psi_0^*(z)^2 \delta \psi(z)^2 + \psi_0(z)^2 \delta \psi^*(z)^2 + 4 |\psi_0(z)|^2 \delta \psi(z) \delta \psi^*(z) \right) \right\},
\]

(3.24)
with $\hat{H}_M = \frac{\hbar^2 \nabla^2}{2m} + V_{\text{tot}}(z) - \mu$. Evaluating equation 3.24 can be facilitated by the use of matrices [34];

$$
\delta E_{\delta \psi(z)} = \frac{1}{2} \int d^3 z \left\{ \left[ \delta \psi^*(z) \delta \psi(z) \right] \hat{M}_{\text{inst}} \left[ \begin{array}{c} \delta \psi(z) \\ \delta \psi^*(z) \end{array} \right] \right\},
$$

(3.25)

where

$$
\hat{M}_{\text{inst}} = \left[ \begin{array}{cc} \hat{H}_M + 2g|\psi_0(z)|^2 & g\psi_0(z)^2 \\ g\psi_0^*(z)^2 & \hat{H}_M + 2g|\psi_0(z)|^2 \end{array} \right].
$$

(3.26)

Determination of the behavior of the system, when a small perturbation $\delta \psi(z)$ is introduced, has thus been reduced to finding the eigenvalues of $\hat{M}_{\text{inst}}$. If all eigenvalues are positive, the system will gain energy by a perturbation $\delta \psi(z)$. If there are negative eigenvalues, $\delta E_{\delta \psi(z)}$ will lower the energy of the system, and $\psi_0(z)$ is thus an energetically unstable state.

**Dynamical instability**

The onset of dynamical instability is governed by the exponential growth in amplitude of the perturbations $\delta \psi(z, t)$. Inserting the perturbed wavefunction, $\psi(z, t)$, from 3.22 into the time dependent GP equation 2.20, yields equations for the time dependence of $\delta \psi(z, t)$ and its complex conjugate. By linearizing the two equations, they can be written on matrix form [34]:

$$
i\hbar \frac{\partial}{\partial t} \left[ \begin{array}{c} \delta \psi(z, t) \\ \delta \psi^*(z, t) \end{array} \right] = \hat{\sigma}_z \hat{M}_{\text{inst}} \left[ \begin{array}{c} \delta \psi(z, t) \\ \delta \psi^*(z, t) \end{array} \right],
$$

(3.27)

where

$$
\hat{\sigma}_z = \left[ \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right].
$$

(3.28)

Since the combined operator $\hat{\sigma}_z \hat{M}_{\text{inst}}$ can have complex eigenvalues, the time evolution of $\psi(z, t)$ can become unstable. Looking at a hypothetical state $\delta \psi(z, t)_{\text{inst}}$, with the eigenvalue of $\hat{\sigma}_z \hat{M}_{\text{inst}}$ being $E_{\text{inst}} = E_{\text{Re}} + iE_{\text{Im}}$, the time evolution will be governed by

$$
i\hbar \frac{\partial}{\partial t} \delta \psi(z, t)_{\text{inst}} = (E_{\text{Re}} + iE_{\text{Im}}) \delta \psi(z, t)_{\text{inst}},
$$

(3.29)

having the solution

$$
\delta \psi(z, t)_{\text{inst}} = \delta \psi(z, 0)_{\text{inst}} \exp \left( \frac{E_{\text{Im}} t - iE_{\text{Re}} t}{\hbar} \right),
$$

(3.30)

which for positive $E_{\text{Im}}$, grows exponentially in time. The BEC will break up in many different wave functions, which at the end leads to its depletion. This exponential growth of other momentum modes is called dynamical instability.

From theoretical studies [36], the parameter regions for dynamical and energetic instabilities has been found. It has been shown that the dynamical instability is a subregion of the energetic instability in parameter space. As a
consequence, whenever the BEC experience dynamical instability, it will also experience energetic instability, and there are parts of the energetic instability region where there is no dynamical instability.

3.4 BEC in a Three-Dimensional Cubic Optical lattice

The optical lattice potential, in a three-dimensional simple cubic case, can be written as

\[ V(r) = V(x, y, z) = V(x) + V(y) + V(z), \]  

which can be treated as three separate one-dimensional problems. The one-dimensional eigenfunctions combined give the three-dimensional solution to equation 3.9;

\[ \Psi_{nq}(r) = \exp \left( \frac{i}{\hbar} \mathbf{q} \cdot \mathbf{r} \right) u_{nq}(r) = \exp \left( \frac{i}{\hbar} \left[ q_x x + q_y y + q_z z \right] \right) u_{n_x q_x}(x) u_{n_y q_y}(y) u_{n_z q_z}(z), \]  

where the subscripts \( x, y \) and \( z \) refer to the three separate, one-dimensional solutions. The band index for the three-dimensional case, \( n \), is actually a set of the three band indices \( n_x, n_y \) and \( n_z \), but it is traditionally written in the short form of as a scalar \( n \).

3.4.1 Weak lattice regime

If the optical lattice potential is weak, and the BEC wave packets are delocalized over several potential wells, the band structure picture of figure 3.1 is a useful model. If the BEC is moving in the lattice reference frame, its velocity is projected into three different quasimomenta and energy bands. As long as it is not affected by instabilities of other depletion mechanisms, it will occupy a quasimomentum state in a band specific for each Cartesian direction.

3.4.2 Localization in Optical Lattices

Bloch states describe systems with delocalized particles, moving around in a periodic potential. If the potential is increased, the atoms will become more and more localized. The energy band gaps will then open up more and more, until they reach the same values as for a potential well without coupling to other wells. For such a well, the lowest energy levels can be approximated the eigenenergies of the harmonic potential,

\[ V \approx \frac{m}{2} \omega_{\text{harm}}^2 (z - z_j)^2, \]  

having a bandgap of \( \hbar \omega_{\text{harm}} \).
When the atoms are in the localized regime, they can be described by another set of functions, localized at position $z_j$, called Wannier functions

$$w_n(z - z_j) = \frac{1}{\sqrt{Z}} \sum_{q} e^{iq_z z_j / \hbar} \Psi_{nq_z}(z), \quad (3.34)$$

where $Z$ provides normalization, and the sum is taken over all Bloch waves with a phase factor. As the phase of the individual solutions of the Bloch functions can vary, care has to be taken during the summation.

For the case where a three-dimensional lattice is separable into three orthogonal lattices, the solution of the three-dimensional problem is given by the product of the three one-dimensional cases;

$$w_n(r - r_j) = w_n(x - x_j)w_n(y - y_j)w_n(z - z_j). \quad (3.35)$$

In the non separable cases, the full three-dimensional problem of equation 3.11 must be solved.

**The Bose-Hubbard Model**

For the case with very cold atoms, only the lowest band is populated and the bosonic field operator in the Wannier basis can be approximated as [37]

$$\Psi(z) = \sum_j w_1(z - z_j) \hat{b}_j, \quad (3.36)$$

where $\hat{b}_j$ is the boson annihilation operator for site $j$. In the limit of strongly localized particles, the Hamiltonian can be discretized;

$$\hat{H}\Psi(z) = \left[\hat{H}_J + \hat{H}_U + \hat{H}_{\text{ext.pot.}}\right]\Psi(z). \quad (3.37)$$

Instead of working with atomic wavefunctions delocalized along the optical lattice, the atom will have a well defined assignment to a potential well $j$ of the optical lattice. Delocalization will be included into the model by tunneling probabilities between neighboring wells.

The kinetic, or tunneling part can be written as

$$\hat{H}_J = -\sum_{i,j} J_{i,j} \hat{b}_i^\dagger \hat{b}_j + \text{h.c.}, \quad (3.38)$$

where $J/\hbar$ is the jumping, or tunneling, rate from site $j$ to site $i$, and h.c. is the Hermitian conjugate. The nonlinear interaction term can be written as

$$\hat{H}_U = \frac{1}{2} \sum_j U_j \hat{n}_j + \frac{1}{2} \sum_{i,j} U_{i,j} \hat{n}_i \hat{n}_j, \quad (3.39)$$

where $\hat{n}_j$ is the boson number operator, and $U_j$ is the atom-atom repulsion energy on site $j$. This term is nonzero for cases where more than one atom occupy a
site. If many atoms occupy a single site, the system can lower its energy from the repulsive part of the Hamiltonian, by atomic tunneling to neighboring sites.

The last term, caused by the external potential, is the term giving rise to effects not present for homogeneous systems. It can be written as

\[ \hat{H}_{\text{ext.pot}} = \sum_j (\epsilon_j - \mu)\hat{n}_j, \quad (3.40) \]

where \( \epsilon_j \) is the potential energy on site \( j \) caused by a slowly varying external potential, and including the chemical potential, \( \mu \), fixes the number of atoms. Without an external potential, the system can reduce its energy, gained from the atom-atom repulsion, by spreading out until there are no sites with more than one atom left.

**The Mott Insulating regime**

By tuning the relations between the tunneling, the atom-atom interaction and the external potential, the system can undergo quantum phase transitions. The two phases mainly involved are; the superfluid phase, where the atoms are delocalized in the lattice, and the Mott insulating phase, where repulsions between the atoms lead to a localization phenomena. The phase transition can be predicted to happen at \( \eta \approx 5.8 \), where \( \eta \) is a dimensionless quantity depending on the number of nearest neighbors \( \tilde{N} \), and defined as [38]:

\[ \eta = \frac{U}{\tilde{N}J}. \quad (3.41) \]

For \( \eta < 5.8 \), the system is superfluid and particle fluctuations are dominant. Crossing into the regime where \( \eta > 5.8 \) will cause the bosons to localize, reducing particle number fluctuations and therefore increasing phase fluctuations.

The crossover is a quantum phase transition affecting the uncertainties of the number of particles per site in an optical lattice, \( N \), and inter-site phases, \( \phi \) [37]. A BEC is a coherent sample, with exceedingly small phase fluctuations between particles. From Heisenberg’s uncertainty relation for particle number \( N \) and phase \( \phi \),

\[ \Delta N \Delta \phi \geq \frac{\hbar}{2}, \quad (3.42) \]

it can be seen that the number fluctuation \( \Delta N \) is, as a consequence, large in a BEC. The opposite case, with large fluctuations in phase, \( \Delta \phi \), and infinitesimal fluctuations in the number of particles, \( \Delta N \), is called a Mott insulator [37, 39]. For bosons in a lattice, relation 3.42 means that the superfluid bosons tunnel freely between potential wells, maintaining high coherence. In Mott insulators, on the other hand, atoms will not tunnel. This is an effect caused by a competition between the tunneling term \( J \), in equation 3.43, and the interatomic interaction \( U \), in equation 3.44. For large \( U \) and small \( J \), the lowest energy for the system is found for an integer filling of potential wells. In an untrapped system, this requires an precise total number of atoms in order to avoid lack or excess of
particles in the system, leading to tunneling. For an experiment with an optical lattice and a magnetic trap potential, the system has layers with integer particle numbers, with superfluid sheets between each integer level [39]. The particle per site distribution is often related to as wedding cake structures. At each level in the cake there is an integer number of atoms per site, increasing while moving towards the center of the trap [37].

To calculate $J$, $U$, and $\epsilon_j$, the solutions for the Wannier functions 3.35 for two neighboring sites can be used. Because of the periodicity of the lattice, the whole solution for one direction is known if the tunneling probability between two sites along that direction has been found.

The three terms can be calculated with the following equations [38]:

$$J_{i,j} = - \int d\mathbf{r} \, w^\dagger_0(\mathbf{r} - \mathbf{r}_i) \hat{H} w_0(\mathbf{r} - \mathbf{r}_j),$$

(3.43)

$$U_j = g \int d\mathbf{r} \, |w_0(\mathbf{r} - \mathbf{r}_j)|^4,$$

(3.44)

and

$$\epsilon_j = \int d\mathbf{r} \, w^\dagger_0(\mathbf{r} - \mathbf{r}_j)V_{\text{pot}} w_0(\mathbf{r} - \mathbf{r}_j),$$

(3.45)

where $g$ is the interaction strength from equation 2.16, and $V_{\text{pot}}$ is the slowly varying external potential, in most cases equal to a magnetic trapping potential $V_{\text{ho}}(\mathbf{r})$.

In the deep lattice regime, for three-dimensional lattices, with the angular wave vector $k$ and the lattice potential depth $V_0$ being the same in all three directions, it can be shown that the tunneling parameter $J$ and the onsite repulsion $U$ can be approximated as [40]:

$$J = \frac{4}{\sqrt{\pi}} E_{\text{rec}} \left( \frac{V_0}{E_{\text{rec}}} \right)^{3/4} \exp \left\{ -2 \left( \frac{V_0}{E_{\text{rec}}} \right)^{1/2} \right\},$$

(3.46)

$$U = \sqrt{\frac{8}{\pi}} ka_s E_{\text{rec}} \left( \frac{V_0}{E_{\text{rec}}} \right)^{3/4}.$$

(3.47)

When the lattice barriers are raised, the tunneling drops exponentially and the onsite repulsion increases. Therefore it is possible to reach regimes where the two terms are comparable. For a critical value in equation 3.41, the sample will cross a phase transition from a superfluid to a Mott insulator, see figure 3.2. The transition will not be infinitely sharp, an effect caused by the finite size of the sample [39, 40].
3.5 Double wells

A double well potential is ideally an isolated system with two wells separated by a finite potential barrier. In this section the theory of a system being close to an ideal case is introduced, as the system starts from a Mott insulator potential (equation 3.31). By putting a potential barrier inside each well, in one direction, the system can be described by a three-dimensional array of double well systems. The dynamics of the system will be governed by the tunneling through the barrier inside the well, and the onsite repulsion on each side of the barrier. In chapter 6 and in Paper VI, this system is studied experimentally.

3.5.1 Band properties of a double well potential

The double well potential presented here benefits from the same potential as in equation 3.15 in two of the three Cartesian directions. In the third direction, the standing wave is replaced by two superimposed standing waves having the wavelengths $\lambda_{\text{short}}$ and $\lambda_{\text{long}} = 2\lambda_{\text{short}}$. Also, the angular wave vectors will differ by a factor of two, $k_{\text{short}} = 2k_{\text{long}}$, and the phase difference $\phi_{\text{short}}$ between the two standing waves can be chosen arbitrarily. The total lattice potential in the double well potential can be written as equation 3.31, with $V(y)$ and $V(z)$ both
given by the one-dimensional potentials in equation 3.15 and

\[
V(x) = -\frac{V_{\text{short}}}{4} \left( e^{4ik_{\text{long}}x + 2i\phi_{\text{short}}} + e^{-4ik_{\text{long}}x - 2i\phi_{\text{short}}} + 2 \right) \\
-\frac{V_{\text{long}}}{4} \left( e^{2ik_{\text{long}}x} + e^{-2ik_{\text{long}}x} + 2 \right).
\]  

(3.48)

Figure 3.3: The principle of a two-color lattice for double well potentials and the role of the phase difference between the two composite standing waves. For the left figures, the phase difference between the short (blue) and long (red) wavelength lattices, \( \phi_{\text{short}} = \pi/2 \); and on the right side figures \( \phi_{\text{short}} = 0 \). The combined potentials are shown in black in the lower part of the figure.

In figure 3.3, the role of the phase difference \( \phi_{\text{short}} \) between the two standing waves is illustrated. The double well potential is created when the lattice with short wavelength has a maximum at the same position as the long wavelength lattice minimum. For other phase differences, the lattice will either be asymmetric (tilted double wells) or symmetrical deep single wells with a small well on the top of the potential barrier.

The problem of double well potentials can also be solved using the methods of band structure described earlier. Instead of three non-zero terms left in equation 3.12, there are now two extra terms given by the short lattice. In figures 3.4 (a)-(d), the lowest bands for a double well lattice are shown. As both lattices are periodic, there are two choices of Brillouin zones to use for the illustrations. The first and the second zone for the long wavelength lattice corresponds to the first zone of the short wavelength lattice, which is shown in figure 3.4 (a) and (b). As the potential of the short lattice is increased, the lowest two bands tend to group up, becoming a single band for a non-existing long lattice.
Figure 3.4: Band structure for the double well potential presented in the long wavelength lattice zone scheme. The first Brillouin zone of the short lattice covers the first two zones of the long lattice, which is illustrated in (a) and (b), where only one of the lattices is on in each figure. In (c) the short lattice is more intense than in (d), forcing the two lowest bands to group. All energies are in units of $E_{\text{rec}}$ for the long lattice.

Equivalent to the case of the cubic lattices described in section 3.4, the eigenenergies of the Hamiltonian 3.11 are the allowed energies of the Bloch functions of the system. In the tight binding regime of a double well system, the Wannier functions can be computed from the Bloch functions, with equation 3.34. In figures 3.5 (a) and (b), examples of the two lowest energy Wannier functions $w_1(x)$ and $w_2(x)$, for the double well are plotted for two different potential depths.

