# Projektpraktikum 

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# Bose-Einstein Condensation 

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## Contents

1 Thermodynamical Basics of the Ideal Bose Gas ..... 5
2 Interacting Bosons ..... 8
2.1 Free particles - Calculating the fluctuations ..... 10
2.2 Arbitrary potential $V(R)$ - Multi-Mode Bogoliubov Transfor- mation ..... 18
3 Results ..... 25
3.1 Free Particles in 1 Dimension ..... 25
3.2 Particles in a Harmonic Potential ..... 28
A Substituting the Bogoliubuv approximation into the Hamil- tonian ..... 35
B Performing the Fourier transformation for the free particles ..... 37
C Proof of conservation of bosonic- commutation relation ..... 39

# D Calculating the $2 L \times 2 L$ matrix for the multi-mode Bogoliubov transformation 

## E Derivation of the condition for the commutation relations for the multi-mode Bogoliubov transformation <br> 44

## Abstract

In this work an attempt to describe Bose-Einstein Condensation (BCE) for a 1 dimensional system is made. In chapter 1 a brief introduction to BCE out of statistical physics can be found.
In chapter 2, starting from the Bose-Hubbard Hamiltonian, a derivation for the Gross-Pitaevski Equation 2.6 which is one of the central equations for this description of BCE is done.
With the GPE the problem is solved for free particles in chapter 2.1. There a Bogoliubov transformation is done, given in equation 2.15. The conditions for this transformation, that the Hamiltonian is diagonal and that the bosonic commutation relations are conserved, are other important equations in solving the problem.
Chapter 2.2 finally describes how to solve the problem for an arbitrary potential $\mathrm{V}(\mathrm{R})$ via a Multi-Mode Bogoliubov transformation (MMB transformation), which is the extension of the Bogoliubov transformation in the previous chapter. Here, in addition to the GPE also the 2 already mentioned conditions have to be fulfilled.
Results of the two worked out problems can be found in chapter 3.1 and 3.2. Because of the work intensity of the MMB transformation I stopped at the point where the Hamiltonian was diagonal and didn't calculate any properties like I did in the zero potential case.

## Introduction

When Einstein developed the quantum statistics for indistinguishable particles, based on a work of the Indian physicist Nathanel Bose, he discovered, that a dilute gas of such particles can undergo a phase transition named Bose-Einstein condensation. The fascinating thing about BCE is, that the strange world of quantum mechanics and its effects actually can be seen by the pure eye. This makes it interesting from a theoretical as well as from a experimental point of view.
In this work the problem is solved for a one dimensional lattice using a field theory approach. In principle, a contradiction occurs due to the mean field nature of the present approximation: according to the Mermin- WagnerHohenberg theorem which forbids spontaneously broken symmetry in systems with less than three dimensions. [3]
Nevertheless it is interesting to consider and spend time with such a problem since it shows a way how to actually solve problems which are more complicated as e.g.: the harmonic oscillator and it gives an insight in the big field of mean field theory.

## Chapter 1

## Thermodynamical Basics of the Ideal Bose Gas

The following short introduction to BCE is, concerning the content, a summary of [2].
We consider noninteracting bosons with zero spin and mass m . The occupation of an energy level with energy $\epsilon_{p}=\frac{p^{2}}{2 m}$ is then given by the Bose-Einstein-statistics:

$$
\begin{equation*}
\left\langle n_{p}\right\rangle=\bar{n}_{p}=\frac{1}{e^{\beta\left(\epsilon_{p}-\mu\right)}-1}, \tag{1.1}
\end{equation*}
$$

with the inverse temperature $\beta=\frac{1}{k_{b} T}$ and the chemical potential $\mu$.
Hence the total particle number is given by:

$$
\begin{equation*}
N=\sum_{p} \bar{n}_{p}=N_{0}+\sum_{p \neq 0} \bar{n}_{p} \tag{1.2}
\end{equation*}
$$

From equation 1.1 we can see, that the chemical potential $\mu$ has to be smaller than the smallest energy $\epsilon_{p}$, which can be taken zero without loss of generality. If the chemical potential approaches this smallest energy the
occupation of the ground state $N_{0} \rightarrow \infty$. Because of this problem we from now on treat it separately.

For $\epsilon_{p}-\mu>0$ we can expand 1.1 as a Taylor series:

$$
\begin{equation*}
\bar{n}_{p}=\sum_{l=1}^{\infty}\left(e^{-\beta\left(\epsilon_{p}-\mu\right)}\right)^{l} \tag{1.3}
\end{equation*}
$$

The total particle number is then given by:

$$
\begin{equation*}
N=N_{0}+\frac{V}{(2 \pi \hbar)^{3}} \sum_{l=1}^{\infty} e^{\beta \mu l} \int e^{-\frac{p^{2} l}{2 m k_{b} T}} d^{3} p \tag{1.4}
\end{equation*}
$$

Where we already replaced the sum over all discrete states by an integral $\frac{V}{(2 \pi \hbar)^{3}} \int \cdots d^{3} p$. This integral can be solved easily and leads to:

$$
\begin{equation*}
N=N_{0}+\frac{V}{\lambda^{3}} \sum_{l=1}^{\infty} \frac{e^{\beta \mu l}}{l^{3 / 2}}=N_{0}+\frac{V}{\lambda^{3}} g_{3 / 2}\left(e^{\beta \mu}\right), \tag{1.5}
\end{equation*}
$$

with the thermal de Broglie wavelength $\lambda=\frac{2 \pi \hbar}{\sqrt{2 \pi m k_{b} T}}$ and the generalized zeta-function $g_{3 / 2}\left(e^{\beta \mu}\right)$. For a given particle number, equation 1.5 determines the chemical potential $\mu$. At high temperatures $T \rightarrow \infty$, the chemical potential has to approach $-\infty$. For lower temperatures, on the other hand, it has to approach zero. Equivalent to the chemical potential approaching zero the limit for $e^{\beta \mu} \rightarrow 1$ can be taken. Then the generalized zeta function can be replaced by the Riemann zeta function $\zeta(3 / 2)$. As seen above the chemical potential cannot be positive, why there has to be a certain temperature $T_{c}$ where $\mu=0$ for $T<T_{c}$. When the temperature exceeds this critical temperature the number of particles in the ground state is still $N_{0}=\mathcal{O}(1)$ and can be neglected. With this condition we can calculate the critical temperature from equation 1.5:

$$
\begin{equation*}
k_{B} T_{c}=\frac{2 \pi \hbar^{2}}{m}\left(\frac{N}{\zeta(3 / 2) V}\right)^{3 / 2} \tag{1.6}
\end{equation*}
$$

For temperatures lower than $T_{c}$ the fraction of particles in the ground state or condensed particles can be calculated from 1.5 as:

$$
\begin{equation*}
\frac{N_{0}}{N}=1-\left(\frac{T}{T_{c}}\right)^{3 / 2} \tag{1.7}
\end{equation*}
$$

This means, that at a temperature lower than $T_{c}$ a macroscopic amount of particles occupies the ground state and the fraction of condensed particles approaches one as T becomes zero. On the other hand for temperatures higher than $T_{c}$ the number of condensed particles can be neglected.

## Chapter 2

## Interacting Bosons

We now consider a simple model for interacting bosons described by the one dimensional Bose-Hubbard-Hamiltonian:

$$
\begin{equation*}
H=\sum_{R=1}^{L}(V(R)-\mu) \hat{\psi}_{R}^{\dagger} \hat{\psi}_{R}-t \sum_{R=1}^{L}\left(\hat{\psi}_{R}^{\dagger} \hat{\psi}_{R+1}+\hat{\psi}_{R} \hat{\psi}_{R+1}^{\dagger}\right)+\frac{U}{2} \sum_{R=1}^{L}\left(\hat{\psi}_{R}^{\dagger}\right)^{2}\left(\hat{\psi}_{R}\right)^{2} . \tag{2.1}
\end{equation*}
$$

Where the first term corresponds to an external potential, which in this work is chosen to be: $V(R)=\alpha\left(R-\frac{L}{2}\right)^{2}$. This term also contains the chemical potential, which insures particle conservation. The second term describes the movement of the particles, where just hopping from a lattice point to its nearest neighbors is included. The last part is the interaction potential between 2 particles, where the potential $V\left(R-R^{\prime}\right)$ acts only on particles on the same site:

$$
\begin{equation*}
V\left(R-R^{\prime}\right)=U \delta_{R R^{\prime}} \tag{2.2}
\end{equation*}
$$

The bosonic field-operators $\hat{\psi}_{R}$ and $\psi_{R}^{\dagger}$ obey the bosonic commutation relations:

$$
\begin{align*}
{\left[\psi\left(R^{\prime}\right), \psi(R)^{\dagger}\right] } & =\delta_{R, R^{\prime}} \\
{\left[\psi\left(R^{\prime}\right)^{\dagger}, \psi(R)^{\dagger}\right] } & =0  \tag{2.3}\\
{\left[\psi\left(R^{\prime}\right), \psi(R)\right] } & =\left[\psi\left(R^{\prime}\right)^{\dagger}, \psi(R)^{\dagger}\right]=0 .
\end{align*}
$$

In the condensed phase these are split into a term $\phi(R)$ describing the condensate and one operator $\hat{b}_{R}$ which treats the fluctuation around this value [4, p. 350].

$$
\begin{align*}
\hat{\psi}_{R} & =\phi(R)+\hat{b}_{R} \\
\hat{\psi}_{R}^{\dagger} & =\phi(R)+\hat{b}_{R}^{\dagger} \tag{2.4}
\end{align*}
$$

Where $\phi(R)$ is a real number, not an operator. A problem with that approach is, that it violates particle conservation, since $\hat{\psi}_{R}$ acting on a vector destroys a particle at R . The number $\phi(R)$ however leaves the state unchanged.
Substituting 2.4 into the Hamiltonian 2.1 leads to ${ }^{1}$ :

[^0]\[

$$
\begin{align*}
H= & \sum_{R}\left[(V(R)-\mu)|\phi(R)|^{2}+\frac{U}{2}|\phi(R)|^{4}-2 t \phi(R+1) \phi(R)\right]+ \\
& \hat{b}_{R}\left[(V(R)-\mu) \phi(R)+U|\phi(R)|^{2} \phi(R)-t(\phi(R-1)+\phi(R+1))\right]+ \\
& \hat{b}_{R}^{\dagger}\left[(V(R)-\mu) \phi(R)+U|\phi(R)|^{2} \phi(R)-t(\phi(R-1)+\phi(R+1))\right]+ \\
& \left.\hat{b}_{R}^{\dagger} \hat{b}_{R}\left((V(R)-\mu)+2 U|\phi(R)|^{2}\right)+\frac{U}{2} \phi(R)^{2}\left(\hat{b}_{R}^{2}+\hat{( }^{\dagger} b_{R}^{\dagger}\right)^{2}\right)-t\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right)+ \\
& \frac{U}{2}\left(2\left(\hat{b}_{R}^{\dagger}\right)^{2} \hat{b}_{R} \phi(R)+2 \hat{b}_{R}^{\dagger} \hat{b}_{R}^{2} \phi(R)+\left(\hat{b}_{R}^{\dagger}\right)^{2} \hat{b}_{R}^{2}\right) . \tag{2.5}
\end{align*}
$$
\]

Because of the Hamiltonian being stationary in the operators $\hat{b}_{R}$ and $\hat{b}_{R}^{\dagger}$, the terms linear in these have to vanish. This leads to the Gross-Pitaevskii equation (GPE), which can be used to determine the condensate amplitude $\phi(R)$ :

$$
\begin{equation*}
\left.\left((V(R)-\mu)+U|\phi(R)|^{2}\right)\right) \phi(R)-t(\phi(R+1)+\phi(R-1))=0 \tag{2.6}
\end{equation*}
$$

### 2.1 Free particles - Calculating the fluctuations

It has to be emphasized that the general approach made in this chapter is not my idea and can be found a variety of literature e.g.: [4]. All the calculations for this specific problem on the other hand were done by myself.

The GPE determines the condensate density on lattice site $\mathrm{R},|\phi(R)|^{2}$. Despite that, the size of fluctuations around this value is interesting. There-
fore it's the next step to solve this problem by including terms up to the second order in the annihilation and creation operators $\hat{b}_{R}$ and $\hat{b}_{R}^{\dagger}$.
To simplify the problem it is first solved for free particles, where $V(R) \equiv 0$. With that there is no dependency on R in the Hamiltonian and therefore the average occupation of the lattice is also independent of the lattice site. This means $\phi(R)$ is the same for all R and from now on it will simply be written as $\phi$. Consequently the GPE reads:

$$
\begin{equation*}
\left(U|\phi|^{2}-\mu\right) \phi-2 t \phi=0, \tag{2.7}
\end{equation*}
$$

or

$$
\begin{equation*}
|\phi|^{2}=\frac{2 t+\mu}{U} \tag{2.8}
\end{equation*}
$$

With the condensate density $|\phi|^{2}$ being the same on every place, an expression for the chemical potential can be found:

$$
\begin{equation*}
\mu=\frac{N}{L} U-2 t=n U-2 t \tag{2.9}
\end{equation*}
$$

with N the total number of particles and n the particle density.
With 2.8 the Hamiltonian 2.5 simplifies to:

$$
\begin{align*}
H= & \sum_{R}\left[-\mu|\phi|^{2}+\frac{U}{2}|\phi|^{4}-2 t \phi^{2}\right]+ \\
& \left.\hat{b}_{R}^{\dagger} \hat{b}_{R}\left(-\mu+2 U|\phi|^{2}\right)+\frac{U}{2} \phi^{2} \hat{b}_{R}^{2}+\frac{U}{2} \phi^{2} \hat{\left(b_{R}^{\dagger}\right.}\right)^{2}-t\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right), \tag{2.10}
\end{align*}
$$