The lowest Wannier function, $w_1(x)$, is symmetric and the next $w_2(x)$ is antisymmetric. Their superpositions are relevant for the double well potential as they describe a particle localized to the left and to the right of the barrier respectively. These functions are given by

$$w_{L,R}(x) = \frac{1}{\sqrt{2}} [w_1(x) \mp w_2(x)],$$

(3.49)
and they are shown in figures 3.5 (c) and (d) for the same potentials as in figures 3.5 (a) and (b) respectively.

A single atom loaded into the left well can, following equation 3.36, be written as

$$|L\rangle = w_L(x - x_j)\hat{b}_j, \quad (3.50)$$

where the subscript $j$ on $|L\rangle = \Psi(x)\rangle$ is dropped, as the interactions with adjacent double wells are mostly neglected. The state $|R\rangle$ is defined accordingly.

If a single atom is originally loaded into one side of the double well, the wavefunction will develop according to

$$w(x, t) = \frac{1}{\sqrt{2}} \left[ w_1(x) - \exp\{-i(E_1 - E_2)t/\hbar\} w_2(x) \right], \quad (3.51)$$
where the energies $E_1$ and $E_2$ are the energies of the two lowest Wannier functions. This leads to an oscillatory behavior, where the particle wavefunction will tunnel back and forth between the wells in the double well potential.

### 3.5.2 The Bose-Hubbard model for double wells

The Bose-Hubbard model can be extended to the double well problem, where the complete model will include many auxiliary terms, of which in practice many often can be neglected \cite{41, 42, 43}. A reasonably complete picture is given by the Hamiltonian:

$$
\hat{H}_\Psi(z) = \left[ \hat{H}_{LR} + \hat{H}_{adj} + \hat{H}_{UL} + \hat{H}_{ULR} + \hat{H}_{tilt} + \hat{H}_{ext.pot.LR} \right] \Psi(z),
$$

(3.52)

where the different parts are defined in analogy with the three-dimensional case of equation 3.37. There are two different tunneling processes, the stronger one is for tunneling from $|L\rangle$ to $|R\rangle$ and vice versa, and the other is between neighboring double wells. They can both be computed from the wave function overlap. Therefore the tunneling terms of the Hamiltonian can be written as:

$$
\hat{H}_{LR} = -J_{LR} \sum_i \left( \hat{b}_{iL}^\dagger \hat{b}_{iR} + \text{h.c.} \right),
$$

(3.53)

$$
\hat{H}_{adj} = -J_{adj} \sum_i \left( \hat{b}_{iR}^\dagger \hat{b}_{(i+1)L} + \hat{b}_{iL}^\dagger \hat{b}_{(i-1)R} + \text{h.c.} \right),
$$

(3.54)

where the tunneling energy, $J$, can be derived from equation 3.43, replacing $w_0$ with $w_{L,R}$ for the sites surrounding the relevant potential barrier.

The onsite repulsion will mainly be due to two atoms being on the same side in a double well, but there can also be a small repulsion between an atom pair with one atom on each side in the double well. The following two terms in equation 3.52 are due to these repulsions and are given by:

$$
\hat{H}_{UL} = \frac{U_L}{2} \sum_i \left( \hat{n}_{iL}^\dagger \hat{n}_{iL} - 1 \right) + \hat{n}_{iR}^\dagger \hat{n}_{iR} - 1),
$$

(3.55)

$$
\hat{H}_{ULR} = U_{LR} \sum_i \hat{n}_{iL} \hat{n}_{iR},
$$

(3.56)

with $U_L$ derived from equation 3.44 for the Wannier function $w_L$, and

$$
U_{LR} = g \int \text{d}r |w_L(r - r_j)|^2 |w_R(r - r_j)|^2.
$$

(3.57)

If the phase difference between the double wells is slightly changed from the symmetric case, the left and right wells will have different offsets in energy. This is here referred to as tilt, and is included in the Hamiltonian by:
\[ \hat{H}_{\text{tilt}} = -\Delta_{\text{tilt}}(n_{iL} - n_{iR}). \] (3.58)

Ignoring the fact that a deep harmonic potential will lead to a positive tilt on one side of the system and a negative tilt on the opposite side, the external potential, \( \hat{H}_{\text{ext, pot, LR}} \), is given by equation 3.40 by adding the contribution from the left and right side of the double well.

All the above energies are illustrated in figure 3.6. As mentioned before, many of the terms in the Hamiltonian 3.52 are small, and for simplicity we will in the following ignore \( \hat{H}_{\text{adj}} \) and \( \hat{H}_{U_{LR}} \).

Figure 3.6: An illustration of the energies relevant to the Hamiltonian 3.52. \( J \) is a tunneling strength between the wells in the double well and between adjacent double wells. The barriers crossed during the tunneling are indicated with double arrows, whose sizes are not to scale in the figure. \( U_L \) and \( U_{LR} \) are the repulsions between two atoms in the same well, and on different sides of a double well respectively. The energy difference, \( \Delta_{\text{tilt}} \), between two wells due to a phase shift between the two standing waves creating the double well potential is shown in the inset.

### 3.5.3 Single atom tunneling

The description of a single atom in a double well potential was introduced in section 3.5.1, and will here be extended to the Bose-Hubbard model, as an introduction for the correlated tunneling description of section 3.5.4.
For a single atom, all repulsions in the Hamiltonian 3.52 are zero, as there is no other atom to repel. Treating only one double well as an isolated system, the external potential term can be dropped, as it affects both wells equally, and therefore only offsets the system energy. Left in the Hamiltonian is only the tilt and the inter-well tunneling. If the state of the system is described by the vector $|L⟩, |R⟩$, then the Hamiltonian is given by:

$$\hat{H}_{\text{atom}} = \begin{bmatrix} -\Delta_{\text{tilt}}/2 & -J_{LR} \\ -J_{LR} & \Delta_{\text{tilt}}/2 \end{bmatrix}.$$ (3.59)

The eigenenergies of the system with zero tilt will be $E_+ = -J_{LR}$ and $E_- = J_{LR}$, with the corresponding symmetric and antisymmetric eigenstates:

$$|±⟩ = \frac{1}{\sqrt{2}} (|R⟩ ± |L⟩).$$ (3.60)

As in the example of equation 3.51, a particle originally located in the left well will have a time evolution, which can be rewritten as

$$ψ_{dw}(t) = \frac{1}{\sqrt{2}} (|L⟩ ± i |R⟩),$$

having an oscillatory motion between the wells, with a period set by the inter-well tunneling.

### 3.5.4 Correlated tunneling

By introducing a second atom into the double well, the onsite interaction, $\hat{H}_{U_L}$, of the Hamiltonian 3.52 can no longer be neglected. All other approximations used, regarding neglected terms, are the same as in the single atom case.

The states of a double well system have to be symmetric under the interchange of two indistinguishable bosonic atoms, leading to a basis of three different states for the system; $|LL⟩, |SS⟩, |RR⟩$, where $|LL⟩$ and $|RR⟩$ are states with both atoms located to the left and right respectively. The state $|SS⟩ = \frac{1}{\sqrt{2}} (|LR⟩ + |RL⟩)$ is the symmetric superposition of the two atoms. The Hamiltonian for a system including a tilt is given by:

$$\hat{H}_{\text{pair}} = \begin{bmatrix} U_L - \Delta_{\text{tilt}} & -\sqrt{2}J_{LR} & 0 \\ -\sqrt{2}J_{LR} & 0 & -\sqrt{2}J_{LR} \\ 0 & -\sqrt{2}J_{LR} & U_L - \Delta_{\text{tilt}} \end{bmatrix}.$$ (3.62)

For a system without tilt, the eigenenergies are given by

$$E_1 = U_L,$$

$$E_{2,3} = \frac{1}{2}U_L \left( 1 ± \sqrt{1 + 16 \left( \frac{J_{LR}}{U_L} \right)^2} \right),$$ (3.63)

with the three corresponding eigenfunctions:
\[ |1\rangle = (-1, 0, 1) = \langle - - | = \frac{-1}{\sqrt{2}} (|LL\rangle - |RR\rangle), \]
|2\rangle, |3\rangle = \left( \frac{\sqrt{2}J_{LR}}{E_{3,2}}, 1, \frac{\sqrt{2}J_{LR}}{E_{3,2}} \right). \tag{3.64} \]

In the case of a system with high potential barrier between the wells, *i.e.*, \( J_{LR}/U_L \to 0 \), the eigenenergy for both \(|1\rangle\) and \(|3\rangle\) will be equal to \( U_L \), whereas for \(|2\rangle\) it will be 0. The eigenfunctions for \(|1\rangle\) stay unchanged and the others can then be simplified to:
\[
\lim_{J_{LR}/U_L \to 0} |2\rangle = |SS\rangle
\]
\[
\lim_{J_{LR}/U_L \to 0} |3\rangle = |++\rangle = \frac{1}{\sqrt{2}} (|LL\rangle + |RR\rangle). \tag{3.65} \]

If the eigenenergies in equation 3.63 are evaluated in the low tunneling regime, then
\[
E_3 \approx U_L \left( 1 + 4 \left( \frac{J_{LR}}{U_L} \right)^2 \right). \tag{3.66} \]

Analogous to the single atom case, where the system was oscillating between the state \(|R\rangle\) and \(|L\rangle\), the atom pair will oscillate between the state \(|RR\rangle\) and \(|LL\rangle\) with an effective tunneling strength
\[
J_{eff} = 2 \frac{J_{LR}^2}{U_L}. \tag{3.67} \]

The atom pair can not break up, since populating the state \(|SS\rangle\) would not conserve energy [44]. An atom pair originally located on one side of the double well will therefore oscillate back and forth through the potential barrier. A scheme for the tunneling processes for the three level system \(|LL\rangle\), \(|RR\rangle\) and \(|SS\rangle\) is shown in figure 3.7

3.5.5 Tilted double wells

If the double well system has a tilt, the resonance for the pair tunneling described in the earlier section will be altered. If the tilt is tuned to the value \( \Delta_{\text{tilt}} = U_L \), another resonance will occur. In this case a single atom can tunnel resonantly, always leaving the other atom in the original well. The situation is illustrated in figure 3.8. In this figure the doubly occupied state \(|LL\rangle\) has equal energy as the state with one atom on each side of the double well potential. To make an atom pair tunnel completely through the barrier, the system energy must now be raised by \( U_L \). The same situation is valid in the case of a double well, containing just one atom. The atom will always occupy the lowest level in each well, as there is no onsite repulsion. The single atom will then have to gain the energy \( U_L \) in
Figure 3.7: The tunneling processes in a symmetric double well potential containing two atoms. \( J_{\text{eff}} \) couples the states with double occupancy of a single well. The state \(|SS\rangle\) can be coupled to either of the states \(|LL\rangle\) or \(|RR\rangle\) by the tunneling \( J_{LR} \), but the process is off-resonant by the onsite repulsion energy \( U_L \).

order to be able to tunnel to the other side of the well, leading to a localization on the original side.

The requirement of having an atom pair in the lowest lying well of the tilted system is referred to as conditional tunneling. The system will have a transistor-like behavior, where the presence of one atom will decide the tunneling probabilities of the other. However it is not a real transistor for indistinguishable bosons, since there is no way to determine which atom that tunneled.

3.6 Anisotropic lattice strength in cubic lattices

For the cubic lattice theory of section 3.4, the problem was split up into three separable one-dimensional systems. The theory will here be generalized for an anisotropic system having different lattice parameters in one or more dimensions. The system is also studied more in detail in chapter 7, in paper VII and in paper VIII.

3.6.1 Tunneling rates and onsite repulsion

To compute the tunneling rates of an anisotropic optical lattice, the same method as for the symmetric case is used. The system is split up into three separate one-dimensional systems, one for each Cartesian direction.

For each one-dimensional case, the one-dimensional Wannier function can be computed using equation 3.34. The tunneling rate in one dimension can then be computed using the one-dimensional version of equation 3.43,

\[
J_z = -\int dz w_0^\dagger(z - z_i)\hat{H}w_0(z - z_{i+1}),
\]

(3.68)
where the $x$ and $y$ directions can be computed in the same way. In this calculation the index $i$ on $J$ is dropped and replaced with $z$, since the tunneling rate will be equal for all neighboring sites in the $z$-direction.

The onsite repulsion will depend on the total three-dimensional wave function. Therefore all three one-dimensional Wannier functions will have to be computed using equation 3.34. The onsite repulsion can thus be computed using equation 3.44, and it is the same for all wells.

### 3.6.2 Reducing dimensionality

In equation 3.46 and equation 3.47, the approximate values of the tunneling rate and the onsite repulsion were presented. Since the tunneling is decreased exponentially with the potential strength, while the repulsion increases as $V_0^{3/4}$, the ratio $J/U$ can be chosen very differently for the three directions $x$, $y$ and $z$.

If all tunneling is frozen out in one of the directions, the system will start to act more like an array of two-dimensional system. When a second direction is tuned to deeper potentials, the system can become a two-dimensional array of one-dimensional systems. The dimensional crossover can be of different character, since various experiments have different requirements on the definition of a true transition. Low-dimensional systems are thus often mentioned with the prefix quasi.

Quasi one-dimensional systems of strongly correlated bosons are in the literature called Tomonaga-Luttinger liquids (TLL) [45]. Experiments in the Tonks gas regime of TLL, where bosons show fermionic behavior have drawn special attention to the field [46, 47]. The central point of the low-dimensional physics included into this thesis is the crossover between one- and two-dimensional systems, where the emphasis is put on how to characterize and detect this tran-
sition. Even though optical lattices would be one suitable test bench for such an experimental system, our theoretical study is only loosely bound to such an experimental set-up, and could be adapted to other suitable experiments with only small changes. Due to this loose connection to optical lattices, the theoretical study is presented separately in chapter 7. It is also the basis of paper VII and VIII.

3.7 Superradiant Rayleigh scattering

The range of experimental systems possible to construct with optical lattices is nearly infinite. So far, all topics have concerned a set of interfering laser beams for the atoms to evolve in. There is however another field of research, closely related to optical lattices, that only involves one laser beam interacting with a BEC, namely superradiant Rayleigh scattering [48].

Rayleigh scattering, is somewhat more fundamental than other excitation-emission processes involving several beams. In a Rayleigh scattering process, an atom is excited by a photon, followed by a spontaneous emission in a random direction [8]. Superradiant Rayleigh scattering is a special case of Rayleigh scattering, where the scattering processes from several absorption-emission cycles interfere, causing the spontaneous emission to be directional dependent.

The scattering of a photon involves two recoils. When excited, the atom gains the photon recoil $\hbar k_{abs}$, directed along the photons path. When emitting, the atom gains the second recoil $-\hbar k_{em}$, in the opposite direction of the new photons path. In the case of a BEC, this will excite a new momentum mode of the condensate, with recoil momentum $p = \hbar (k_{abs} - k_{em})$.

A matter interference pattern of the two BEC modes is equivalent to a moving grating, of angular wave vector $k_g = p/\hbar$. A second photon from the laser source can thus be diffracted from this grating, which lead to a diffracted angular wave vector, $k_{diff} = k_{abs} - k_g = k_{em}$. The second photon will thus lead to an addition of amplitude of the recoiled mode, further amplifying the diffraction process for the following absorption-emission cycles.

The growth of the recoiled mode will be exponential in time. Even though the first absorption-emission process might seem random, the growth rate being largest in the longest direction of the BEC, will lead to constructive interference of all random processes. Working with an elongated (cigar shaped) BEC, this process have preferential directions for the $k_{em}$ angular wave vectors, with a nearly complete domination of modes along the axial direction of the BEC. It has been recorded in experiments, both by detection of recoiled photons, and of recoiled atoms in the two axial directions [48, 49].

Superradiant Rayleigh scattering have been studied extensively in both theory and experiments, and a complete description of the phenomenon is beyond the scope of this thesis. In paper IV and in section 4.7.3, an experiment concerning the role of spurious reflections causing the superradiant Rayleigh scattering to be disguised by the effect of an optical lattice, is introduced.
Chapter 4

Experimental set-ups

The work presented in this thesis has been performed on three different experimental systems. A considerable part of the time has been spent on designing and building the set-up at Umeå University. This set-up has been planned for experiments including a $^{87}\text{Rb}$ BEC in optical lattices in non-cubic geometries.

The other two set-ups used, are the $^{87}\text{Rb}$ BEC apparatus at LENS at Florence University in Italy, and the $^{87}\text{Rb}$ BEC experiment at Johannes Gutenberg University in Mainz, Germany. These two experimental apparatuses are only briefly introduced here, and more detailed information can be found in, i.e., [42, 50].