Here, terms of third and fourth order in the fluctuation operators have been neglected, what is correct in the low density limit.
2.10 can be written as:

$$
\begin{equation*}
H=C+\sum_{R} A \hat{b}_{R}^{\dagger} \hat{b}_{R}+B\left(\hat{b}_{R}^{2}+\hat{\left(b_{R}^{\dagger}\right)^{2}}\right)-t\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right), \tag{2.11}
\end{equation*}
$$

with the position independent constants:

$$
\begin{align*}
C & =\sum_{R}\left(-\mu \phi^{2}+\frac{U}{2} \phi^{4}-2 t \phi^{2}\right)=\frac{L(\mu+2 t)(\mu-2 t)}{2 U} \\
A & =-\mu+2 U \phi^{2}=\mu+4 t  \tag{2.12}\\
B & =\frac{U}{2} \phi^{2}=t+\frac{\mu}{2} .
\end{align*}
$$

Now the creation and annihilation operators are expanded into the basis of the free particle (in other words, we perform a Fourier transformation):

$$
\begin{align*}
\hat{b}_{R} & =\frac{1}{\sqrt{L}} \sum_{k} e^{i k R} \hat{b}_{k} \\
b_{R}^{\dagger} & =\frac{1}{\sqrt{L}} \sum_{k} e^{-i k R} \hat{b}_{k}^{\dagger} \tag{2.13}
\end{align*}
$$

Because of the periodic boundary conditions $k$ is restricted to $k=\frac{2 \pi}{L} n, n \in$ $\mathbb{N}$. Normally n would be chosen to be in $[0, L-1]$, in this work however it is convenient to take n symmetric from $\left[-\frac{L-1}{2}, \frac{L-1}{2}\right]$ if L is odd or from $\left[-\frac{L}{2}, \frac{L}{2}-1\right]$ if it is even.
Substituting the Fourier transformation into the Hamiltonian 2.11 leads to ${ }^{2}$ :

$$
\begin{equation*}
H=C+\sum_{k}(A-2 t \cos k) \hat{b}_{k}^{\dagger} \hat{b}_{k}+B\left(\hat{b}_{k} \hat{b}_{-k}+\hat{b}_{k}^{\dagger} \hat{b}_{-k}^{\dagger}\right) \tag{2.14}
\end{equation*}
$$

[^1]The goal, to diagonalize this Hamiltonian, will be achieved by using a Bogoliubov transformation:

$$
\begin{align*}
& \hat{b}_{k}=u_{k} \hat{a}_{k}+v_{k} \hat{a}_{-k}^{\dagger} \\
& \hat{b}_{k}^{\dagger}=u_{k}^{*} \hat{a}_{k}^{\dagger}+v_{k}^{*} \hat{a}_{-k} \\
& \hat{b}_{-k}=u_{-k} \hat{a}_{-k}+v_{-k} \hat{a}_{k}^{\dagger}  \tag{2.15}\\
& \hat{b}_{-k}^{\dagger}=u_{-k}^{*} \hat{a}_{-k}^{\dagger}+v_{-k}^{*} \hat{a}_{k}
\end{align*}
$$

The parameters $u_{k}$ and $v_{k}$ have to be determined in a way that, assuming one set of operators already obeys the commutation relation 2.3 (this operators will be $\hat{a}_{k}$ and $\hat{a}_{k}^{\dagger}$ ), the other set ( $\hat{b}_{k}$ and $b_{k}^{\dagger}$ ) also obeys it. The last requirement for the coefficients will be that the Hamiltonian gets diagonal. Nevertheless this turns out to be possible only for indices $k \neq 0$, because for $k=0$ :

$$
\begin{array}{r}
(A-2 t) \hat{b}_{0}^{\dagger} \hat{b}_{0}+B\left(\hat{b}_{0} \hat{b}_{0}+\hat{b}_{0}^{\dagger} \hat{b}_{0}^{\dagger}\right)= \\
(\mu+2 t) \hat{b}_{0}^{\dagger} \hat{b}_{0}+\frac{\mu+2 t}{2}\left(\hat{b}_{0} \hat{b}_{0}+\hat{b}_{0}^{\dagger} \hat{b}_{0}^{\dagger}\right)
\end{array}
$$

A Bogoliubov transformation is for such an arrangement of coefficients not possible. This can also be seen by looking at equation 2.21 where $k=0$ would lead to a singularity, because of dividing by zero.
The state $k=0$ corresponds to the ground state where in 2.4 the creation and annihilation operators have been replaced by the condensate amplitude $\phi(R)$, where $\sum_{R}|\phi(R)|^{2}=N_{0}$.
Since we are interested in BEC, where a big fraction of particles is in the ground state, there is no big difference between the Fock-states:

$$
\begin{align*}
\hat{b}_{0}\left|N_{0}, N_{1}, \ldots\right\rangle & =\sqrt{N_{0}}\left|N_{0}-1, N_{1}, \ldots\right\rangle \\
\hat{b}_{0}^{\dagger}\left|N_{0}, N_{1}, \ldots\right\rangle & =\sqrt{N_{0}+1}\left|N_{0}+1, N_{1}, \ldots\right\rangle \tag{2.16}
\end{align*}
$$

Here the above mentioned violation of particle conservation can be seen: The replacement of the operators by a number leads to a violation of particle conservation. For that reason we work in the grand-canonical ensemble and ensure particle conservation by introducing the chemical potential as a Lagrange multiplier [3, p. 23].

The Bogoliubov transformation is now done for all indices except $k=0$. First the numbers $u_{k}$ and $v_{k}$ are chosen to be real. Then the commutator $\left[\hat{b}_{k}, \hat{b}_{k}^{\dagger}\right]$ is calculated and it is assumed, that $\hat{a}_{k}$ and $\hat{a}_{k}^{\dagger}$ already are bosonic operators:

$$
\begin{align*}
{\left[\hat{b}_{k}, \hat{b}_{k}^{\dagger}\right] } & =u_{k}^{2}\left[\hat{a}_{k}, \hat{a}_{k}^{\dagger}\right]+v_{k}^{2}\left[\hat{a}_{-k}^{\dagger}, \hat{a}_{-k}\right]+u_{k} v_{k}\left(\left[\hat{a}_{k}, \hat{a}_{-k}\right]+\left[\hat{a}_{-k}^{\dagger}, \hat{a}_{k}^{\dagger}\right]\right)  \tag{2.17}\\
& =u_{k}^{2}-v_{k}^{2} \stackrel{!}{=} 1 .
\end{align*}
$$

Now the commutator $\left[b_{k}, b_{-k}\right.$ ] is calculated which has to vanish:

$$
\begin{align*}
{\left[\hat{b}_{k}, \hat{b}_{-k}\right] } & =u_{k} u_{-k}\left[\hat{a}_{k}, \hat{a}_{-k}\right]+v_{k} v_{-k}\left[\hat{a}_{k}^{\dagger}, \hat{a}_{-k}^{\dagger}\right]+\left[\hat{a}_{k}, \hat{a}_{k}^{\dagger}\right]\left(u_{k} v_{-k}-u_{-k} v_{k}\right) \\
& =u_{k} v_{-k}-u_{-k} v_{k} \stackrel{!}{=} 0 \tag{2.18}
\end{align*}
$$

This condition can be fulfilled by:

$$
\begin{align*}
& v_{k}=v_{-k}  \tag{2.19}\\
& u_{k}=u_{-k}
\end{align*}
$$

Plugging the Bogoliubov transformation 2.15 into the Hamiltonian 2.14 leads to:

$$
\begin{align*}
H= & C+\frac{3}{2}(\mu+2 t) N_{0} \\
& \sum_{k \neq 0} \hat{a}_{k}^{\dagger} \hat{a}_{k}\left(u_{k}^{2}(A-2 t \cos k)+B u_{k} v_{k}\right)+B u_{k} v_{k} \hat{a}_{-k}^{\dagger} \hat{a}_{-k}+ \\
& \sum_{k \neq 0} \hat{a}_{k} \hat{a}_{k}^{\dagger} B u_{k} v_{k}+\hat{a}_{-k} \hat{a}_{-k}^{\dagger}\left(v_{k}^{2}(A-2 t \cos k)+B u_{k} v_{k}\right)+  \tag{2.20}\\
& \sum_{k \neq 0} \hat{a}_{k}^{\dagger} \hat{a}_{-k}^{\dagger}\left((A-2 t \cos k) u_{k} v_{k}+B\left(v_{k}^{2}+u_{k}^{2}\right)\right)+ \\
& \sum_{k \neq 0} \hat{a}_{k} \hat{a}_{-k}\left((A-2 t \cos k) u_{k} v_{k}+B\left(v_{k}^{2}+u_{k}^{2}\right)\right)
\end{align*}
$$

To get rid of the restrictions to the sums $u_{0}=v_{0}=0$ can be defined, because with that the sum can again be over all allowed k values.
Demanding the Hamiltonian to be diagonal, $u_{k}$ and $v_{k}$ have to satisfy the equation:

$$
\begin{aligned}
& (A-2 t \cos k) u_{k} v_{k}+B\left(v_{k}^{2}+u_{k}^{2}\right)=0 \\
& (A-2 t \cos k) v_{k} \sqrt{1+v_{k}^{2}}+B\left(2 v_{k}^{2}+1\right)=0
\end{aligned}
$$

where condition 2.17 was used to get to the second line.
Hence the coefficients $u_{k}, v_{k}$ for the transformation for all $k \neq 0$ are given by:

$$
\begin{align*}
& v_{k}=\sqrt{-\frac{1}{2}+\frac{(\mu+4 t-2 t \cos k)}{2 \sqrt{(\mu+4 t-2 t \cos k)^{2}-(2 t+\mu)^{2}}}} \\
& u_{k}=\sqrt{\frac{1}{2}+\frac{(\mu+4 t-2 t \cos k)}{2 \sqrt{(\mu+4 t-2 t \cos k)^{2}-(2 t+\mu)^{2}}}}  \tag{2.21}\\
& u_{-k}=u_{k} \\
& v_{-k}=v_{k}
\end{align*}
$$

To diagonalize the Hamiltonian 2.20 we use the bosonic commutation relation and replace $\hat{a}_{k} \hat{a}_{k}^{\dagger}$ with $1+\hat{a}_{k}^{\dagger} \hat{a}_{k}$ :

$$
\begin{align*}
H= & \left(C+v_{k}^{2}(A-2 t \cos k)+2 B u_{k} v_{k}\right)+\frac{3}{2}(\mu+2 t) N_{0} \\
& \sum_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}\left(u_{k}^{2}(A-2 t \cos k)+2 B u_{k} v_{k}\right)  \tag{2.22}\\
& \sum_{k} \hat{a}_{-k}^{\dagger} \hat{a}_{-k}\left(v_{k}^{2}(A-2 t \cos k)+2 B u_{k} v_{k}\right)
\end{align*}
$$

Because of the allowed values for k , and the coefficients at the creation and annihilation operators in the second line of 2.22 being symmetric around zero ${ }^{3}$ the Hamiltonian can be simplified to:

$$
\begin{align*}
H= & \left(C+v_{k}^{2}(A-2 t \cos k)+2 B u_{k} v_{k}\right)+ \\
& \sum_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}\left(\left(u_{k}^{2}+v_{k}^{2}\right)(A-2 t \cos k)+4 B u_{k} v_{k}\right) \tag{2.23}
\end{align*}
$$

The minimum energy is obtained by setting all excitations $\hat{a}_{k}^{\dagger} \hat{a}_{k}=0$, therefore the constant term in the first line in this equation is the ground

[^2]state energy. The final resulting Hamiltonian is given by:
\[

$$
\begin{align*}
H= & \frac{L(\mu+2 t)(\mu-2 t)}{2 U}+\sum_{k}+v_{k}^{2}[(\mu+4 t)-2 t \cos k]+(\mu+2 t) u_{k} v_{k}+ \\
& \frac{3}{2}(\mu+2 t) N_{0}+\sum_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}\left(\left(u_{k}^{2}+v_{k}^{2}\right)(\mu+4 t-2 t \cos k)+2(\mu+2 t) u_{k} v_{k}\right) \tag{2.24}
\end{align*}
$$
\]

Again reminding, that for the index $k=0$ the Bogoliubov transformation was impossible. Just formally the transformation coefficients $u_{0}$ and $v_{0}$ were defined zero, to be able to let the summation go over all allowed values of k . This means although in equation 2.24 it looks like there is a number operator of the ground state $\hat{a}_{0}^{\dagger} \hat{a}_{0}$, the energy of that state is zero and therefore that term doesn't contribute.
Equation 2.24 is mathematically identical to several harmonic oscillators with the ground state energy $E_{0}$ and different excitation energies $E_{k}$ which would correspond to the energiesteps $\hbar \omega_{k}$ in the harmonic oscillator.
Beside the energies, also the eigenstates can be constructed. There the occupation of a certain normal mode k is introduced as a quantum number and the state itself is given by the occupation of all accessibly states: $\left|N_{k_{1}}, N_{k_{2}}, \ldots, N_{k_{L-1}}\right\rangle$

$$
\begin{align*}
E_{0}= & \frac{L(\mu+2 t)(\mu-2 t)}{2 U}+v_{k}^{2}[(\mu+4 t)-2 t \cos k] \\
& +(\mu+2 t) u_{k} v_{k}+\frac{3}{2}(\mu+2 t) N_{0}  \tag{2.25}\\
E_{k}= & \left(u_{k}^{2}+v_{k}^{2}\right)((\mu+4 t)-2 t \cos k)+2(\mu+2 t) u_{k} v_{k}
\end{align*}
$$

Therewith it is possible to calculate the expectation value of the occupation of different states, excluding the ground state, using the Bose-Einstein-
statistics 1.1 for different temperatures T . But we have to be careful doing that, because the chemical potential $\mu$ is in this case already included in the energy in a non linear way. This means instead of $\epsilon_{p}-\mu$ just $\epsilon_{p}$ has to be taken.
With that the occupation of the ground state can be calculated using equation 1.2:

$$
\begin{equation*}
N_{0}=N-\sum_{p \neq 0} \bar{n}_{p} . \tag{2.26}
\end{equation*}
$$

In the continuous case the sum over all nonzero momenta would be replaced by $\frac{V}{(2 \pi \hbar)^{D}} \int \cdots d \vec{p}$, with D the number of spatial dimensions.
In the discrete case it is possible just to add them together since the number of k -states is limited.