4.1 Requirements to reach BEC

To reach the phase transition to BEC, the phase space density $\rho_{ph}$, defined in equation 2.1, of the atoms used needs to be increased by orders of magnitude. As stated in chapter 2, the onset of BEC has a critical value of $\rho_{ph} = 2.612$, which can be compared to a rubidium gas at room temperature and atmospheric pressure, where $\rho_{ph} \approx 10^{-8}$.

Increasing $\rho_{ph}$ can be achieved either by increasing the density or by cooling the sample, and thereby increasing the thermal deBroglie wavelength. When cooling, care has to be taken not to enter into the solid phase, where undesired interactions between the atoms will dominate.

A technique used worldwide today is a combination of optical and evaporative cooling of dilute atomic samples. In a first step of cooling, enough atoms can be cooled and trapped in a MOT, typically reaching densities of $10^{10}$ atoms/cm$^3$ and typical temperatures of 10 $\mu$K for $^{87}\text{Rb}$, reaching $\rho_{ph} \approx 10^{-6}$. To reach BEC, another six orders of magnitude in $\rho_{ph}$ is needed, and this is typically achieved by evaporative cooling. In figure 4.1 some typical conditions for the $^{87}\text{Rb}$ gas in the experiments are shown.

To reach BEC, a number of prerequisites need to be fulfilled. The experiment is performed in an ultra-high vacuum set-up, where a small background pressure of rubidium is available. By having a dilute sample, the losses of atoms through
Figure 4.1: Phase space density, temperature and particle density for different experimental conditions calculated for $^{87}\text{Rb}$. The black solid line at $\rho_{ph} = 2.612$ marks the phase transition to BEC, and the red dashed lines are phase space densities separated consecutively by three orders of magnitude. A typical position of a MOT, the Rb getter source, and Rb at room temperature and atmospheric pressure are shown.

inelastic three-body collisions are reduced. A MOT needs to collect a large number of atoms from the background and to cool the sample several orders of magnitude in temperature. When the MOT is fully loaded, the atoms are transferred to a magnetic trap, where they are further cooled by evaporative cooling.

The MOT is very efficient in loading, trapping and cooling the atomic sample. The same cannot be said about the evaporative cooling, since while cooling the sample, the majority of the atoms are ejected from the trap. Therefore the original quantity of atoms loaded into the magnetic trap, from the MOT, will be of importance for successful evaporation. As earlier stated in section 2.4, the rethermalization rate of the sample needs to be higher than the rate of trap losses. This will be most crucial in the initial part of the evaporation, when the sample is dilute, reducing the two-body collision rates and thus the rethermalization rate. By computing the density of the cloud loaded into the magnetic trap, and requiring a ratio between good and bad collisions (rethermalization and losses) of more than one hundred, the experimental conditions for a successful evaporation can be formulated as [51]:

$$\frac{24m a_s^2 N \omega_{ho}}{\pi k_B T} \gg \frac{100}{\tau_{trap}}.$$  \hspace{1cm} (4.1)

The most stretched states of $^{87}_{37}\text{Rb}$ has, $a_s \approx 100 a_0$, where $a_0$ is the Bohr radius [52]. Knowing the data for the atoms used, the relations between the experimentally required parameters can be computed. From equation 4.1 it can be found...
be seen that a system having good vacuum (high $\tau_{\text{trap}}$), can achieve BEC with less stringent demands on temperature, number of atoms and stiffness of the trap.

### 4.2 Vacuum System

The vacuum system used in Umeå is divided into two main chambers. In the first chamber, atoms are collected from the background gas by a MOT. The pressure is typically of the order of $10^{-7}$ Pa. This chamber is equipped with an Ionivac ITR90 vacuum gauge from Leybold Vacuum, providing a measurement range from atmospheric pressure down to $5.5 \cdot 10^{-1}$ Pa with a Pirani manometer, and in the range of 2 Pa down to $5 \cdot 10^{-8}$ Pa with an ionization probe. The vacuum is maintained by an 81/s ion pump from Varian.

The first chamber has an evacuation valve, open only during preparation of the vacuum, when it is connected to an external Turbotronik NT340M turbomolecular pump, backed by a Trivac rotary vane pump, both from Leybold Vacuum.

The chamber has ten flanges, of which eight have viewports attached, providing optical access for laser beams and for optical detection such as with CCD cameras. On one flange, four electrical feed-throughs are installed for the rubidium getter sources.

There are two different getter sources installed, providing the possibility of comparisons. The getters are provided by SAES getters and Alvatec, both having a controllable yield of rubidium for the experiment. The partial pressure can be controlled by varying the current fed through the getters. The main differences between the getters are size and purity. The getter provided by Alvatec contains a larger quantity of rubidium, and the amount of contamination is lower; desirable properties for an experiment running for many years under good vacuum conditions. The other getter, from SAES getters, has the advantage of having a protecting seal maintained during the entire lifetime of the getter. This is an advantage if the vacuum needs to be broken and the system rebaked. The Alvatec getter would need to be replaced, and care has to be taken for reactions between the getter material and H$_2$O vapor in the air.

Atoms from the MOT in the first chamber can be transferred to a second MOT via a differential pumping stage connecting the two chambers of the vacuum system. This stage is a cylindrical tube having 50 mm length and 5 mm diameter. The tube is mounted to provide a clean view from the position of the first to the second MOT, allowing transfer, while unintentional flow of atoms between the two chambers is limited, maintaining a pressure difference. To improve the vacuum further, a valve is installed in series with the differential stage. The valve is kept closed when the experiment is not running.

The second chamber is a custom made glass cell by Hellma. It is shaped as a right rectangular prism having two sides of 25 mm and one of 65 mm. The cell does not have anti-reflection coating. It is bakeable to 300°C. In figure 4.2, two different cells are shown. The older set-up (left) used a larger second chamber,
only bakeable to 90°C, with drawbacks for both vacuum and magnetic coil access (chamber size).

In the second chamber the pressure is lower than in the first. There is no vacuum gauge installed, but measurements of the lifetime of the magnetic trap to 9 s suggest comparable pressure to other running set-ups, such as the one in Florence [50] having a lifetime of 17 s, providing a vacuum below $10^{-8}$ Pa. The lifetime in the magnetic trap is not only limited to background pressure, since stray light, vibrations, magnetic field fluctuation etc., can reduce the lifetime.

The low pressure of the second chamber is maintained by a combination of two pumps, a 1000 l/s Non-Evaporative-Getter (NEG) pump and a 20 l/s Starcell ion pump from Varian. The NEG pump is passive and require no external power supply, while the two ion pumps both have electric power supplies.

The vacuum components used can be mounted with different geometries, of which two have been used extensively in the laboratory in Umeå (see figure 4.2). The older set-up was horizontal, providing optical mounting close to the stable optical table. In the new set-up, the configuration is vertical, with the second chamber below the first. Care has been taken in the design to avoid instability problems by using rigid supports. The second chamber, which is more sensitive to vibrations, is mounted closest to the table. The main advantage with the vertical set-up is to avoid the trouble of mounting optics in a cramped space between the chamber and the table.

When remounting a vacuum system, all parts need to be rebaked, meaning
heated to high temperatures for a time being in the order of magnitude of days, while pumping with the external turbo molecular pump. All pieces have been baked at temperatures as close to the maximally allowed possible. For most parts of the system the maximal temperature is in the range of 300°C.

The main differences between the set-up in Umeå and the ones in Florence and Mainz are mounting choices for different optical access. The set-up in Florence have magnetic coil mounts very close to the center of the cell, with the drawback of lack of optical access in non-Cartesian directions. The set-up is also mounted close to the table, creating a stable system, but having a cramped space for optical access from below. In Mainz, the vacuum system is L-shaped, and the corner in the vacuum system provides both the differential vacuum, and the possibility to have good optical access in all Cartesian directions.

There is no NEG pump in neither the Florence, nor in the Mainz set-ups. Instead, an ion pump is accompanied by a titanium sublimation pump. The lifetime of the magnetic trap in Florence is 17 s [50] and in Mainz it is 90 s [42].

4.3 Lasers and optics

In the Umeå set-up, two laser sources are used for trapping and cooling. One is a Toptica DLX high power diode laser system used to cool and trap, and the other is a home built external cavity diode laser [53], used for repumping atoms from a state that is dark for the cooling and trapping laser. These lasers will from here and on be called cooling and repumper lasers respectively.

Saturation spectroscopy with a feedback loop is used to lock both lasers to desired frequencies [54]. Frequency modulated light is used in the saturation spectroscopy to produce the desired error signal for the feedback loop [55]. Since the two light sources have different demands on frequency stability, two different procedures are used. For cooling and trapping atoms, a more stable frequency is required. Therefore, the modulation of the frequency for the saturation spectroscopy is achieved with an acousto optic modulator (AOM) before the saturation spectroscopy. An AOM can be seen as a moving grating, where the period of the grating, and therefore the frequency of the diffracted beams can be varied by applying an electric voltage [56]. For the repumper laser, frequency stability demands are low, and the modulation can be done on the laser itself, saving equipment and reducing complexity of the experimental set-up.

Different steps in the cooling and trapping sequence require different frequencies and irradiances. Light from the cooling laser is split up into several beams, and the frequency of each beam can be controlled with AOMs. The repumper laser light can be adjusted in irradiance, and is aligned directly onto the two traps. A schematic drawing of the laser frequency generation is shown in figure 4.3, and the corresponding atomic resonance frequencies for the \(^{87}\text{Rb D2-line}\) are presented in figure 4.4.

To mechanically decouple different parts of the experiment, as-well as to clean the spatial mode of the laser beam, single mode optical fibers are used. Typically, a fiber is installed after frequency and irradiance manipulating optics, and before
Figure 4.3: A schematic view of the optical set-up. The two lasers are locked to desired frequencies with servo loops using saturation spectroscopy. The laser light is set to correct frequencies, irradiances, polarizations, and spatial modes, by a system of optics. The MOT beams are three retro-reflected beams for each MOT.

beamsplitters and polarization controlling optics. Mechanical shutters installed before the fibers make it possible to completely shield of all laser light from the experiment, increasing the lifetime of the magnetic trap, by stopping resonant photons from arriving to the trapping regions.

Even though a MOT works also with non-perfect spatial modes, a clean mode facilitates the alignment procedure. For the absorption imaging introduced in section 4.6, introducing a fiber for mode cleaning drastically reduces the amount of interference fringes in the final image.

For alignment purposes, fibers generally facilitates handling of the laboratory. Whenever some equipment is changed before the fiber, the experiment can be repositioned at its previous alignment just by realigning the fiber coupling. Without a fiber, a change in the initial stage of a beam path will require a complete realignment of the entire optical path.

For optical lattice experiments, two MBR 110 Ti:sapphire ring cavity lasers, pumped by Verdi V18 solid-state diode pumped frequency doubled Nd:YV04 lasers, from Coherent are used. The lasers are tuneable in a large wavelength interval from visible to far into the infrared. Using a similar scheme as for the cooling and repumper lasers, they can be locked to atomic resonances, which is useful for near resonant optical lattices. The irradiance is controlled with AOMs and shutters placed before fibers.

The laser systems in Florence and Mainz are very similar to the ones used in Umeå, as the principle is widely standardized for this kind of experiments.
Figure 4.4: To the left, a partial $^{87}\text{Rb}$ level scheme (not to scale), showing the D2 line used in cooling and trapping, with the hyperfine splittings noted. To the right the laser frequencies used in the set-up are shown relative to the hyperfine levels they excite.

### 4.4 Electronics and computer control

The experimental sequences are computer controlled. A typical measurement cycle last for several minutes, and for most parts timing is uncritical, as many steps last for several seconds. There are however sections of the experiments that require sub-millisecond precision on the control voltages from the computer. The combination of a long overall sequence and the occurrence of high precision timing disqualifies many modern computer systems, often running in program time blocks of tens of milliseconds.

In Umeå the choice have been a NI-6229 digital data acquisition card from National Instruments. This card provides direct memory access, where a processor on the card reads a memory buffer, and feeds the output accordingly. The memory buffer is fed by the computer processor, and as long as the buffer never empties, the system will have the desired timing all through the experiment.

To feed the memory buffer, a custom made Labview program reads a text file containing all the desired output voltages for each time step. The text file is created by a script system based on Gnu Octave.

The electrical signals from the NI-6229 card are fed to different parts of the experiment, controlling shutters, AOMs, lasers, current supplies, etc., either directly, or via home built electronics. Some of these circuits have detailed descriptions in experimental theses such as [57, 58, 59, 60].
4.5 Atomic traps

The atomic traps used in the experiments in this thesis, are MOTs to precool and collect atoms, and magnetic traps in which the atoms are trapped and further cooled to the BEC transition using evaporative cooling. Optical lattices can also be treated as atomic traps, but are treated in a separate section in this chapter.

4.5.1 MOTs

In the set-up in Umeå, the MOT realized in the part of the vacuum chamber having a background pressure of rubidium atoms is hereby referred to as the first MOT [61]. It serves as a source of atoms for the experiment, as it collects and cools thermal atoms from the background gas.

The magnetic field gradient of this MOT is tunable around 0.1 T/m by changing the current through a pair of anti-Helmholtz coils having 300 windings each. The magnetic field minimum in the vacuum system is centered by three pairs of Helmolz coils, one in each Cartesian direction.

The laser light of the first MOT is red detuned 12.5 MHz from the $^8_{37}$Rb transition; $5s^2S_{1/2} \rightarrow 5p^2P_{3/2}$, $F = 2 \rightarrow F = 3$, during a growth phase of about 500 ms, see figure 4.4. The light is composed of three retro-reflected beams, resulting in six, pairwise counter-propagating laser beams with circularly polarized light.

The cooling transition is cyclic and the atoms should, after an excitation-emission cycle, return to the $5s^2S_{1/2}, F = 2$ state. However there is a small, but important loss of atoms ending up in the ground-state $5s^2S_{1/2}, F = 1$, which is not resonant with the cooling light. The repumper laser is used to optically pump atoms back to $5s^2S_{1/2}, F = 2$ by resonant excitation on the $5s^2S_{1/2} \rightarrow 5p^2P_{3/2}, F = 1 \rightarrow F = 2$ transition. The frequency of the repumper laser is fixed, but the irradiance can be varied with an AOM and blocked completely with a shutter. Both the cooling and the repumper light are fiber coupled through the same fiber, which facilitates the alignment.

When the first MOT has reached a sufficiently large load of atoms, the detuning is increased for a couple of milliseconds in order to further cool the sample. Thereafter, the cooling and repumping light are turned off and the atomic cloud will start to expand for a short moment, until a push laser beam is pulsed on. The push is resonant with the same transition as used for the cooling, and accelerates the atoms down to the second chamber. The irradiance and the exposure time of the push beam, are both optimized in order to accelerate the atoms to velocities in the range of 20 m/s, being within the capture range of a second MOT in the center of the glass cell in the lower part of the vacuum system [58], see figure 4.2.

The anti-Helmholz coils of the second MOT only have four windings each, leading to much higher currents being used (220 A). The advantage of such a configuration is the reduction of the inductive load, giving fast switching of the coils. A drawback is the need of water cooling as the power dissipation is large.

The optics for the second MOT is arranged in a similar way as for the first MOT. There are three retro-reflected beams, yielding six counter propagating...
beams with circular polarization. The light is fiber coupled, and the irradiance and detuning is set by an AOM, and a shutter installed before the fiber.

The transfer of cold atom clouds from the first MOT to the second is cycled, keeping the second MOT on for several cycles. For each cycle, the second MOT cloud will achieve a number of atoms closer to its maximum load. Upon saturating the second MOT, the atomic sample can be further cooled by increasing the detuning, and decreasing the cooling irradiance. For the experiments performed in paper V, the MOT is switched off and the atomic sample is loaded into an optical lattice, see section 4.7. When the experiment is used for further cooling towards BEC, the atoms are instead transferred to the magnetic trap at this stage.

4.5.2 Magnetic trapping

The atoms are cooled further with evaporative cooling in a magnetic trap, see section 2.3 and 2.4. The magnetic trap configurations used in the experiments covered by this thesis are all IP traps of various designs.

A clover-leaf magnetic trap has been implemented in the set-up in Umeå [57, 62]. Compared to other IP traps, the clover-leaf configuration have increased optical access in one plane, making it useful for experiments where optical lattice beams are to be aligned in arbitrary angles. The trap consist of three types of coils; gradient, curvature, and anti-bias, all shown schematically in figure 4.5.

The main responsibilities of the eight gradient coils are to produce the magnetic field in the radial direction. They are all mounted in anti-Helmholtz configuration, with alternating current directions between neighboring pairs, giving a radial quadrupole field. The field along the \( z \) axis has a magnetic minimum created by the two curvature coils, mounted essentially in Helmholtz configuration, but with a distance larger than their coil radii. To compensate for the offset field \( B_0 \), induced by the curvature coils in the trap center, two anti-bias coils are run in exact Helmholtz configuration, with the current direction opposing the curvature coils. By varying the current in the anti-bias coils, \( B_0 \) can be changed in order to vary the trapping frequencies for trap loading and evaporation.

During the MOT phase, the anti-bias coils are used in anti-Helmholtz configuration by reversing the current direction in one of the coils. To alternate between MOT and magnetic trap, switches shown in the right part of figure 4.5 are used in order to reverse the current direction, and turn the coils on or off.

All coils are connected in series, to ensure that current fluctuations, induced by the power supplies, are equal in all coils. This minimizes the drift of the offset \( B_0 \) during the experiment. The use of the current dump, to vary the anti-bias coil current, will thus be a major noise source for \( B_0 \), see figure 4.5.

Power dissipation from the trap is controlled by water cooling. All coils are made by hollow copper tubes with a constant internal flow of water. The cooling is over dimensioned, as the trap was designed for currents in the 400 A range. Currently two parallel Delta Elektronik SM 15-200D, 0−200 A DC power supplies can only deliver 220 A due to the high voltage drop over the switch.
Figure 4.5: The magnetic trap coils (left) and the current switching (right). A clover-leaf configuration trap consist of a pair of composite coils packets. Each packet is made of six coils. To start with, there are four gradient coils, symmetrically placed around the central curvature coil. The outermost coils are used as anti-bias coils for the magnetic trap, as-well as for quadrupole coils for the MOT. The coil configuration along the $z$-axis is shown in the top left part. In the lower left, the $z$-axis is turned vertically. On the right, a simplified drawing of the current switch for the magnetic trap and the MOT is shown. The current source can deliver around 220 A. The current dump is a home built high precision current sink with a fixed value, in parallel with a Delta Elektronik SM7020-D 0–20 A DC power supply for tunability. The switches are all Powerex IGBT CM400HA-12H, computer controlled via a custom designed circuit. Missing in the electronic current switch drawing are the diodes and resistors used to dissipate the magnetic energy during switching.

circuit. This current is however large enough to achieve trapping frequencies of $\omega_r/2\pi = 170\text{Hz}$ and $\omega_z/2\pi = 12\text{Hz}$.

The transfer from MOT to magnetic trap is still under optimization. Currently the MOT is first cooled and compressed by reducing the MOT beam irradiance and increasing their detuning. The MOT light and the magnetic field is then turned off, and a uniform magnetic field along the $z$-axis is quickly ramped up to provide a quantization axis for the atoms. Circularly polarized light, resonant with the transition $5s^2S_{1/2} \rightarrow 5p^2P_{3/2}$, $F = 2 \rightarrow F = 2$ is pulsed in the
z-direction in order to optically pump the atoms to the $|F = 2, M_F = 2\rangle$ state, being a low field seeking state. After pumping, the magnetic trap is ramped up with a large $B_0$ offset, in order to accomplish an optimum overlap between the shape of the atomic cloud and the trap. When the atoms are trapped, $B_0$ is reduced to increase the trapping frequency for the evaporative cooling.

Evaporation is done with a simple antenna, consisting of a small copper wire loop fed by an Agilent 8648A signal generator amplified by a Mini-circuits amplifier ZHL-3A. The evaporation frequency is set by a Labview program, controlling the signal generator via a GPIB interface.

For the set-up used in Florence, the magnetic trap consist of four coils. Along the $x$-axis, there are two quadrupole coils, and along the $z$-axis there is one curvature and one anti-bias coil. The trap is fitted onto the vacuum system, leaving high quality optical access mainly in the Cartesian directions. This trap is discussed more in detail in [50, 63].

The magnetic trap in Mainz is a Quic trap [42, 64], consisting only of three coils. Along the $x$-axis, there are coils in an anti-Helmholtz configuration, and on the $z$-axis there is a single curvature coil. The loading of the magnetic trap differs significantly from the set-ups in Umeå and Florence, since there is never any second MOT. The atoms are loaded into a quadrupole field magnetic trap from the first, and only MOT. The trap shape is changed, and the atoms are moved with a conveyor belt of overlapping quadrupole traps, covering the distance between the MOT and the Quic trap [65].

4.6 Imaging

The atomic cloud is detected by resonant absorption imaging after a variable time of flight [21, 66]. The detection is destructive, i.e., every data point extracted will be from a separate sample.

4.6.1 Detected signal

A laser beam, resonant with the $5s^2S_{1/2} \rightarrow 5p^2P_{3/2}$, $F = 2 \rightarrow F = 3$, transition is collimated and directed through the atomic cloud. The atoms will cast a partial shadow in the beam, locally damping the irradiance according to Beer’s law,

$$I_t(x, z) = I_0(x, z) \exp \left\{ -\sigma_c \int dy \varrho(x, y, z) \right\} + I_{bg}(x, z),$$

(4.2)

where $I_t(x, z)$ and $I_0(x, z)$ are transmitted and incident irradiances respectively, $I_{bg}$ is any background light source that may contribute to the signal after the cloud, $\sigma_c$ is the resonant absorption cross section and $\varrho(y)$ is the column density along the probe path, see figure 4.6. In the experiment, a plot of the density in the $x$ and $z$ directions can be calculated from equation 4.2;

$$\varrho(x, z) = \int dy \varrho(x, y, z) = -\frac{1}{\sigma_c} \ln \left( \frac{I_t(x, z) - I_{bg}(x, z)}{I_0(x, z) - I_{bg}(x, z)} \right).$$

(4.3)
The irradiances \( I_t(y, z) \) and \( I_0(y, z) \) are recorded by acquiring the irradiance profiles of the probe laser beam, with and without a shadow of the atomic sample respectively. A background irradiance, \( I_{bg}(x, z) \) is acquired with the probe light being blocked, thus only recording stray light in the experiment.

In the above calculations, two saturation effects have been ignored. If the probe light has an irradiance above the saturation irradiance of the transition, the atoms will spend a considerable amount of time in the excited state. This will give an underestimation of the number of atoms. Irradiances lower than half the saturation irradiance are used in order to reduce this effect.

The second saturation effect comes from the density of the cloud. The most straightforward way of avoiding density saturation is to let the atomic cloud expand before detection. Both saturation effects can be compensated for, if kept small, by methods presented in \cite{21, 66}. The cross-section, \( \sigma_c \), is corrected for the wavelength and polarization used, according to the same reference.

\[
I_t(x, z) \quad I_0(x, z) \quad I_{bg}(x, z) \quad \rho(x, z)
\]

Figure 4.6: The three images, \( I_t(x, z) \), \( I_0(x, z) \) and \( I_{bg}(x, z) \) recorded to produce the density plot \( \rho(x, z) \). The two leftmost images are acquired by imaging a probe laser beam on the CCD sensor, with and without atoms present in the beam path. To compensate for stray light, an image, \( I_{bg} \), with the probe light blocked, is recorded, and subtracted from the other images. The optical density, according to equation 4.3 is shown in the rightmost picture.

4.6.2 Image analysis

Resonant absorption imaging is a destructive process, where the atomic sample is heated and lost during the acquisition. To be able to study the evolution of the system after release from the trap, several clouds are produced, and recorded after different desired times of flight. The experimental set-up is therefore required to be highly reproducible from shot to shot.

For a MOT, the expansion reveals the original shape and the temperature of the cloud. An atomic cloud, at temperature \( T \), with a Maxwell-Boltzmann velocity distribution will have a width, \( s_\alpha(t_{TOF}) \), after the time of flight \( t_{TOF} \), in the direction \( \alpha = (x, y, z) \). After a short expansion time, the cloud will be more or less unchanged, since many atoms have their flight directions towards the center of the cloud. For longer times of flight, all velocities are directed outwards, and the atomic cloud will have a size, well approximated by \( v_\alpha t_{TOF} \),
where $\frac{1}{2}mv_\alpha^2 = \frac{1}{2}k_B T$. For all times the expansion, in a system without collisions and without an external potential, is given by [67]:

$$s_\alpha(t_{TOF}) = \sqrt{s_\alpha(0)^2 + v_\alpha^2 t_{TOF}^2}. \quad (4.4)$$

A two-dimensional Gaussian profile is fitted to the density profile obtained by equation 4.3 in order to obtain information about the atomic sample at each $t_{TOF}$. For an anisotropic cloud, the fit function is

$$\rho_{O.D.}(x, z) = B + A \exp \left\{ \left( \frac{x - x_c}{s_x} \right)^2 + \left( \frac{z - z_c}{s_z} \right)^2 \right\}, \quad (4.5)$$

where $B$ is the background level, $A$ is the maximum column density, $x_c, z_c$ are the cloud centers in $x$ and $z$, and $s_x, s_z$ the clouds’ $1/e$-radius. A similar function, but with a rotated coordinate system, is used if the anisotropy is tilted relative to the CCD camera sensor. To prevent interference fringes in the probe, caused by multiple reflections, the probe is inclined relative to the normal of flat surfaces, such as the camera window and the vacuum chamber walls. The curve fitting is therefore done with a coordinate rotation, in order to compensate for the inclination angles.

A freely expanding BEC, without an optical lattice, is analyzed in a similar way, by fitting an inverted parabola to the optical density image. Integrating the three-dimensional density of a condensate in the TF limit, see equation 2.23, along the $y$-axis, here being the projection axis, results in the column density:

$$\rho_{O.D.}(x, z) = B + A \left\{ 1 - \frac{x^2}{R_{R\perp}^2} - \frac{z^2}{R_z^2} \right\}^{3/2} \Theta_H \left( 1 - \frac{x^2}{R_{R\perp}^2} - \frac{z^2}{R_z^2} \right), \quad (4.6)$$

where $R_\perp$ and $R_z$ are the time dependent radii in the radial and axial direction of the BEC respectively, and $\Theta_H$ is the Heaviside step function. Experimentally, there can be a thermal fraction of atoms remaining when an image of the BEC is acquired. As the image of the thermal atoms is fitted according to equation 4.5, and the pure BEC to equation 4.6, a mixed cloud will contain a Gaussian mode and an inverted parabola. By fitting a bimodal distribution, the thermal fraction can be estimated.

Adding an optical lattice to the experiment might alter the shape of the detected cloud. Several different optical lattice experiments are presented in this thesis. A conservative optical lattice in combination with a MOT have been used in paper V and section 4.7.1 to alter the anisotropy of the expanding MOT, changing the coordinate rotation. In papers I, II, III and in chapter 5, the momentum distribution of the BEC, as-well as its size and condensed fraction is used to detect the onset of instabilities. In paper VI and chapter 6, the transition to a Mott insulator, having the Gaussian profile of a non-correlated cloud is studied. Also the momentum distribution of a double-slit experiment is detected and studied. Such a profile can neither be fitted with a simple Gaussian,
nor with an inverted parabola. In paper VII and chapter 7, interference peaks in the momentum distribution is suggested in order to reveal information about the dimensionality of the system, whereas in paper IV, the momentum distribution reveals the onset of superradiance.

All of the above experimental signals can be detected with time of flight absorption imaging. The shape of the momentum distribution will be studied more in detail in the appurtenant sections of the thesis and the corresponding papers.

4.7 Optical lattices

In all papers included in this thesis, both experimental and theoretical, optical lattices played a central role. The three experimental apparatuses used were built with the aim on different kinds of optical lattice experiments.

In Florence, a BEC moving in a one-dimensional optical lattice was studied, and the alignment could be made by overlapping two counter-propagating beams on the BEC position. The lattice light originated from a single laser, and was split up into two beams. The amplitude of the two beams and the frequency difference between them were controlled by two phase-locked AOMs. When the two beams were overlapped with opposing wave-vectors, a standing wave was produced, whose position was moving in the laboratory frame with the velocity

\[ v_L = \frac{\Delta \omega_L}{2k}, \]

where \( \Delta \omega_L \) is the difference in angular frequency between the lattice beams.

The set-up in Mainz has been customized for three-dimensional cubic lattices, which consisted of three separate one-dimensional lattices, all aligned along the Cartesian axes of the set-up. The laser beams of the separate lattices had orthogonal polarizations, and differed in frequency by more than any inherent frequencies of the trapped atoms.

For the experiments of paper VI, a double well potential was created by including a second one-dimensional lattice in one of the Cartesian directions, having twice the wavelength of the first. In this direction the two lattice wavelengths used were \( \lambda_{\text{blue}} = 765 \text{ nm} \) and \( \lambda_{\text{red}} = 1530 \text{ nm} \). The two laser sources used, were frequency locked to each other by detecting the beating between \( f_{\text{blue}} = c/\lambda_{\text{blue}} \) and a frequency doubled portion of \( f_{\text{red}} = c/\lambda_{\text{red}} \). A feedback system locked \( f_{\text{red}} \) to a desired beat frequency [43, 68].

Since all three lattice directions had retro-reflecting mirrors for the beams, they had fixed anti-nodes at the mirror. Two lattices having a periodicity differing by roughly a factor of two, thus have common anti-nodes at the mirror. If the BEC is situated a distance \( D_{\text{dw}} \) from the mirror, the resulting phase difference at the BEC would be

\[ \phi_{\text{short}} = 2\pi \frac{\Delta \omega_{\text{dw}}}{\omega_{\text{blue}}} \frac{D_{\text{dw}}}{\lambda_{\text{blue}}/2} = \frac{2\Delta \omega_{\text{dw}} D_{\text{dw}}}{c}, \]

56
Figure 4.7: The coordinate system for the alignment tool has its origin coinciding with the atomic sample. The iris used for alignment of the beams can be moved in a plane, \( y = y_p \), above the atoms. A beam passing through the origin, and through the iris placed in \((x, y_p, z)\), will have a well defined angular wave vector \( k \). The primed axes represent the projected two-dimensional coordinate system in the alignment tool plane.

where \( \Delta \omega_{dw} \) is the detected difference in angular frequency between the beating beams, and \( \omega_{\text{blue}} = \frac{2\pi c}{\lambda_{\text{blue}}} \). In the experiment \( D_{dw} = 25 \text{ cm} \), and any mechanical or other drift in this distance is compensated for by adjusting \( \Delta \omega_{dw} \) until the desired phase difference is achieved.

The set-up in Umeå has been built for optical lattices not being limited to cubic geometries. The geometry of such a lattice will depend on the wave vectors of the included lattice beams (see section 3.1). The precise control of the beam geometry was the motivation for the work of paper V. Quasiperiodic optical lattices is one example of experiments that will require precision alignment of the lattice geometry [69].

### 4.7.1 Alignment of lattices with arbitrary geometry

An alignment tool for optical lattices has been realized, and this is reported on in paper V. This tool consists of an iris that can be moved to a specific coordinate in a plane above an atomic trap. A laser beam passing through the iris and striking the atomic cloud will have a well defined wave vector if the distance from the plane to the cloud is known.

The atomic cloud defines the origin, and the axes constitutes a right hand Cartesian coordinate system with the \( z \)-axis horizontal, through the symmetry axis of the magnetic trap, and the \( y \)-axis being the vertical axis, positive upwards, see figure 4.7.

The wave vector of the beam is specified by letting the beam pass through an iris in a horizontal plane above the atomic cloud. If the iris coordinates \((x, y_p, z)\) are known, the direction of an angular wave vector is given by the line passing
through the origin and these coordinates. The experimental procedures, to define
the coordinate system in the plane, and to align the beams, are both described
as follows.

**Calibration**

The movement of the iris in the plane is controlled by two translation stages with
millimeter scales. Two of the axes are for simplicity defined to be the axes of
movements of the translational stages, here called the $x$- and $z$-axes. To define
the rest of the coordinate system, and relate it to the values read on the scales,
a few measurements are needed;

- the projection of the origin in the plane, $(0, y_p, 0)$, and
- the distance between the atomic cloud and the plane.

To find the projection of the origin in the plane, a vertical beam passing
through the atomic cloud is used. The values read on the scales of the translation
stages for the iris, when the vertical beam passes through it, define the desired
point.

The distance between the lattice plane and the atomic sample cannot be
easily measured directly, because of equipment blocking the way. Instead, two
beams are aligned through the atomic cloud. The distance between the beam
coordinates in the iris plane is easily derived. Also, the distance between the
intersections with another, well defined plane, parallel to the iris plane, is mea-
sured. By measuring the distance between those two planes, and using geometric
rules for triangles, the value of $y_p$ is found. The optical table is here taken as the
reference plane.

All alignments are done with a resonant beam with variable size and irra-
diance. This allows the user to see when the beam hits the atomic sample by
looking at the decrease in fluorescence, proportional to the decrease in number of
atoms in the trap. This beam can later be overlapped with another beam, used
for the lattice, which may be tuned further away from resonance.

The alignment tool has as its main limitations the fact that horizontal beams
cannot be aligned with it. However, this problem is solved by introducing an-
other, similar set-up in a vertical plane. The choice of wave vectors is limited by
the coils from the magnetic trap and other equipment, but is almost unlimited
in the $z = 0$ plane.