### 2.2 Arbitrary potential $V(R)$ - Multi-Mode Bogoliubov Transformation

The next step is to diagonalize the Hamiltonian, including terms up to second order in the fluctuation operators with an external potential $V(R)$. This will be achieved using a multi-mode Boguliubov Transoformation.
The Hamiltonian, from where we start in this chapter, is given in equation $2.5^{4}$ :

$$
\begin{align*}
H= & \sum_{R}\left[(V(R)-\mu)|\phi(R)|^{2}+\frac{U}{2}|\phi(R)|^{4}-2 t \phi(R+1) \phi(R)\right]+ \\
& \left.\hat{b}_{R}^{\dagger} \hat{b}_{R}\left((V(R)-\mu)+2 U|\phi(R)|^{2}\right)+\frac{U}{2} \phi(R)^{2}\left(\hat{b}_{R}^{2}+\hat{\left(b_{R}^{\dagger}\right.}\right)^{2}\right)-  \tag{2.27}\\
& t\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right)+\mathcal{O}\left(\hat{b}^{3}\right) .
\end{align*}
$$

[^3]This Hamiltonian is written in vector notation:

$$
\begin{equation*}
H=\Delta+\vec{B}^{\dagger} M \vec{B}+\mathcal{O}\left(\hat{b}^{3},\left(\hat{b}^{\dagger}\right)^{3}\right) \tag{2.28}
\end{equation*}
$$

With the vectors $B$ and $B^{\dagger}$ defined as (Nambu-notation):

$$
\begin{align*}
\vec{B}^{\dagger} & =\left(b_{1}^{\dagger}, \ldots, b_{L}^{\dagger}, \hat{b}_{1}, \ldots, \hat{b}_{L}\right) \\
\vec{B}=\left(\vec{B}^{\dagger}\right)^{\dagger} & =\left(\hat{b}_{1}, \ldots, \hat{b}_{L}, b_{1}^{\dagger}, \ldots, b_{L}^{\dagger}\right)^{T} \tag{2.29}
\end{align*}
$$

We could, at this point, try just to take the Hamiltonian from equation 2.5 and construct the matrix M, but would soon discover that the matrix is not hermitian. Therefore we have to remember, that this particular Hamiltonian was obtained using the bosonic commutation relations and with that the internal symmetry of the Hamiltonian was lost. This has to be cured by replacing following terms in 2.5 with:

$$
\begin{aligned}
\hat{b}_{R}^{\dagger} \hat{b}_{R} & =\frac{1}{2}\left(\hat{b}_{R}^{\dagger} \hat{b}_{R}+\hat{b}_{R} \hat{b}_{R}^{\dagger}+1\right) \\
\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right) & =\frac{1}{2}\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R+1} \hat{b}_{R}^{\dagger}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}+\hat{b}_{R+1}^{\dagger} \hat{b}_{R}\right)
\end{aligned}
$$

If the goal is just to make the matrix hermitian, replacing $\hat{b}_{R}^{\dagger} \hat{b}_{R}$ would not be necessary. Nevertheless it has to be done, because otherwise the energies would be negative. The problem with that is, that the energy gets lower the more particles are in the state, what would result in an infinite occupation of this state.

This whole procedure produces a constant term $\Delta$ :

$$
\begin{equation*}
\Delta=\sum_{R}\left[(V(R)-\mu) \phi(R)^{2}+\frac{U}{2} \phi(R)^{4}-2 t \phi(R+1) \phi(R)+\zeta(R)\right] \tag{2.30}
\end{equation*}
$$

and the $2 L \times 2 L$ dimensional matrix ${ }^{5} \mathrm{M}$ (for detailed calculation see Appendix D):

$$
M=\left(\begin{array}{cccc|cccc}
\zeta(1) & -\bar{t} & & -\bar{t} & \eta(1) & & &  \tag{2.31}\\
-\bar{t} & \ddots & \ddots & & & \ddots & & \\
& & \ddots & -\bar{t} & & & \ddots & \\
-\bar{t} & & -\bar{t} & \zeta(L) & & & & \eta(L) \\
\hline \eta(1) & & & & \zeta(1) & -\bar{t} & & -\bar{t} \\
& \ddots & & & -\bar{t} & \ddots & & \\
& & \ddots & & & & \ddots & -\bar{t} \\
& & & \eta(L) & -\bar{t} & & -\bar{t} & \zeta(N)
\end{array}\right),
$$

with the place dependent functions

$$
\begin{aligned}
\zeta(R) & =\frac{1}{2}\left[(V(R)-\mu)+4 \phi(R)^{2}\right] \\
\eta(R) & =\frac{U}{2} \phi(R)^{2} \\
\bar{t} & =\frac{t}{2}
\end{aligned}
$$

The multi-mode Bogoliubov transformation transforms the operators B into a set of quasiparticle creation and annihilation operators P via an in general not unitary transformation U where $B=U P$. The transformation U has to conserve the bosonic commutation relation:

$$
\begin{equation*}
S_{i j}:=\left[\vec{B}_{i}, \vec{B}_{j}^{\dagger}\right]= \pm \delta_{i j} . \tag{2.32}
\end{equation*}
$$

The sign of the distribution depends on the order of multiplication of the operators $\hat{b}_{i}$ and $\hat{b}_{i}^{\dagger}$ and is with the chosen definition of the vectors $B$ and $B^{\dagger}$ positive for the first L entries and negative from $L+1$ to $2 L$.

[^4]Consequently the matrix S is an involution ${ }^{6}$ and given by:

$$
S=\left(\begin{array}{c|c}
I & 0  \tag{2.33}\\
\hline 0 & -I
\end{array}\right) .
$$

With I the L-dimensional identity matrix. This leads to the first condition for the transformation ${ }^{7} \mathrm{U}$ :

$$
\begin{equation*}
\left[\vec{B}, \vec{B}^{\dagger}\right]=U\left[\vec{P}, \vec{P}^{\dagger}\right] U^{\dagger}=U S U^{\dagger} \stackrel{!}{=} S \tag{2.34}
\end{equation*}
$$

At this point it is worth mentioning, that the commutator of two vectors of creation and annihilation operators has to be defined first, what is done in equation E.2. Furthermore U has to be a real transformation for this condition.
Using $S^{2}=I$, this relation can be rewritten as:

$$
\begin{align*}
U S U^{\dagger} & =S \\
U S U^{\dagger} S & =I \\
U^{-1} U S U^{\dagger} S U & =U^{-1} U \\
U^{\dagger} S U & =S \tag{2.35}
\end{align*}
$$

The second condition is, that the Hamiltonian has to be diagonal:

$$
\begin{align*}
& \vec{B}^{\dagger} M \vec{B}=\vec{P}^{\dagger} U^{\dagger} M U \vec{P} \stackrel{!}{=} \vec{P}^{\dagger} D \vec{P} \\
& \quad \Longrightarrow U^{\dagger} M U=D \tag{2.36}
\end{align*}
$$

[^5]with a diagonal matrix D .