Fine alignment of the lattice beam overlap with the atomic cloud can be made
by methods such as presented in sections 4.7.2, 4.7.4 and 4.7.5.

**Fidelity test of the alignment tool**

In paper V, a test of the reproducibility of the alignment tool was performed,
both for the overlap of the beams in the region of atoms and for the reproducibil-
ity of lattice beam angles. The tests were made with a MOT, cooled down to
temperatures in the range of 20 µK, having energies lower than the potential barrier heights of the optical lattices used.

Using three beams, a two-dimensional optical lattice potential was created. The lattice potential was ramped up just after the MOT potential was switched off. The ramping sequence was controlled by a computer, aiming for an adiabatic ramp-up. Due to the lack of feedback from the actual potential to the ramp-up electronics, small deviations from the adiabaticity criteria might have been present, but they ought not to have affected the outcome of the measurement.

The optical lattice has been kept on for a variable time, followed by detection by absorption imaging, where the cloud sizes in two orthogonal directions, within the lattice plane, were recorded. The cloud did not expand within the lattice, and the cloud sizes with and without lattice beams are presented in figure 4.8(a). If any of the beams would have been severely misaligned, it would have resulted in a lattice potential being too shallow to catch a cloud having temperatures of 20 µK. A freely expanding MOT will expand according to equation 4.4, and soon after release it has become too dilute for detection with our imaging system.

![Figure 4.8: Validation of optical lattices produced by the alignment tool. In (a) expansion in the lattice plane of a two-dimensional lattice was studied. When the lattice was present, the size of the atomic cloud stays constant (filled and hollow circles). Fluctuations in cloud size depend on the initial size. Without lattice, the cloud expands (triangles), and after 8 ms expansion, the cloud was too dilute for our detection system. The lines are fits to equation 4.4. In (b) cloud expansion is measured in one-dimensional lattices, having different incident angles set by the alignment tool. The lattice potential prevents the cloud to from expanding along the lattice. The expansion angle, θatom is compared to θtool, set by the alignment tool. The line is a linear fit, with slope 0.98 ± 0.02. The inset in (b) shows an example of a cloud expanding in the one-dimensional lattice.](image-url)

To test the angular reproducibility of the alignment tool, a measurement was done using one-dimensional optical lattices. The measurement procedure was the same as in the two-dimensional lattice experiment above. The optical lattice potentials were made deep enough to prevent the atoms from expanding
along the lattice, resulting in a cylindrically expanding cloud, with the short axis being constant, and the other growing with time. By aligning different one-dimensional lattices within a plane, and detecting the expansion within the same plane, a verification of the alignment tool angular precision could be made, see figure 4.8(b). Making a linear fit to the experimental data yields a slope of $0.98 \pm 0.02$, verifying that the actual angle of the potential, $\theta_{\text{atom}}$ is the same as the one intended, $\theta_{\text{tool}}$.

### 4.7.2 Fine alignment using Bragg scattering

Several experiments with optical lattices require some method to measure the lattice potential depth. In the experiments of Paper I, II and III, the lattice depth is shallow, and can thus be calibrated with Bragg spectroscopy, within the lowest energy band [50, 70, 71].

An optical lattice of two laser beams, with an inclination angle difference of $\theta_{\text{diff}}$, where $\theta_{\text{diff}} = \pi$ for anti-parallel beams, will transfer the recoil momentum $p_{\text{rec}} = 2\hbar k \sin(\theta_{\text{diff}}/2)$ to an atom, in a two-photon Raman process. Energy conservation will thus require

$$\frac{p^2}{2m} - \frac{p_o^2}{2m} = \frac{(p_o + p_{\text{rec}})^2 - p_o^2}{2m} = \Delta E,$$

where $\Delta E$ is the energy difference between the original and the final energy states.

For a condensate moving in the lattice frame, with $\theta_{\text{diff}} = \pi$, this process includes two states of the system having momenta $\pm \hbar k$. The Raman process will excite via a virtual level, red detuned by the energy $\hbar \Delta$, see figure 4.9.

![Figure 4.9: Using Raman excitations between atoms having momenta $\pm \hbar k$, the optical lattice potential is determined. The blue rings mark the two atomic states involved; the black parabolas are the ground and the excited state. Red arrows mark the transition from $-\hbar k$ to $\hbar k$ via the virtual level marked with a red dash-dotted line, being off resonant by the energy $\hbar \Delta$.](image-url)
Starting in the state, having the momentum $-\hbar k$, will thus lead to a time dependent population of the state with momentum $+\hbar k$ of the type:

$$N_{+\hbar k} = \frac{N}{2} (1 - \cos(\Omega_R t_{\text{latt}})),$$

(4.10)

where $t_{\text{latt}}$ is the time the BEC has spent in the lattice, and

$$\Omega_R = \frac{\Omega_0^2}{2\Delta},$$

(4.11)

is the effective Rabi frequency, related to the detuning $\Delta$ and the Rabi frequency $\Omega_0$.

Since the effective Rabi frequency will be dependent on the strength of the driving field, the potential depth can be extracted by fitting a sine wave to the measured population of atoms in one of the states. The amplitude of the potential will thus be [50]

$$V_{1D} = 2\hbar \Omega_R.$$

(4.12)

Optimizing the overlap of two beams at the position of a BEC can thus be done by selecting $\Omega_R t_{\text{latt}} < \pi$, by using a combination of low enough lattice irradiance, and time spent in the lattice. If the number of atoms $N_{+\hbar k}$ increases when the lattice alignment is altered, the effective Rabi frequency, and thus the potential has increased.

### 4.7.3 Bragg scattering for seeding superradiant Rayleigh scattering

In a superradiant Rayleigh scattering experiment, only one laser beam (here called pump beam) is used to stimulate a scattering process, where spontaneous emission is suppressed, in favor of coherent scattering along one direction in a BEC [72].

In an experiment, where the scattered direction is chosen to be the reverse direction of the pump beam, special care has to be taken to avoid back reflected beams in optical components or in the vacuum chamber itself. If spurious back-reflected light is present, with high enough irradiance, Bragg scattering would disguise any superradiant Rayleigh scattering signal. Both effects would result in the same, detectable signal, being a momentum separation of the atoms in the BEC into one state having the original momentum, and another which gained two photon recoils.

In an experiment, presented in paper IV, a one-dimensional lattice set-up, similar to the one used for Bragg scattering in section 4.7.2, was used to verify the absence of spurious back-reflected light in superradiant Rayleigh scattering experiments.

The main difference between the alignment experiment of section 4.7.2, and the verification of the superradiant Rayleigh scattering experiment, is in the power balance between the two beams of a moving one-dimensional optical lattice. By lowering the irradiance of one of the beams (the seed), by a factor of
$10^{-3}$ to $10^{-5}$, compared to the pump laser beam, the onset of Bragg scattering could be detected.

The characteristics that determined the onset of Bragg reflection was a Rabi oscillation between the original momentum state, and the other state having gained two photon recoils. For a correct alignment of the pump laser beam, causing no back reflections in the experimental set-up, the Rabi oscillations ceased to appear when the seed laser beam had low enough irradiance. Blocking the seed laser beam in such an experiment, a recoiled atomic cloud, was associated with superradiant Rayleigh scattering. In the case of persistent Rabi oscillations, even with the seed beam completely blocked, realignment of the pump beam direction was necessary, as back reflections from the experimental set-up was present.

4.7.4 Rough alignment by displacement

For tightly focused lattice beams, where the beam waist is of the same order of magnitude as the diameter of the BEC, alignment of the intersection between the beams and the BEC becomes more sensitive than for larger beams. In the set-up in Mainz, where the lattice beams were aligned along the Cartesian axes, the effect of attractive and repulsive forces from the lattice could be followed by imaging along the three axes.

A red detuned beam will, as shown in section 3.1, attract atoms. This effect is used for alignment by recording the movement of the BEC as a function of lattice beam alignment. The lattice beams are applied to a BEC, one by one, always blocking the retro-reflection. The displacement of the BEC position is recorded with absorption imaging, with a CCD camera in the lattice direction. Minimizing the movement of the BEC, caused by the beam gives an indication of the overlap of the beam with the BEC. The retro-reflection can then be overlapped with the lattice beam on a point far back in the experimental set-up.

For a blue detuned lattice, a similar procedure is performed. The forces will however be repulsive, and instead of a displacement of the cloud, the optimized signal will show a blowup of the BEC. The repulsion will, for intense enough beams, make the cloud expand. If the beam is slightly out of alignment, the cloud expands asymmetrically away from the beam. The retro-reflected beam is blocked while detecting the expansion, and it is aligned on-top of the incoming beam by overlapping on a point far away.

4.7.5 Fine alignment by higher band excitation

In the experiments of paper VI, the lattice used was deep enough to enter the Mott insulating phase. The basis of Wannier functions instead of Bloch functions require another method for fine alignment, rather than that presented in section 4.7.2. Instead of measuring Rabi oscillations, the atomic sample is excited to higher bands, and the excitation probability is monitored [73, 74].

A principle sketch of the higher band excitations procedure is shown in figure 4.10. The optical lattice is adiabatically ramped up to $V_0$, the value which is to be verified. An amplitude modulation of a variable frequency is added to the
Figure 4.10: Higher bands are excited by modulating the lattice potential height for a time $t_{\text{mod}}$.

potential for a time $t_{\text{mod}}$, followed by a rethermalization time before the lattice is ramped down. The modulation will create two frequency sidebands, allowing a frequency selective Raman transition to the second excited band. When the frequency of the modulation is tuned to resonance for the excitation, energy will be added to the system. Detection of the excitation is thus measured by measuring the size of the atomic cloud by time of flight. The cloud size as a function of modulation frequency, can be fitted to a Lorentzian distribution, where the peak position is recorded as the frequency of the resonant transition to the higher band. From this value, the lattice potential depth can be extracted, using band structure calculations.
Chapter 5

Detection of unstable regimes for a BEC

Using a BEC as a probe for experiments with optical lattice potentials have become an increasingly strong subfield in the field of cold atoms and in BEC research [7]. The coherence properties of the BEC, as well as the possibility to address a narrow momentum state of the BEC in the periodic potential, have triggered a range of experimental ideas. Theoretical models, such as the band structure picture, where the BEC can be described as a Bloch state, have been adapted from solid state physics by introducing only slight modifications.

In certain regimes, the standard theoretical models will however fail due to the inherent non-linearity of a BEC. This non-linear term, caused by the s-wave scattering, lets the different atoms interact with each other without an external medium, which would be needed for non-linear interactions between photons. The non-linear term can in many cases be neglected, or by expanding the BEC before the lattice experiment, it can be reduced enough in order to become unimportant.

The experiments presented in this chapter, and in papers I, II and III, provide deeper knowledge into the effects caused by this non-linearity. The experiments dealt with the topics of instabilities, which caused the BEC to break down, either by being heated, or by chaotic growth of additional states of the system. A theoretical model has been introduced for comparison with the experiments [36]. These experiments have also been presented in [50, 75].

5.1 Experimental model

The system under scrutiny consisted of a three-dimensional anisotropic harmonic potential, with cylindrical symmetry, where the axial trapping frequency was lower than the radial (cigar shaped potential). Added to this potential was a one-dimensional periodic potential, with a periodicity along the axial direction.
of the cigar potential. The periodic potential was moving with a controllable velocity.

In the experiment, a BEC was introduced in a selected quasimomentum state in any band of the potential. The evolution of this cloud in the potential was detected and the depletion of the BEC as a function of initial state and time spent in the trap could be compared with models for energetic and dynamical instability.

5.2 Experiments on energetic and dynamical instabilities

The experiments were performed using one of the BEC apparatuses in Florence. For a more detailed information about this apparatus, references are made to [50, 63]. The optical lattice set-up used is presented in detail in [76]. A selection of other related experiments that used the same apparatus is [50, 77, 78].

5.2.1 Preparing a BEC in a Bloch state

In the experiment, cigar shaped BECs, magnetically trapped with aspect ratios $\omega_r/\omega_z = 10$, were created. A typical sample had $3 \times 10^5$ atoms of $^{87}$Rb, trapped in the $|F = 1, M_F = -1\rangle$ ground state. While being magnetically trapped, the cloud density was high enough for the non-linear term, $(g|\psi(r, t)|^2)$, in equation 2.20, to be of importance.

An optical lattice, overlapping a periodic potential with the magnetic trap in the axial ($z$) direction, was ramped up adiabatically. Due to the possibility to control the frequency difference between the two laser beams used for the lattice, the BEC could have a well determined velocity, $v_L$, in the optical lattice frame of reference (see section 4.7).

When the optical lattice was ramped up adiabatically, the atomic momentum, $mv_L$, was transformed into a quasimomentum and a band index of the lattice, according to the theory of section 3.2. This loading method was examined more in detail in [76], and it was shown to give precise results when loading into states far away from the Brillouin zone edges.

When the lattice was applied, a bandgap opened up at the edge of the Brillouin zones. The energy of the system did no longer vary with the parabolic shape of a free particle, when changing the quasimomentum. The relation between quasimomentum and the BEC group velocity, $v_B$, became more complicated, as earlier stated in equation 3.16. Ramping up the lattice adiabatically [79] would however conserve the quasimomentum, loaded from the free particle state.

The difference between $v_L$ and $v_B$ resulted in a movement of the BEC in the magnetic trap. The presence of the magnetic trap led to an external restoring force, accelerating the cloud, and thus an acceleration according to equation 3.18. Close to the Brillouin zone edges, the motion ceased to be oscillatory, and the BEC was accelerated away, thus making experiments in the vicinity of the zone
edges a difficult task. In the parameter range where measurements were possible, the effect of changing quasimomentum \( q \), was treated as an uncertainty in \( q \).

### 5.2.2 Measurement procedure

Through the loading procedure the BEC was prepared into a precise quasimomentum state of the system. The height of the potential \( V_{1D} \) was also selected, with high precision, and the magnetic trap was left on in order to maintain high density. The experimental apparatus was stable enough to provide good reproducibility of the initial conditions; an important issue as a new BEC was created for each measurement point.

A series of experiments could thus be performed, letting the BEC evolve for a variable time in the combined potential of the magnetic trap and the one-dimensional optical lattice. The time spent in the lattice ranged from milliseconds to seconds.

At the end of the experiment, the lattice was ramped down adiabatically, followed by the magnetic trap being switched off. The number of atoms remaining in the BEC was detected by letting the cloud expand freely for 28 ms followed by an absorption imaging sequence, see section 4.6.

The lifetime of the BEC, for various optical lattice potential heights and initial system states, could be recorded. Destructive effects from thermal, non-condensed atoms could be examined by either maintaining the evaporative cooling during the lattice phase, or by turning it off before the BEC was loaded into the lattice. The lifetime of the BEC could also be varied by setting the evaporation to different final frequencies during the experiment, and thus varying the condensed fraction of the sample.

### 5.2.3 Results

The results displayed in figures 5.1(a) and (b) show the rate of atom losse from the BEC. This loss rate is defined as the reciprocal lifetime of the BEC in the combined optical lattice and magnetic trap potential. The experiment was performed with a nearly pure BEC, keeping the evaporative cooling on during the entire lattice sequence, to ensure that any thermal component of the cloud was suppressed.

As stated in section 5.2.1, the loaded quasimomentum state is not as pure around the Brillouin zone edges, as it is far inside the zone, reducing the possibility to reproduce experimental data at the edge. The lattice potential height, \( V_{1D} \), affects the band structure that sets the size of the bandgap, leading to larger zones without data in figure 5.1(b), where \( V_{1D} = 1.15 \, E_{\text{rec}} \), than in (a) where it is \( 0.2 \, E_{\text{rec}} \).

In figures 5.1(c) and (d) the growth rate of the most unstable mode, due to dynamical instability is shown as a comparison to (a) and (b) respectively. Due to differences in the simulated system and the actual experiment, a direct comparison is not possible in this case. However, the similarity in shape between
Figure 5.1: (a) and (b): Experimental loss rates (reciprocal lifetimes) of atoms for a BEC loaded into an optical lattice, measured for various $q$ for two lattice depths $V_{1D} = 0.2 E_{rec}$ and $V_{1D} = 1.15 E_{rec}$. (c) and (d): Theoretically predicted growth rate for the most dynamically unstable mode computed with methods from [36]. The lines were added as guides to the eye.

the theoretical curves and the experimental data points suggests that the onset of dynamical instability is detected.

For the theoretical study, equation 2.20 has been solved using the non-polynomial Schrödinger equation (NPSE) [36]. This method gives a more reliable result than solving a pure one-dimensional problem. It is also less demanding when it comes to computer resources, compared to solving the full three-dimensional Schrödinger equation.

As dynamical instability is manifested by exponential growth of new modes (with other quasimomenta), the difference between a stable and an unstable system can be seen directly in the recorded time of flight images. This is shown in figure 5.2(a), for an optical lattice with $V_{1D} = 1.15 E_{rec}$, for an initial state being stable ($q = 0.40 \hbar k$), and a dynamically unstable initial state ($q = 0.55 \hbar k$). In the stable case, the condensate shape stays smooth for optical lattice interaction
times even in the range of seconds. For the unstable case, interference patterns, caused by the presence of several quasimomentum states appear already after a very short interaction time of a couple of milliseconds.

Figure 5.2: Density profiles after time of flight detection. In (a), the BEC have been loaded into two different states, where \( q = 0.4 \hbar k \) is dynamically stable, and \( q = 0.55 \hbar k \) is dynamically unstable. The instability causes growth of additional momentum states, visible as interference fringes after time of flight. The time spent in the lattice before release is noted under each image. (b) is an illustration of the relaxation of dynamically unstable modes after switching off an optical lattice. The lattice has been on for 5 ms, and the time noted under each image is the relaxation time in the magnetic trap, after the lattice have been turned off.

In figure 5.2(b), the BEC had been left to relax in the magnetic trap after the introduction of unstable modes. The image shows that the unstable modes will relax back into a uniform BEC after a time, in the range of seconds.

For a mixed cloud, containing both a thermal component and a BEC, the sample depletes much quicker than for a pure BEC. This is shown in figure 5.3, where two different evaporative cooling ramps were used in the experiment. In the upper part of the figure, evaporative cooling was applied to produce a pure BEC before the sample was loaded into an optical lattice with potential height \( V_{1D} = 0.2 E_{rec} \). The BEC was loaded into different quasimomentum states, all within the dynamically stable region. After 15 s, there was still a large fraction of atoms left in the BEC sample.

In the case of a mixed cloud, energetic instability could be triggered by the thermal atoms being present. The mixed cloud was depleted for quasimomentum states that are stable for a pure BEC. Such depletion of the cloud could also be detected if the evaporative cooling was turned off while the BEC interacted with the optical lattice. The evaporation effectively removed all traces of heated atoms that could have masked the signal from the dynamical instability.
Figure 5.3: Density profiles for two different condensed fractions, achieved by stopping the radio frequency ramp of the evaporative cooling at different values. The atoms were loaded with different quasimomenta into an optical lattice with $V_{1D} = 0.2 \, E_{\text{rec}}$. The lattice was applied for 15 s. A thermal fraction induces losses due to energetic instability, whereas the pure BEC stays unaffected by the lattice.

### 5.3 Conclusions

In a series of three papers, instabilities for BEC in optical lattices have been reported. Different detection techniques, such as loss rates and direct observation of interference fringes, have been used, and the results have successfully been described by theoretical models.

Paper I is a detailed study for the time scales of dynamical instability of a BEC in a one-dimensional optical lattice. A more extensive study of the onset of both energetic and dynamical instability, have been presented in paper II, where also theory and experiments are presented more in detail. As a comparison between the linear regime, where the BEC is expanded in order to reduce its density before interacting with the lattice, paper III reviews a series of experiments ranging from the examination of band structure to dynamical and energetic instabilities.

This study of instabilities in optical lattices clarifies limitations of the direct use of the band structure picture from solid state physics. The results can both be used in experiments where the effect should be avoided, as well as for a further study of the phenomena themselves. The research field could benefit from even deeper studies of the phenomena, where the onset of an instability could become a useful measurement tool in the laboratory. A deeper knowledge about the onset of energetic instability, could for instance be used as a probe for the thermal fraction of a mixed cloud of cold thermal atoms and a BEC.
Chapter 6

Double well potentials

An isolated double well potential, loaded with only one or two atoms, could be modeled by a simplified theoretical picture, where few possible energy states are involved. The system can be seen as a miniaturized optical lattice, including only two wells, where the tunneling and repulsion effects can be studied. In an experiment containing more than two wells, the results of individual atom tunneling is often acquired by extrapolation from effects on the entire system state in all wells. To study the miniaturized lattice, a theoretical description for double wells containing one or two atoms, based on methods inspired by solid state physics, was presented in section 3.5. The theory includes both non-interacting atoms, and atoms bound by repulsive interactions. For the latter, one atom out of a pair can be prevented from tunneling to a neighboring empty site by the repulsive interaction with the other atom of the pair. The tunneling of only one atom would reduce the repulsion, and thereby the energy of the system would not be conserved during a single atom tunneling event. An atom pair can however tunnel as a whole, without modifying the total energy. In the experiment presented in this chapter, and in paper VI, this effect is studied in detail, for different tunneling strengths and atom-atom repulsions of the atoms in double wells created by loading a BEC in an optical lattice.

From another point of view, double wells can also be seen as a Josephson tunneling junctions [80]. Such a model is used for some of the data analysis, and is described more in detail in [81], and in references therein.

6.1 Experimental Model

The experimental system was an array of singly and doubly occupied double wells. All wells were prepared in the same way and at the same time. The atoms started tunneling between the two wells of each double well simultaneously, when the experiment was initiated. A measurement of the system was instantaneously made on all double wells, adding up to one single signal.

In an initiation step, the state $|L\rangle$ and/or $|LL\rangle$ was prepared (see equa-
tion 3.50). For technical reasons, while it was possible to prepare a system containing only $|L\rangle$ sites, measurements on $|LL\rangle$ always contained a fraction of singly occupied double wells having $|L\rangle$ occupation.

During a variable tunneling time, the physics of the Hamiltonians 3.59 and/or 3.62 was tested by decreasing the potential barrier between the two wells in each double well. At the end of the tunneling sequence, the state of the system was frozen by increasing the barrier. This was followed by a readout of the phase difference between the wells, and the number of atoms being in the right and left well respectively. The experiment was cycled for different tunneling times, and tunneling and repulsion parameters.

6.2 Correlated pair tunneling experiment

The preparation of the double well optical lattice had many steps in common with experiments on Mott insulators, presented more in detail in [39, 42]. The same experimental apparatus was used for the creation of a BEC of $^{87}$Rb in the $|F = 1, M_F = -1\rangle$ state. The optical lattice ramping sequence for the double well lattice was somewhat different from the Mott insulator experiment.

To describe all the steps included in the experiment is beyond the scope of this thesis. A more detailed description can be found in [43, 81]. Described below are the main parts needed to prepare a dynamic double well potential suitable for the experiment.

6.2.1 Preparation of the initial state

The desired experimental condition was double well lattices in one Cartesian direction, created by superimposing a long and a short lattice, and deep single well lattices along the orthogonal axes, see sections 3.5 and 4.7. The double well potential created should have one or two atoms loaded into the left side of each double well.

Starting from the creation of the BEC, all four lattice potentials were ramped up in 160 ms, using an adiabatic ramp [82]. The potential barriers in the orthogonal directions were large enough to prevent tunneling in those directions. In the direction of the double well, all tunneling processes to adjacent wells were blocked by the long period lattice, whereas tunneling within one double well was still possible by keeping the short period lattice at a moderate height, which created a low barrier inside the double well. The phase difference between the long and short wavelength lattices was kept such that a symmetric double well configuration was maintained, see figure 6.1(a). The number of atoms in the original BEC was tuned such that the production of states having two atoms per double well was most likely (one atom in each well). As in the case of the Mott insulator experiments [39], the site occupancy was larger in the center of the sample, leading to a situation where the doubly occupied double wells in the center were surrounded by singly occupied double wells in the outer parts of the
system. This effect is caused by the harmonic potential, extending over many double wells, and being deepest in the center of the atomic sample.

Going from homogeneously distributed atoms to $|LL\rangle$ was done using the following procedure: By adiabatically removing the shorter wavelength lattice, the barrier in the double well potential was eliminated, and the atoms were combined in single wells having large periods, see figure 6.1(b). The phase difference between the lattices was changed, followed by an increase of the irradiance of the short lattice, as shown in figure 6.1(c). Due to the changed phase, the combined potential then became a single well. When ramped up, the blue lattice irradiance was high enough to suppress tunneling for a symmetric configuration of the double wells.

For measurements with single occupancy of the double well, all doubly occupied sites were emptied by a filtering sequence, which will be explained shortly. After this filtering sequence, the initiation sequence was again common for both single atom, and two atom experiments.

The phase difference between the lattice beams was again changed to the symmetric double well configuration. As illustrated in figure 6.1(d), the atoms followed the potential in which they were merged in the earlier step. The final configuration was an empty right well, and a left well occupied by one or two atoms, which depended on the localization of the well in the system, and it also depended on if the filtering was used or not. The potential barrier between the two wells of each double well was kept large until the experiment was started. This ensured that the atoms remained in the left well.

![Figure 6.1: The preparation steps for the double well system. The black lines outline the local potential; the red illustrate of energy levels (not to scale). Atoms are shown in blue. (a) Atoms loaded into a symmetric double well. The condensate size was tuned to make two atoms per double well most probable. In the outer region there were sites with one atom per double well. (b) Removing the short lattice merged the wells. (c) The short lattice was ramped up again with a non-centered phase, leaving both atoms in the left well. (d) The phase was adjusted to reform symmetric double wells.](image)

**Filtering**

Tunneling properties of singly, as well as of doubly occupied double wells, were investigated in the experiment. With the preparation sequence described above, the initial system would contain both types of systems, which would make analysis of the results difficult. To improve on this point, a filtering sequence was
used to separate the effect of singly occupied double wells from the other results. The filtering sequence emptied all sites occupying an atom pair.

The atoms, initially in the state $|F = 1, M_F = -1\rangle$, were transferred to the state $|F = 2, M_F = 0\rangle$ using a microwave adiabatic rapid passage [14, 83]. Atoms in doubly occupied sites of the lattice were affected by spin changing collisions, where the projection of the spin will change, while the sum was kept constant at $\sum M_F = 0$ [84, 85]. The spin changing collisions released enough energy to eject the atoms from the trap. After 40 ms hold time, this left atoms only in the singly occupied sites, as they were not affected by any collisions. Transferring the atoms back to the $|F = 1, M_F = -1\rangle$ state brought the system back to the conditions prior to the filtering sequence, except for all doubly occupied sites having been emptied.

In the cases where doubly occupied sites were to be examined, the microwave pulse was not turned on. To avoid to introduce systematic errors, all the lattice manipulations used during the filtering sequence were also made for the non-filtered sequence.

A more detailed description of the underlying processes can be found in [86], and in references therein.

6.2.2 Tunneling

When the initial state has been successfully prepared, the tunneling sequence could be initiated by lowering the barrier in the double well, which was accomplished by decreasing the short lattice power, see figure 6.2.

The barrier was lowered by an exponential ramp, in order to avoid excitations of the system. Even though the ramping was made in just 200 $\mu$s, it was slow enough for the tunneling process to initiate before the barrier had reached the desired height. This caused an uncertainty in the knowledge of the starting time of the tunneling evolution.

By letting the system evolve for a variable tunneling time $t_{\text{tun}}$, and then raising the barrier in order to freeze out any further tunneling, the dynamics of both single atoms and of atom pairs could be studied. All double wells in the system were studied during each experimental cycle. If the filtering was used, only singly occupied systems were studied, otherwise both singly and doubly occupied systems were studied in parallel.

Figure 6.2: The tunneling started when the short optical lattice was lowered. The local potential was then changed from the dashed configuration to the solid black line. Red lines illustrate energy levels (not to scale) and atoms are shown in blue.
6.2.3 Detection techniques

Two different methods were used for detection of the properties of the atomic wave packets in the double wells. To measure the difference in phase between the two sides in each well, an interference technique was used. The average position of the atoms in each double well was measured by a combined excitation and Brillouin zone mapping technique.

**Interference measurement**

To gain basic knowledge about the state of the double well systems, a time of flight technique was used. The optical lattice was turned off fast, and the atoms were left to expand for a time $t_{\text{tof}}$ in the millisecond regime. For a coherent sample, such as the BEC, interference fringes from the overlapping wave packets in different lattice sites could be detected as distinct momentum components of the expanding cloud. For an incoherent sample, such as a Mott insulating state, the different wave packets also interfered, but as there was no fixed phase relation between the wells, any interference pattern would average out due to the large amount of atoms, and only a Gaussian distribution would be detected.

For the double well system, an intermediate regime was achieved. The atoms inside each double well formed a coherent sample in miniature, which lead to interference fringes. The signal from one well was small, and would be difficult to detect in an experiment. Adjacent wells, were however not coherent, which lead to an overall signal from the sample composed of an addition of all double well signals. Since all double wells were affected by the same Hamiltonian during the experiment, they would all share the same double well signal, adding up to a strong composite signal that revealed information about the double well states.

The state of a single double well can be written as

$$\Psi_{\text{DW}} = \Psi_L \exp\{i\phi_L\} + \Psi_R \exp\{i\phi_R\},$$

where $\Psi_L, R$ contain information, about the left and right states respectively, including the amplitude of the states. For a released atomic cloud, both $\Psi_L$ and $\Psi_R$ had Gaussian envelopes, centered in their respective wells. The sizes of the Gaussian envelopes increased during expansion when the cloud was released. Within a short time, the distance between the wells had become small compared to the size of the envelope, and a common Gaussian envelope could be used.

The detected signal was dependent on the density of the expanding cloud, thus being:

$$\rho_{\text{O.D.}}(r) = \sum_i |\Psi_{\text{DW}}|^2_i = \sum_i |\Psi_L \exp\{i\phi_L\} + \Psi_R \exp\{i\phi_R\}|^2_i$$

$$= \sum_i [ |\Psi_L|^2 + |\Psi_R|^2 + 2 |\Psi_L||\Psi_R| \cos(\phi_L - \phi_R) ].$$

Time of flight images of the cloud yielded two-dimensional density distributions as shown in figure 6.3, where the third dimension was integrated out during
the exposure. Adding all data points orthogonal to the interfering direction led to a one-dimensional distribution, governed by a Gaussian envelope and an oscillating term. This signal was fitted to

![Image of typical interference data from the experiment.](image)

\[ \rho_{\text{O.D.}}(x) = B + A \left[ 1 + \mathcal{V} \cos \left( \frac{x - x_0}{\Lambda} + \phi_{\text{sp}} \right) \right] \exp \left\{ -\frac{(x^2 - x_0^2)}{s_x^2} \right\}, \quad (6.3) \]

where different double well configurations led to different fringe visibilities \( \mathcal{V} \), and spatial phases \( \phi_{\text{sp}} \) [87]. The amplitude \( A \), the size \( s_x \), and the center of the envelope \( x_0 \) were mainly dependent on the overall size and position of the BEC. The background \( B \) was an experimental artifact, \( \Lambda \) was the fringe spacing, and \( x_0 \) was the center of the cloud.

**Brillouin zone mapping**

When the tunneling sequence was ended, all further inter-well motion was stopped by ramping up the potential barrier between the two wells. Counting the number of atoms located on each side of the barrier, was performed by dumping the population of the left well into a higher band [87], and then detecting by Brillouin zone mapping.

In practice this was done by adiabatically tilting the lattice by the amount

\[ -\Delta_{\text{tilt}} = E_{\text{eig}} \left( 3^{\text{rd}} \text{ band} \right) - E_{\text{eig}} \left( 1^{\text{st}} \text{ band} \right), \quad (6.4) \]

by slightly tuning the phase \( \phi_{\text{short}} \) of the double well lattices (see section 3.5), which lifted the atoms in the left well enough to give them the same energy as the third band of the right well, see figure 6.4. By slowly ramping down the potential barrier of the double well, the atoms originally in the left well would all transfer to the third band of a single well system with the long lattice periodicity. The atoms originally in the right well, stayed in the lowest (first) band of this single well potential. The same procedure happened in all double wells in parallel.

Adiabatically ramping down an optical lattice preserved the quasimomentum. When the lattice had reached zero amplitude, the different bands were mapped.
Figure 6.4: Manipulations of the double well for the dumping technique. (a) An atom population originally to the left is marked with a green, and to the right by a blue dot. (b) Lifting the left well, first band, to the same height as the right well third band, by tilting the potential. (c) Ramping down the short wavelength lattice, merged the two wells, leaving the green population in the third excited band.

onto different Brillouin zones, as shown in figure 6.5 [79, 88, 89]. The total number of atoms in right wells, \( N_R \), was recorded by counting the number of atoms of the first Brillouin zone, whereas the number of atoms in the third zone gave the total number of atoms originally in the left wells, \( N_L \).

Figure 6.5: Typical image acquired from a dumping measurement using Brillouin zone mapping. The middle section shows atoms from the right well, occupying the first Brillouin zone. The outer clouds were atoms from the left well, which have been excited to the third Brillouin zone.