The following construction of the transformation $U$ and the proofs that both conditions can be fulfilled are taken from [1].
Note that some variables are defined differently as it is done in the cited work. For example the matrix M was there defined as SM.

Multiplying equation 2.36 from the left with $U S$ and using equation 2.34 leads to:

$$
\begin{align*}
U S U^{\dagger} M U & =U S D  \tag{2.37}\\
S M U & =U S D
\end{align*}
$$

Because of S and D being both diagonal matrices, also their product is diagonal. Hence equation 2.37 is an eigenvalue equation of the matrix SM with eigenvalues $e_{i}=(S D)_{i i}= \pm D_{i i}$. The sign of the diagonal elements is again positive for the first L entries and negative for the last $\mathrm{L}+1$ to 2 L ones. Since the Matrix SM is not hermitian its not guaranteed, that it has real eigenvalues, but that is necessary from a physical point of view, because the eigenvalues $e_{i}$ represent the excitation energies, which, of course, have to be real. In addition to this they also must not be negative, because otherwise the energy would not be bound from below.

When the eigenvalues $e_{i}$ turn out to be complex or negative this indicates an instability in the the system, which means that the approximation done here of neglecting third and fourth order terms in the fluctuation operators was insufficient. In this work however the energies are real and positive for the harmonic potential.
We are left with the proof, that condition 2.35 can really be fulfilled:

It should be shown that:

$$
\begin{equation*}
X:=U^{\dagger} S U=S \tag{2.38}
\end{equation*}
$$

The eigenvalue equation can be written as:

$$
U^{-1} S M U=D,
$$

exploiting the hermiticity of $\mathrm{M}, \mathrm{X}$ and D leads to:

$$
X D=U^{\dagger} S S M U=U^{\dagger} M U=\left(U^{\dagger} M U\right)^{\dagger}=(X D)^{\dagger}=D X
$$

or with other words:

$$
[X, D]=0 .
$$

Commutating operators can be diagonalized simultaneously, we have just to be careful when the eigenvalues of SM are degenerated to use a proper linear combination of the eigenvectors of the subspace.
With X being diagonal its not hard to transform it into S where all diagonal elements are $\pm 1$. It's enough just to replace $U$ by UV where:

$$
V_{i i}=\frac{1}{\sqrt{\left|X_{i i}\right|}} .
$$

This is only possible if $X_{i i} \neq 0 \forall i$. But thats always fulfilled, because if we assume $X_{l l}=\vec{U}_{l} S \vec{U}_{l}=0$ where $\vec{U}_{l}$ is the l-th column of U , then $S \vec{U}_{l}$ would be orthogonal to $\vec{U}_{l}$ and hence be an element of the $2 N-1$ dimensional space $R_{l}$ orthogonal to $\vec{U}_{l}$. From 2.38 we get that the vectors $\vec{U}_{1}, \ldots, \vec{U}_{l-1}, \vec{U}_{l+1}, \vec{U}_{2 N}$ also belong to the space $R_{l}$ and hence, assuming that all eigenvectors are orthogonal ${ }^{8}$, span $R_{l}$. From 2.38 also follows, that $S \vec{U}_{l}$ is orthogonal to all of these vectors $\vec{U}_{1}, \ldots, \vec{U}_{l-1}, \vec{U}_{l+1}, \vec{U}_{2 N}$ and thus cannot be part of the space $R_{l}$. Which proves that the assumption $\vec{U}_{l} S \vec{U}_{l}=0$ cannot be true.

Since the product of two diagonal matrices commutes (VD=DV) the

[^6]eigenvalue equation is still valid, but the transformation UV is not guaranteed to be unitary, since the eigenvectors may not be normalized:
$$
M(U V)=(M U) V=(U D) V=(U V) D
$$

But now:

$$
\begin{equation*}
\bar{X}_{i i}=\left(V U^{\dagger} S U V\right)_{i i}=(V X V)_{i i}=\frac{X_{i i}}{\sqrt{X_{i i}^{2}}}=\operatorname{sgn}\left(X_{i i}\right) \tag{2.39}
\end{equation*}
$$

The only problem which has to be faced is, that for all diagonal values of X which are negative also the corresponding energies have to be negative. Furthermore the number of negative eigenvalues has to be $L$, since in SD half of the entries are negative. But this turns out to be true for this model with the harmonic potential for all tested cases.

Having insured, that both conditions, the bosonic commutation relations and the Hamiltonian being diagonal can be fulfilled, the Hamiltonian is given by:

$$
\begin{align*}
H=\Delta+ & \vec{P}^{\dagger} D \vec{P}=\Delta+\sum_{i=1}^{L} D_{i i} \hat{p}_{i}^{\dagger} \hat{p}_{i}+\sum_{i=L+1}^{2 L} D_{i i} \underbrace{\hat{p}_{i} \hat{p}_{i}^{\dagger}}_{1+\hat{p}_{i}^{\dagger} \hat{p}_{i}}  \tag{2.40}\\
& =\Delta+\operatorname{tr}(D)_{i>L}+\sum_{i=1}^{L}\left(D_{i i}+D_{i+L, i+L}\right) \hat{p}_{i}^{\dagger} \hat{p}_{i}
\end{align*}
$$

$\operatorname{tr}(D)_{i>L}$ means, that the trace of D , which is given by $\sum_{i} D_{i i}$, is performed just over indices i which are greater than $L$.

## Chapter 3

## Results

### 3.1 Free Particles in 1 Dimension

The average value of the number operators $\left\langle\hat{\psi}_{R}^{\dagger} \hat{\psi}_{R}\right\rangle$, which were first introduced in 2.1 and were split in a condensate contribution $\phi(R)$ and a operator $\hat{b}_{R}$ in equation 2.4, is given by:

$$
\begin{equation*}
\left\langle\hat{\psi}_{R}^{\dagger} \hat{\psi}_{R}\right\rangle=|\phi(R)|^{2}+\left\langle\hat{b}_{R}^{\dagger} \hat{b}_{R}\right\rangle \tag{3.1}
\end{equation*}
$$

Since the external potential $V(R)$ is zero this values are place independent and can be calculated for any index R . For convenience $R=0$ is chosen and the place will not be denoted any more.

The simple expression for the condensate density $\phi^{2}$ reads from 2.8:

$$
\phi^{2}=\frac{2 t+\mu}{U}
$$

The expectation value of the fluctuation operators $\left\langle\hat{b}^{\dagger} \hat{b}\right\rangle$ has to be calculated
since only the expectation values for the set of operators $\hat{a}_{k}$ is known:

$$
\begin{aligned}
\left\langle\hat{b}_{0}^{\dagger} \hat{b}_{0}\right\rangle & =\frac{1}{L}\left\langle\sum_{k, k^{\prime}} e^{-i k^{\prime} 0} e^{i k 0} \hat{b}_{k^{\prime}}^{\dagger} \hat{b}_{k}\right\rangle \\
& =\frac{1}{L} \sum_{k, k^{\prime} \neq 0}\left\langle\left(u_{k} \hat{a}_{k}^{\dagger}+v_{k} \hat{a}_{-k}\right)\left(u_{k^{\prime}} \hat{a}_{k^{\prime}}+v_{k^{\prime}} \hat{a}_{-k^{\prime}}^{\dagger}\right)\right\rangle \\
& =\frac{1}{L} \sum_{k, k^{\prime} \neq 0}(u_{k} u_{k^{\prime}}\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{k^{\prime}}\right\rangle+v_{k} v_{k^{\prime}}\langle\underbrace{}_{\left.\left.\delta_{k, k^{\prime}+\hat{a}_{-k^{\prime}}^{\dagger} \hat{a}_{-k}}^{\hat{a}_{-k} \hat{a}_{-k^{\prime}}^{\dagger}}\right\rangle+u_{k} v_{k^{\prime}}\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{-k^{\prime}}^{\dagger}\right\rangle+u_{k^{\prime}} v_{k}\left\langle\hat{a}_{-k} \hat{a}_{k^{\prime}}\right\rangle\right)} \\
& =\frac{1}{L} \sum_{k, k^{\prime} \neq 0}\left(\left(u_{k} u_{k^{\prime}}+v_{k} v_{k^{\prime}}\right)\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{k^{\prime}}\right\rangle+v_{k} v_{k^{\prime}} \delta_{k, k^{\prime}}\right) \\
& =\frac{1}{L} \sum_{k \neq 0}\left(\left(u_{k}^{2}+v_{k}^{2}\right)\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{k}\right\rangle+v_{k}^{2}\right)
\end{aligned}
$$

Since the values $\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{-k^{\prime}}^{\dagger}\right\rangle$ and $\left\langle\hat{a}_{-k} \hat{a}_{k^{\prime}}\right\rangle$ are zero anyway, because they transform one orthogonal basis state into another. With the same argument the expression $\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{k^{\prime}}\right\rangle$ can be replaced by $\left\langle\hat{a}_{k}^{\dagger} \hat{a}_{k}\right\rangle \delta_{k, k^{\prime}}$.
From this point these average values can be calculated using the BoseEinstein statistics 1.1 for a given temperature T. For $T=0$ all these values are zero and the fluctuation reduces to:

$$
\begin{equation*}
\left\langle\hat{b}_{0}^{\dagger} \hat{b}_{0}\right\rangle=\frac{1}{L} \sum_{k \neq 0} v_{k}^{2} \tag{3.2}
\end{equation*}
$$

If the number of lattice sites L is increased the number of k-states increases, what means there are more states closer to $k=0$. So it is interesting to calculate the behavior of $v_{k}^{2}$ for small values of k . Therefore the cosine terms
are expanded into its series up to second order in k :

$$
\begin{aligned}
v_{k}^{2} & =-\frac{1}{2}+\frac{\mu+2 t\left(1+\frac{k^{2}}{2}+\mathcal{O}\left(k^{4}\right)\right)}{2 \sqrt{\left(\mu+2 t+t k^{2}+\mathcal{O}\left(k^{4}\right)\right)^{2}-(\mu+2 t)^{2}}} \\
& =-\frac{1}{2}+\frac{\mu+2 t\left(1+\frac{k^{2}}{2}+\mathcal{O}\left(k^{4}\right)\right)}{2|k| \sqrt{4 t^{2}+2 \mu t+\mathcal{O}\left(k^{2}\right)}|\tilde{k \mid \ll}| \frac{1}{|k|}}
\end{aligned}
$$

This means, that even at zero temperature the fluctuations will diverge as the thermodynamic limit is made since the sum over all discrete k states becomes a integral which diverges. This behavior is illustrated in figure 3.1. That this happens is not surprising since BEC can only take place in systems with more than one dimension. To be precise it occurs in the two dimensional case if the gas is trapped or in the free case just at zero temperature. For three dimensions BEC can take place also for a free gas for higher temperatures than zero [3].


Figure 3.1: Expectation value of the fluctuation $\left\langle\hat{b}_{R=0}^{\dagger} \hat{b}_{R=0}\right\rangle$ for different values of L. The model parameter were set to: $t=U=1$ and $n=\frac{N}{L}=10$. As expected the fluctuation diverges logarithmically with growing $L$.

### 3.2 Particles in a Harmonic Potential

In that case a potential $V(R)=\alpha\left(R-\frac{L}{2}\right)^{2}$, with arbitrary constant $\alpha$, was used. Again the expectation value of the number operator can be calculated as:

$$
\begin{equation*}
\left\langle\hat{\psi}_{R}^{\dagger} \hat{\psi}_{R}\right\rangle=|\phi(R)|^{2}+\left\langle\hat{b}_{R}^{\dagger} \hat{b}_{R}\right\rangle . \tag{3.3}
\end{equation*}
$$

$\phi(R)$ is determined by the Gross-Pitaevskii equation:

$$
\left.\left((V(R)-\mu)+U|\phi(R)|^{2}\right)\right) \phi(R)-t(\phi(R+1)+\phi(R-1))=0 .
$$

This equation has ot be solved numerically, because the particle interaction term $U|\phi(R)|^{2}$ makes an analytical approach impossible. Finding the solutions can be done using an iteration, where we start with a certain $\phi_{0}$ calculate with that the particle interaction term $U|\phi(R)|^{2}$. After doing that a simple eigenvalue equation remains. Then we use the eigenvector to the smallest eigenvalue $\mu$ as the new $\phi_{0}$ and iterate until it converges.
The eigenvalue equation for each iteration step is then given by:

$$
\begin{equation*}
\underline{\underline{M}} \phi=\mu \phi . \tag{3.4}
\end{equation*}
$$

With the hermitian and real matrix:
$\underline{\underline{M}}=\left(\begin{array}{ccclc}V(1)+U\left|\phi_{0}(1)\right|^{2} & -t & 0 & \cdots & -t \\ -t & V(2)+U\left|\phi_{0}(2)\right|^{2} & -t & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -t & 0 & \cdots & -t & V(L)+U\left|\phi_{0}(L)\right|^{2}\end{array}\right)$.

However this procedure is not very stable and just gives results for a very limited range of parameters U, t and $N_{0}$. Because of this I decided to use another approach. The normalization of the condensate amplitude is:

$$
\begin{equation*}
N_{0}-\sum_{R}|\phi(R)|^{2}=0 \tag{3.6}
\end{equation*}
$$

Together with the GPE this can be considered as a $\mathrm{L}+1$ dimensional function $\vec{F}(\vec{y})$ from which we want to know the zeros. $\vec{y}$ is a $\mathrm{L}+1$ dimensional vector with $\phi(1), \ldots \phi(L)$ as the first L entries and with the chemical potential $\mu$ as the last.
The zeros of this function can be easily found using the Newton algorithm:

$$
\begin{equation*}
\vec{y}_{n+1}=\vec{y}_{n}-\left(J\left(y_{n}\right)\right)^{-1} \vec{F}\left(\vec{y}_{n}\right), \tag{3.7}
\end{equation*}
$$

with J the jacobi matrix of $\vec{F}$.
This procedure works pretty well. However we have to make sure that we truly find a state where the energy is minimal. The left hand side of the GPE is $\frac{d E}{d \phi(R)}$. If the jacobi matrix

$$
J\left(R, R^{\prime}\right)=\frac{d^{2} E}{d \phi(R) d \phi\left(R^{\prime}\right)}
$$

is positive definite (all eigenvalues are positive for hermitic matrices), $\phi(R)$ is a local minimum. Note that the jacobi matrix $J\left(R, R^{\prime}\right)$ is except the last row and column ${ }^{1}$ the same as the one that was used in the Newton algorithm 3.7.