The average position inside a double well could then be computed by

\[
\langle x_{\text{pos}} \rangle = \frac{N_R - N_L}{N_R + N_L}. \tag{6.5}
\]

Detection of the populations in the different Brillouin zones was made with time of flight absorption imaging (see section 4.6). Each Brillouin zone occupied its part of the momentum space, given by the momentum in the extended zone scheme of figure 3.1. When dumping the atoms from the left well into higher bands, the third band was chosen to improve signal to noise in the measurements. Since all atoms from the right wells had momenta \( p_R \leq \hbar k \) and the left well atoms had their momenta \( 2\hbar k \leq p_L \leq 3\hbar k \), they were well separated after some time of flight. Excitation to adjacent zones would increase counting difficulties at the zone boundary \( p = \hbar k \).

The dumping sequence was calibrated in order to avoid systematic effects from collisions during time of flight, and from excitations of other bands (specially when the atoms were well localized on one side of the double well), see further [81].
6.2.4 Results

The central results of the measurements are presented in figures 6.6 and 6.7. In figure 6.6, some examples of tunneling dynamics is presented. For the weak interaction case (figures 6.6a and b), the repulsion between atoms was of the same magnitude as the tunneling ($J_{LR}/U_L = 1.5$). Therefore, the atoms were allowed to tunnel independently of each other. For singly occupied sites, the tunneling behavior is in figure 6.6a, and it was a single frequency oscillation, with an amplitude damping term, in good agreement with the theory of section 3.5.3.

For the doubly occupied sites, presented in figure 6.6b, two processes were

![Figure 6.6: Tunneling dynamics for different experimental conditions. Black dots are single atom tunneling positions, phases and visibilities. Red dots are the position of atom pairs. Blue dots are the phases and visibilities for an atom pair. Two experimental regimes are shown: weakly interacting atoms ($J_{LR}/U_L = 1.5$), (a, b) and strongly interacting atoms ($J_{LR}/U_L = 0.2$), (c-f). The lines show fits to the data, according to methods presented in [81].](image-url)

...
Figure 6.7: The measured tunneling rates as a function of the short lattice depth, which defined the barrier between the two wells in the double well system. Bare tunneling was the result for the initial state being $|L\rangle$, and was quickly reduced as the potential barrier was raised. The bare tunneling was compensated for atom pairs in double wells, which gave a $3 - 10\%$ increase in tunneling rate [81]. First order tunneling was the off-resonant tunneling for one atom out of an initial state $|LL\rangle$, which saturated at $U_L$ for large potential barriers. Second-order tunneling was the correlated tunneling of two atoms as a pair, initially loaded into $|LL\rangle$. The dashed lines were calculated from band structure calculations, including $2\%$ lattice depth uncertainties.

In the opposite regime, where the onsite interaction was larger than the tunneling $J_{LR}/U_L = 0.2$, the system behaved differently. If figure 6.6c, the dynamics of singly occupied sites is shown. The process showed the same behavior as for the weak interaction regime in figure 6.6a, but the tunneling frequency was now lower. This can also be understood from the theory presented in section 3.5.3, where a lower tunneling rate, lead to a longer period of the oscillation. In figure 6.7, the bare tunneling rate, $J_{LR}$ is presented as a function of the height of the potential barrier between the two wells of the double well.

The dynamics of the doubly occupied sites is presented in figure 6.6d. Compared to the case presented in figure 6.6b, the atom pairs tunnelled in a correlated manner, having a slow oscillatory motion governed by $J_{eff}$. On top of this oscillation, there was a fast oscillation of broken pair tunneling, where only one atom out of the pair tunnelled. This process did however have a much lower amplitude, both compared to the case of figure 6.6b, and compared to the correlated pair tunneling amplitude in figure 6.6d.

In figure 6.7, the tunneling rates of single atoms (first-order tunneling) and
correlated pairs (second-order tunneling) have been presented as a function of the potential barrier in the double well.

The visibility and phase, measured with the interference method are presented in figures 6.6e and f, for the case of $J_{LR}/U_L = 0.2$. For the single particle tunneling (black dots), the phase made jumps between $\pm \pi/2$ at the turning points, where the tunneling direction was reversed. These phase jumps came from the difference in phase between the contributions from the two wells (sine and cosine in equation 3.61). The visibility was strongest when the wavefunction was equally distributed between the two wells. When the atom had completely tunneled to one of the sides, the interference pattern disappeared, and the detected distribution had the same Gaussian shape as in the case of a Mott insulator. As the contrast goes to zero, the phase acquired from the fit of the data to equation 6.3 became ambiguous, explaining the noise at these points in figure 6.6e.

Atom pair phase and visibility are also shown in figures 6.6e and f. The interference pattern was no longer as clear as for the singly occupied sites. This was due to the more complicated description of the total wavefunction of the state. The data sets for the atom pairs were fitted to a model of a quantized Josephson Hamiltonian, described more in detail in [81].

6.3 Conditional tunneling experiment

In section 3.5.5, the effect of tilted double wells was introduced. Experimentally this has been studied by shifting the phase difference between the long and the short lattice of the double well, thereby introducing a tilt $\Delta_{\text{tilt}}$. The tunneling behavior for different tilts was examined during an experiment, and the results are presented in figure 6.8.

For singly occupied sites, a tilted potential put the tunneling process out of resonance due to the different energies of the right and left site. This can be seen for the black dots in figure 6.8, where there was a resonance in tunneling amplitude for the non-tilted case, $\Delta_{\text{tilt}} = 0$.

Doubly occupied sites had two resonances; one for correlated pair tunneling, which was centered around $\Delta_{\text{tilt}} = 0$ (red dots); and another centered around $\Delta_{\text{tilt}} = U_L$ (blue dots), where one atom from the pair tunneled resonantly to the other well. Since the resonance only appeared when two atoms initially were present in the same well, the effect was called conditional tunneling. The atoms were however indistinguishable, and it was therefore not possible to tell which one out of a pair that had tunneled.

6.4 Conclusions

The double well system presented here makes it possible to study tunneling phenomena in a simplified potential. It was possible to select the initial state of the system as pairs of atoms or single atom loadings. Tuning the parameters of the potential, it was possible to go from single particle tunneling, to corre-
Figure 6.8: Tunneling amplitude (a), extracted from fitting a damped sine to the average atom position, and tunneling period (b), for a tilted double well potential for strongly interacting atoms. One atom tunneling out of a repulsively bound pair became resonant when $\Delta_{\text{tilt}} = U_L$ (red). Single atom tunneling (black) and correlated tunneling of pairs (blue) became resonant for $\Delta_{\text{tilt}} = 0$, thus being the same experimental conditions as presented in section 6.2.

lated tunneling of atom pairs. The potential could also include a tilt, where a transistor-like behavior could be achieved.

The experiment was performed with an apparatus that proved to be both flexible and stable. The stability was essential for the possibility to measure long sequences of tunneling processes, where different tunneling times were to be tested on an otherwise unchanged potential. Changing the lattice parameters during the run would have made the conditions for atom tunneling and atom-atom repulsion different, leading to a tunneling sequence that would be difficult to predict.
Chapter 7

Phase transition with dimensional dependence in an optical lattice

Changing the dimensionality of a system does not necessarily preserve the physical laws as they are formulated for a three-dimensional system. Some phases, such as the BEC do not exist in infinitely long one-dimensional systems, and in two dimensions it only exist at $T = 0$ [10]. If a system is made finite, these phases reappear, but the phase transitions are smeared out into cross-overs.

In the theoretical study presented here, an optical lattice is the test-bench for the crossover between on one hand superfluidity along only one of the three dimensions, and on the other hand along two of the dimensions. Tunneling has been “frozen out” along one or two dimensions, by increasing lattice potential barriers individually along the three Cartesian directions. The simulated system was finite, and the role of the size of the system could therefore be determined using finite size scaling.

The simulations presented in this chapter are the basis of papers VII and VIII. Complementary information can also be found in [90, 91], and references therein.

7.1 Theoretical Model

The system under consideration was a two-dimensional array of potential wells, where atoms could tunnel between wells in the array. The dynamics was modeled by selecting the ratio between tunneling and atom-atom repulsion, $J/U$, for the two array dimensions $x$ and $y$. For the $x$-direction the ratio was chosen large enough to allow superfluidity in the system, whereas in the $y$-direction it could be varied over a range where the system went from superfluid to Mott-insulating behavior. In figure 7.1, the studied region has been marked with a double arrow.
Figure 7.1: Phase diagram for the two-dimensional system under examination. As described in chapter 3; when the ratio between tunneling and atom-atom repulsion is lowered, the system crosses a transition from a superfluid (here 2D SF) to a Mott insulator (2D MI). Here, another phase transition, marked with a double arrow, between 2D SF and 1D MI was studied, where the latter phase was superfluid along one direction only.

7.1.1 The anisotropic Bose-Hubbard model

The simulations were based on the anisotropic Bose-Hubbard model of section 3.6. All tunneling along the \( z \)-axis was neglected, and the \( \hat{H}_J \) part of the Hamiltonian in equation 3.38 only included the tunneling energies \( J_x \) and \( J_y \). The chemical potential was tuned in order to get an average unit filling of the wells in the simulated system.

7.1.2 Quantum Monte Carlo simulation

To simulate the system, a quantum Monte Carlo (MC) method was used. For the results of paper VII, this method has been described in [90], and for paper VIII a similar code was used, with more details in [91].

The MC simulations were made with the stochastic series expansion algorithm [92, 93], on a grid with size \( L_x \times L_y \), having periodic boundary conditions. Care was taken to ensure that no states with higher energy were excited, by keeping the thermal energy of the system low. The number of available states was kept high enough in order to ensure convergence.

From the MC simulation, numerical results for several physical properties were attained. Most widely used for the evaluation of the properties of the system was the superfluid density. This could be computed from the number of cycles made by a boson in the simulated periodic system, \( i.e., \) the winding number \( W \). The superfluid density needed to be correctly scaled with the size of the system in order to become meaningful. Doubling the path in the direction of \( W \), requires a doubling of the number of cycles made to make a comparison meaningful. Also, reducing the width of the system increases the superfluid density.
Taken along the weakly coupled \( y \) direction, the superfluid density was thus defined as [94]

\[
\rho_s = \frac{\langle W_y^2 \rangle}{L_y \beta}.
\]  

(7.1)

The compressibility, being the variance of the density in the superfluid tubes, given by

\[
\Delta N_{\text{tube}}^2 = \langle N_{\text{tube}}^2 \rangle - \langle N_{\text{tube}} \rangle^2,
\]  

(7.2)

and the boson-boson correlation function, between sites \( i \) and \( j \),

\[
\left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle,
\]  

(7.3)

could also be computed in the MC simulations. In figure 7.2(a), a series of data for \( \rho_s \) is shown for various system sizes. When the tunneling rate was tuned to smaller values, there was a sudden drop in \( \rho_s \), due to a localization effect for the bosons. In the figure, it should be noted that the position of the ”knee”, where the drop starts, depends on the size of the simulated system.

By scaling the ratio \( J_y/U \) with the size of the system, the position of the knee could be made to collapse to the same value for all system sizes. In figure 7.2(b), the three quantities acquired from the MC simulation are shown for a set of simulation parameters, including a finite size scaling, that is motivated in the next section.

### 7.2 Localization of the phase transition

The phase here called 1D-MI is in various references, e.g. [45, 95], described as TLL, as already mentioned in section 3.6. In TLL theory, the positions of bosons in a one-dimensional system have not been fixed at lattice sites, but are allowed to fluctuate around an average position. Using this model, it was shown [96], that a one-dimensional TLL could be characterized by two parameters, being the sound velocity \( v_s \), and the TLL parameter

\[
K = \frac{\hbar k \rho_f}{mv_s},
\]  

(7.4)

where the average number of bosons per lattice site, \textit{i.e.} the filling factor, is denoted \( \rho_f \). For bosons in a lattice, with only on-site interactions, it was also shown that

\[
2 \leq K \leq \infty,
\]  

(7.5)

in the superfluid phase. For lower values of \( K \), the system was shown to enter a MI phase.

An important property of the TLL, which has been further examined both in paper VII and VIII, is the algebraic decay of the boson-boson correlations;

\[
\left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle \propto |\mathbf{r}_i - \mathbf{r}_j|^{-1/2K}.
\]  

(7.6)
Figure 7.2: (a) Superfluid density, according to equation 7.1, from quantum Monte Carlo simulations [91]. The size of the simulated system was varied according to the legend. The superfluid density has a drop at a system-specific ratio $J_y/U$. (b) By scaling the ratio $J_y/U$ with the size of the system, the points where $\rho_s$, $\langle \hat{b}_i \hat{b}_j \rangle$, and $\Delta N_{\text{tube}}^2$ drops could be made to overlap for different system sizes. The simulation in (a) was made with $J_x/U = 0.5$, and in (b) with $J_x/U = 0.3$. 

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For the anisotropic system described here, there are different correlations along the strongly coupled \(x\)-axis and along the weakly coupled \(y\)-axis. For clarity, an index \(x\) or \(y\) is therefore added to dimension dependent parameters such as \(K\).

**The Josephson model**

In a two-dimensional Josephson model [97], the dynamics of the system can be described using only two degrees of freedom. This means considering TLL tubes, with an inherent phase, \(\phi_i\) and number of particles \(N_i\), leading to a Hamiltonian

\[
\hat{H} = -E_J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) + E_C \sum_i (N_i - N_0)^2,
\]

(7.7)

where \(\langle ij \rangle\) is summed over all neighboring pairs, and \(N_0 = L_x \rho_f\) is the equilibrium number of particles per tube. Like for the BH case, the Josephson Hamiltonian contains a tunneling and a repulsion energy (here called charging energy). From [45, 95], the relation between the parameters of these two models is given by:

\[
E_J = J_y N_0^{1-\alpha_x}
\]

(7.8)

and

\[
E_C = \frac{C_0 U}{L_x},
\]

(7.9)

where \(\alpha_x = 1/2K_x\) is the reciprocal of the TLL parameter and \(C_0\) is a constant.

In the Josephson picture, there is a phase transition at

\[
\frac{E_J}{E_C} = \text{constant},
\]

(7.10)

which leads to a critical tunneling in the BH model;

\[
\frac{J_{yc}}{U} \propto L_x^{-2+\alpha_x} \rho_f^{1-\alpha_x}.
\]

(7.11)

In figure 7.2(b), this is shown in a case, where the ratio \(J_y/U\) is rescaled for the different values of \(L_x\). It was thus practical to work with a rescaled tunneling energy, defined as;

\[
\tilde{J}_y = \frac{J_y}{U} L_x^{2-\alpha_x} \rho_f^{1-\alpha_x}.
\]

(7.12)

A rewriting of equation 7.12 at the critical point;

\[
\frac{J_{yc}}{U} = \tilde{J}_{yc} L_x^{-2+\alpha_x} \rho_f^{-1+\alpha_x},
\]

(7.13)

leads to a scaling relation for systems, where \(L_x\) and \(\rho_f\) was varied. In such a system \(\tilde{J}_{yc}\) and \(\alpha_x\) was to be determined from the MC data, as seen in figure 7.2(a) and (b) for a scaled and an unscaled system.
The XY model

To determine the relevant parameters of the quantum phase transition, the Josephson model was further mapped into the classical XY-model [98]. Or more precisely, the one-dimensional Josephson model was mapped into a two-dimensional XY-model. The dimensions in question where \( L_{x,XY}, L_{y,XY} \). According to [99], these parameters, and an inverse thermal energy \( \beta_{XY} \) could be retrieved from the Josephson model, which could in turn be retrieved from the underlying two-dimensional BH model;

\[
L_{x,XY} = \beta \sqrt{E_J E_C} = \beta \sqrt{C_0 U J_y L_x^{-\alpha_x} \rho_1^{1-\alpha_x}},
\]

\[
L_{y,XY} = L_y,
\]

\[
\beta_{XY} = \sqrt{\frac{E_J}{E_C}} = \sqrt{\frac{J_y L_x^{2-\alpha_x} \rho_1^{1-\alpha_x}}{C_0 U}}.
\]  

(7.14)

The superfluid density, of the XY-model, is defined analogously to equation 7.1, and can be mapped to the parameters from the BH model;

\[
\rho_{s,XY} = \frac{\langle W_y^2 \rangle}{L_{x,XY} \beta_{XY}} = \frac{\langle W_y^2 \rangle}{\beta J_y \rho_1^{1-\alpha_x} L_x^{1-\alpha_x}}.
\]  

(7.15)

The two-dimensional XY-model has been shown to have a phase transition of Berezinskii-Kosterlitz-Thouless (BKT) type [98], having a universal jump in superfluid density at \( J_{yc} \). When this jump has been found in the XY-model, it could be mapped to a BKT transition in the underlying BH model.

By using a correct scaling, all system sizes have a coinciding value for \( \rho_{s,XY} \). For higher tunneling energy, the 2D-SF regime was entered, and the mappings to the Josephson and XY-model were no longer valid. For lower tunneling, the mapping was however valid, and a correct scaling of \( L_x \) would make all MC data having a common \( L_y \) coincide.

As a first step, the scaling dependence for \( L_x \) was achieved by minimizing the spread of the MC data for common values of \( L_y \). As a measure of the spread, the variance of the data was used, according to

\[
\text{Var} \left( \rho_{s,XY}(\tilde{J}_y, \alpha_x, L_y) \right) = \sum_{L_x} \left( \rho_{s,XY}(\tilde{J}_y, L_x, L_y) - \bar{\rho}_{s,XY}(\tilde{J}_y, L_y) \right)^2,
\]  

(7.16)

where the superfluid density, averaged over \( N_{L_x} \) sets of different \( L_x \) is given by

\[
\bar{\rho}_{s,XY}(\tilde{J}_y, L_y) = \frac{1}{N_{L_x}} \sum_{L_x} \rho_{s,XY}(\tilde{J}_y, L_x, L_y).
\]  

(7.17)

Using equation 7.16, variances dependent on the tunneling rate could be computed for various trial solutions of \( \alpha_x \), for each set of MC data, sorted by \( L_y \).

Below the phase transition, a correct scaling would lead to a common superfluid density for all \( L_x \). From trial scalings, the critical point was found to be
The average variance in $\rho_{s,XY}$ as a function of $\alpha_x$ for different system sizes $L_y$, for MC data having $J_x/U = 0.5$. The exponent $\alpha_x$ was determined by overlapping the superfluid density $\rho_{s,XY}$ for data having different $L_x$ and $L_y$. Below the phase transition, a correct $\alpha_x$, resulted in a minimal spread of $\rho_{s,XY}$, for systems having the same $L_y$. The minimal variance, for all system sizes $L_x$ and $L_y$, could be achieved for $\alpha_x = 0.15 \rightarrow K_x = 3.4$.

$J_y c \leq \tilde{J}_y c = 0.3$, and the spread in rescaled MC data, as a function of the scaling exponent $\alpha_x$ could thus be defined as

$$\text{Var}(\rho_{s,XY}(\alpha_x, L_y)) = \frac{1}{\tilde{J}_y c} \int_{0}^{\tilde{J}_y c} d\tilde{J}_y \text{Var}\left(\rho_{s,XY}(\tilde{J}_y, \alpha_x, L_y)\right),$$  \hspace{1cm} (7.18)

which is a function having a parabolic shape, with a minimum for each $L_y$, as seen in figure 7.3. From the graph, it can be concluded that $\alpha_x = 0.15$ in the case of $J_x/U = 0.5$, which gives $K_x = 3.4$.

### Weber-Minnhagen Scaling

In the previous section it could be seen that MC data, having different $L_x$ but a common $L_y$, could be made to coincide by a proper choice of $\alpha_x$. When scaling the length of the TLL tubes, $L_y$, the curves would however only collapse in one point, namely $J_y c$. By using a Weber-Minnhagen (WM) scaling [94, 100, 101], which scales the data to $L_y = \infty$, it was possible to get a narrow waist positioned at $J_y c$. In figure 7.4, the MC data has been rescaled according to WM scaling;

$$\rho_{s,XY}(\infty) = \frac{\rho_{s,XY}(L_y)}{1 + 1/[2 \ln(L_y) + 1.8]}.$$  \hspace{1cm} (7.19)
Figure 7.4: MC data for $J_x/U = 0.5$, scaled with $\alpha_x = 0.15$ for the size $L_x$, and with WM scaling for the size $L_y$. As a result, all data curves collapse at the critical point $J_y c$. For lower tunneling, the MC data for different $L_x$, having a common $L_y$, all lie on a smooth curve. Above the transition, the mapping to the Josephson and XY models is not valid, and the data is spread out, as a consequence of improper scaling.

7.3 Experimental realizability

A three-dimensional simple cubic optical lattice, as the one described in section 3.4, has been considered as a test-bench for testing the quantum phase transition described in this chapter. Keeping the lattice potential barrier much higher in one dimension than in the two others freezes out all tunneling efficiently, creating a stack of two-dimensional systems in parallel.

The ratio between the tunneling and the onsite repulsion, at the position of the phase transition, provided information for a band structure calculation, where different lattice configurations could be used to find a suitable optical lattice depth. In paper VII, this calculation was presented for the case of $J_x/U = 0.3$. Varying the optical lattice depth along the $y$-axis near the value for the phase transition would thus tune the system over the phase transition between 2D-SF and 1D-MI.

7.3.1 Detection

The detection of the superfluid to Mott insulator transition is usually done by mapping the velocity distribution $n(k)$ of the atomic sample to positions in space [39]. To map $n(k)$, the magnetic trap and the optical lattice should suddenly be turned off, letting the atomic cloud expand. An image is recorded by absorption imaging after expansion times of typically tens of milliseconds. A more detailed description of absorption imaging can be found in section 4.6, but for now it is enough considering the image as a two-dimensional projection of the
spatial density distribution, \( n(r, t) \). While expanding the cloud, different velocity
groups separate, and \( n(r, t) \) has the same characteristics as \( n(k) \).

Mott insulators and superfluids in optical lattices have fundamental differ-
ences in the appearance of \( n(k) \). In a pure Mott insulator, there are no phase
relations between atoms in different wells. All the atoms will expand indepen-
dently and the density distribution detected is approximated by a Gaussian veloc-
ity distribution. For a superfluid in an optical lattice, the phase coherence leads
to distinct interference peaks in the reciprocal lattice directions. The positions
of the peaks are given by the geometric structure factor [31, 32, 102, 103]:

\[
S(q = \hbar k) = \sum_{i,j} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)/\hbar} \left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle, 
\tag{7.20}
\]

where \( \left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle \) is the correlation function for two bosons in sites \( i \) and \( j \). The interference
pattern will be periodic in \( q \)-space, have the periodicity of the reciprocal
lattice.

Equation 7.20 is valid both for the case of the Mott insulator and the su-
perfluid. In a superfluid the correlation between sites is close to one, giving
a geometric structure factor with delta function peaks, separated periodically,
with \( q \cdot (\mathbf{r}_i - \mathbf{r}_j)/\hbar = 2\pi \). In a Mott insulator the case will be the opposite,
leaving a correlation function of \( \left\langle \hat{b}_i^\dagger \hat{b}_j \right\rangle \) that drops to zero within a couple of
wells [102, 103]. The structure factor will therefore approach unity, when going
deeper into the Mott insulator regime, and no interference fringes will be seen.

In figure 7.5(a), the structure factor for an intermediate regime is plotted.
The system is superfluid along \( x \) and insulating along \( y \). The stucture factor,
given by equation 7.20, will have slow oscillations in the insulating direction and
have distinct peaks in the superfluid direction.

The structure factor does not alone give the particle density \( n(k) \). To get the
full expression, the effect from the wave function of a particle in the potential
must be included. This contribution is given by the Fourier transform of the
Wannier function in equation 3.35, \( \tilde{w}(k) \) [102, 103]. The Fourier transform for
a Wannier function, calculated for the same lattice as used in figure 7.5(a), is
plotted in figure 7.5(b).

The density distribution at time \( t \) is then given by:

\[
n(r, t) = \left( \frac{m}{\hbar t} \right)^3 \left| \tilde{w} \left( k = \frac{m\mathbf{r}}{\hbar t} \right) \right|^2 S \left( k = \frac{m\mathbf{r}}{\hbar t} \right), 
\tag{7.21}
\]

which is plotted in figure 7.5(c) for the same \( S \) and \( \tilde{w} \) as in figure 7.5(a) and
(b). The plot shows the velocity distribution for an arbitrary time, and the
function is not normalized. The relevant information for expansion times long
enough in order to separate the different velocity groups is included. This infor-
mation will not depend on expansion times for longer times, when the velocity
peaks are separated. In figure 7.5(d), cuts in the time of flight simulations along
the low tunnelling axis, for tunneling strengths just above, near and below the
phase transition are plotted. In this graph, the difference in decay of the central
Figure 7.5: The composite parts of a computed hypothetical absorption imaging time of flight picture, for detecting the occurrence of the phase transition from 2D-SF to 1D-MI. In (a), the structure factor $S(k)$, being the Fourier transform of the correlation function is shown. (b) The probability distribution of the Wannier functions computed for the same optical lattice parameters as (a). In (c), the combined 2D time of flight picture, according to equation 7.21 is shown, using the data from (a) and (b). Cuts along the $y$-axis for three cases, below, above, and near the phase transition are shown in (d). This kind of experimental curves could be used for detecting the signatures of the phase transition.

peak can be seen. For the superfluid case, the peaks are sharp, whereas for the insulating case, they are smeared out.

Another way to detect the Mott insulator is by directly imaging the density distribution of the sample as in [104, 105]. This method alone would however leave the problem of distinguishing between one-dimensional superfluids and a three-dimensional superfluid.

### 7.3.2 The role of scaling

Customary, BEC experiments have had harmonic confinements from magnetic traps, optical traps or both. In the proposed experiment special care would have to be taken to avoid this confinement, as it would cause the system lengths $L_x$ and $L_y$ to vary along the lattice. Due to the scaling relation of the phase transition
discussed earlier, this would smear out the phase transition over a range of lattice depths.

Avoiding the harmonic trap is a simple task in theory. In an experiment it would be feasible, but challenging. The most straightforward solution, using contemporary techniques, would be using non-Gaussian beam profiles, or a combination of several overlapping potentials. The former could be achieved by imaging the light transmitted through a square aperture on the BEC position, or by using diffractive optics, i.e., spatial light modulators [106]. The latter from overlapping attractive and repulsive optical traps, such as light potentials being red or blue detuned, with the sample. Using this technique a weak and narrower repulsive potential in the center of the strong and wide attractive potential, could push atoms away from the center part, leading to a combined confining potential being made more boxlike. Finally, the potential should overlapped with an optical lattice to control the tunneling and onsite repulsion.

7.4 Conclusions

A model based on an optical lattice is used to simulate the transition between BEC phases of different dimensionality. The simulated system is kept finite, as the lower dimensional phases do not exist for infinite systems.

A detailed investigation of the anisotropic transition from a one-dimensional to a two-dimensional system is accomplished. The results support the earlier predictions from the TLL theory, opening the choices of simulation methods to be used for future studies. Using finite size scaling, it is also shown that the transition is of BKT-type, having algebraic decay of the boson-boson correlations.

As one of the earlier aims of this theoretical study was to provide information for future experiments, it successfully gives the relevant parameter regimes for the optical lattices to be used. It also makes it clear that special care needs to be taken to the geometry of the trapping potential, in order not to blur the phase transition between 2D SF and 1D MI.

Combining the MC data with band structure calculations is proven useful in order to compute the expected time of flight absorption images for the future experiments.
Chapter 8

Conclusions

The work presented in this thesis spreads out over roughly five years of research, produced in close collaboration with scientists from different parts of the world. It includes experiments with high precision alignments, ranging from arbitrary optical lattice geometries, to overlapping potential minima from different colored laser beams, and moving optical lattice potentials with well defined velocities. The work also includes the design of a new BEC apparatus, currently being built at Umeå University.

One-dimensional optical lattices, with the possibility of velocity selective loading of a BEC into an optical lattice, have been the basis of a series of experiments. By adopting models for periodic potentials from solid state physics, many predictions of how a BEC interacts with an optical lattice could be made. However, as experimentally shown here, the inherent nonlinearity of a BEC limits usability of the band structure picture. For certain parameter regimes, there exist an onset of energetic and/or dynamical instability, causing the BEC to break apart. In collaborations with theoreticians, the onset of these instabilities could be modeled using a three-dimensional GP theory. A direct comparison between the theoretical growth of dynamical instabilities and experimental loss of atoms was possible.

Nonlinearities, giving rise to atom-atom repulsions, will normally cause a BEC to break apart. In experiments with double well potentials, it was however shown that such effects can cause a pair of atoms to move about as a whole. By tuning the strength of the repulsive force, the onset of such correlated tunneling was achieved, and its properties explored in detail. Tailoring the potential even more, a transistor like behavior could be accomplished, where a single atom can only tunnel through a barrier, if another atom is present.

Throughout the experiments of this thesis, optical lattices were used as a tool to manipulate the BEC wave function. In combination with the absorption imaging detection technique, it has been possible to directly measure the result by acquiring an image of the momentum distribution of the released atomic cloud. The versatility of an optical lattice, and the following absorption imaging detection, made it a natural choice as a test-bench for our theoretical study of
dimensional crossovers. Tuning the atom-atom repulsion energy, with individually variable tunneling energies along the three Cartesian directions, opened the possibility to use a system with anisotropic tunneling to create lower dimensional systems. The dimensional crossover between two- and three-dimensional systems was studied, and by implementing finite size scaling, the properties of this phase transition could be simulated.

The work of this thesis have not only provided new experimental and theoretical results in the research field of BEC in optical lattices. The work also provide the possibility for future work on cold atoms in arbitrary aligned optical lattices in the Umeå set-up, where a broad range of experiments on different Bravais lattices, as-well as quasiperiodic lattices are possible.


I en serie experiment som utförts vid laboratoriet LENS i Florens, Italien, har modeller anpassade från fasta tillståndets fysik testats för endimensionella OKG. Modellerna har byggts på växelverkan mellan en periodisk potential och ett vågpaket, i detta fall ett OKG och ett BEC. I undersökningarna kom det fram att dessa modeller var otillräckliga i de fall där den ickelinjära atom-atomväxelverkan hos ett BEC blev dominant. Resultatet blev en uppvärmning, eller ett sönderfall i flera små moder av BEC, så kallad energetisk och dynamisk instabilitet. I samråd med teoretiker kunde nya, mer realistiska modeller skapas, där experimentella data direkt kunde jämföras med de teoretiska.

En övergång till en MI kan i ett OKG skapas genom höga potentialbarriärer mellan koordinatpunkterna i ett tredimensionellt kristallgitter. Potentialbarriärernas höjd kan bestämmas genom irradiansen och graden av sidstämdhet hos laserstrålarna som används för att skapa ett OKG. När atomernas möjlighet att röra sig fritt begränsas, och energin hos atomatomrepslusionen blir dominant, ordnar atomerna upp sig i heltalsmultipler i koordinatpunkterna.

En undersökning av möjligheten för atomer att röra sig genom en potentialbarriär, så kallad tunneleffekt, genomfördes i ett laboratorium på Johannes Gutenberg Universitetet i Mainz; Tyskland, där man specialiserat sig på OKG med MI. Genom att använda tvåfärgade OKG kunde varje koordinatpunkt i det tredimensionella kristallgittert kompletteras med en liten potentialbarriär i mitten. Detta skapade ett system där en stor mängd dubbelbrunnspotentialer kunde undersökas parallellt. En eller två atomer kunde laddas på ena sidan i varje dubbelbrunn, och därefter kunde möjligheten för tunneleffekt undersökas. För atomer som hade stora repellerande krafter, skapades ett bundet tillstånd. På grund av energiskillnaden mellan att ha två atomer på en sida i en dubbelbrunn än ena sidan, och en atom på var sida om potentialbarriären i dubbelbrunnen än andra sidan, tvingades atomerna att röra sig korrelerat genom barriären. Om repulsionskrafterna minskades, ökade sannolikheten för att atomerna skulle röra sig genom barriären individuellt.

En tvådimensionell eller endimensionell modell för ultrakalla atomer går att realisera, både experimentellt och teoretiskt, med potentialbarriärerna i ett OKG. Hur atomerna reagerar i övergången mellan dessa system av lägre dimensioner har studerats med teoretiska simuleringsmetoder. Speciellt övergången mellan ett tillstånd med koherenta atomer i två dimensioner i det ena extremfallet, och parallella endimensionella system i det andra, har simulörats i detalj. Ett beroende av det simulerade systemets storlek kunde härledas till koherenseegenskaper hos atomerna. Genom att härleda skalningsberoendet av koherensen och andra egenskaper för olika systemstorleken kunde övergången mellan en- och tvådimensionella system lokaliseras. Beräkningar gjordes för flera olika egenskaper hos systemet, och en beräkning av en experimentellt mätbar signal har redovisats. Simuleringsarna genomfördes med bland annat Monte-Carlometoder i samarbete med forskare på Kungliga Tekniska Högskolan i Stockholm.

Vid Umeå Universitet har ett experiment för infängning och kylning av isotopen rubidium-87, konstruierats. Experimentet kan fånga mer än 200 miljoner atomer vid en temperatur på cirka 10 µK i en så kallad magnetooptisk falla. För att kyla atomerna ytterligare, och få dem att övergå till ett BEC, så har en magnetisk falla konstruerats. Denna är testad och har en livstid på 9 s. Atomerna som
överförts till denna magnetfalla kan kylas ytterligare genom förågningskylning, en process där de varmaste atomerna avlägsnas, varvid medeltemperaturen sjunker. Funktionaliteten hos denna process är testad, men ännu ej optimerad. Experimentet har även kompletterats med ett system för högprecisionslinjering av OKG med näst intill valfri geometri.
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