In figures 3.2, 3.3 and 3.4 the results of the Newton algorithm for different values of the hopping strength t , the interaction strength U and the number of particles in the ground statet $N_{0}$ can be seen. As expected higher values of these parameters cause the particles to spread out more over the whole lattice, although their potential energy ${ }^{2}$ increases.

[^7]

Figure 3.2: $|\phi(R)|$ as a function of the lattice site R for different values of the hopping strength t . As t increases the particles spread out over the whole lattice, although they have a higher potential energy at the borders. The model parameter for the calculation were set to: $\alpha=1, U=1$ and $N_{0}=100$.


Figure 3.3: $|\phi(R)|$ as a function of the lattice site R for different values of the interaction strength U. Again the particles spread out more the higher the value of U is chosen. The model parameter for the calculation were set to: $\alpha=1, t=1$ and $N_{0}=100$.


Figure 3.4: $|\phi(R)|$ as a function of the lattice site R for different values of number of particles in the ground state $N_{0}$. Like in the cases before a higher value of the parameter $N_{0}$ lets the particles spread out over the whole chain. On first thought one could assume that the form of the curve should stay the same, just the hight differs when changing $N_{0}$. This is because in the GPE $\phi(R)$ contributes quadratically and not just linearly. So instead of increasing $\phi(R)$ at a certain place R much more energy can be saved if the particles move to the borders. The model parameter for the calculation were set to: $\alpha=1, t=10$ and $U=5$.

To calculate the fluctuations $\left\langle\hat{b}_{R}^{\dagger} \hat{b}_{R}\right\rangle$ of the mean occupation $|\phi(R)|^{2}$, first the multi-mode Bogoliubov transformation UV has to be constructed. U consists of the eigenvectors of the matrix SM, with M defined in equation 2.31. This eigenvalue equation arises from the condition of the Hamiltonian to be diagonal. In addition to this a orthogonal basis from a degenerate subspace of SM has to be choosen.

The matrix V, on the other hand, arises from the second condition on the transformation: to conserve the bosonic commutation relation (see equation 2.34). V is a diagonal matrix and insures that the commutator of two poperators is really 1 and not just a number, what normally occurs in the numeric calculations. Furthermore the order of the eigenvectors has to be changed since $S$ is strictly defined with diagonal elements +1 for the first $L$ indices and -1 for the other half.
With that it is known how the operators $\vec{B}$ transforms into the operators $\vec{P}$. From the latter the expectation value (equation 1.1) is known, since the Hamiltonian is diagonal in them.

Since all the above mentioned procedures are pretty time consuming to program I decided not to calculate any of the properties and stop at the point where I have calculated the energies and the Multi-Mode Bogoliubov transformation.

## Appendix A

## Substituting the Bogoliubuv approximation into the Hamiltonian

Starting from the Hamiltonian:

$$
H=\underbrace{\sum_{R}(V(R)-\mu) \hat{\psi}_{R}^{\dagger} \hat{\psi}_{R}}_{H_{1}}-t \underbrace{\sum_{R} \hat{\psi}_{R}^{\dagger} \hat{\psi}_{R+1}+\hat{\psi}_{R} \hat{\psi}_{R+1}^{\dagger}}_{H_{2}}+\underbrace{\frac{U}{2} \sum_{R}\left(\hat{\psi}_{R}^{\dagger}\right)^{2}\left(\hat{\psi}_{R}\right)^{2}}_{H_{3}}
$$

and substituting:

$$
\hat{\psi}_{R}=\phi(R)+\hat{b}_{R},
$$

leads for the first term called $H_{1}$ to:

$$
H_{1}=\sum_{R}(V(R)-\mu)\left(|\phi(R)|^{2}+\phi(R) \hat{b}_{R}^{\dagger}+\phi(R) \hat{b}_{R}+\hat{b}_{R}^{\dagger} \hat{b}_{R}\right),
$$

equally the next term of the Hamiltonian $H_{2}$ is given by:

$$
\begin{array}{r}
H_{2}=-t \sum_{R} 2 \phi(R) \phi(R+1)+\hat{b}_{R+1} \phi(R)+\hat{b}_{R} \phi(R+1)+ \\
\hat{b}_{R+1}^{\dagger} \phi(R)+\hat{b}_{R}^{\dagger} \phi(R+1)+\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger} .
\end{array}
$$

With an index transformation $R+1=R^{\prime}$ and using the periodic boundary conditions in the terms linear in $\hat{b}_{R+1}$ and $\hat{b}_{R+1}^{\dagger}, H_{2}$ can be written as:

$$
\begin{array}{r}
H_{2}=-t \sum_{R} 2 \phi(R) \phi(R+1)+\hat{b}_{R} \phi(R-1)+\hat{b}_{R} \phi(R+1)+ \\
\hat{b}_{R}^{\dagger} \phi(R-1)+\hat{b}_{R}^{\dagger} \phi(R+1)+\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger} .
\end{array}
$$

Similar calculation for the last term $H_{3}$ :

$$
\begin{gathered}
H_{3}=\frac{U}{2} \sum_{R} \phi(R)^{4}+2 \hat{b}_{R} \phi(R)^{2} \phi(R)+2 \hat{b}_{R}^{\dagger} \phi(R)^{2} \phi(R)+ \\
\left.\hat{b}_{R}^{2} \phi(R)^{2}+\hat{\left(b_{R}^{\dagger}\right.}\right)^{2} \phi(R)^{2}+4|\phi(R)|^{2} \hat{b}_{R}^{\dagger} b_{R}+ \\
2\left(b_{R}^{\dagger}\right)^{2} \hat{b}_{R} \phi(R)+2 \hat{b}_{R}^{\dagger} b_{R}^{2} \phi(R)+\left(b_{R}^{\dagger}\right)^{2} \hat{b}_{R}^{2} .
\end{gathered}
$$

Adding those three parts together and collecting terms like exponents in the fluctuation operators results in equation 2.5.

## Appendix B

## Performing the Fourier transformation for the free particles

Starting point is the Hamiltonian:

$$
H=C+\sum_{R} \underbrace{A \hat{b}_{R}^{\dagger} \hat{b}_{R}}_{H_{1}}+\underbrace{B\left(\hat{b}_{R}^{2}+\hat{\left.\left(b_{R}^{\dagger}\right)^{2}\right)}\right.}_{H_{2}} \underbrace{-t\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}\right)}_{H_{3}} .
$$

A Fourrier transformation given in equations 2.13 is performed. Again the Hamiltonian is split up into 3 parts. For the first term called $H_{1}$ :

$$
\begin{align*}
H_{1} & =\sum_{R} A \frac{1}{L} \sum_{k, k^{\prime}} e^{i\left(k-k^{\prime}\right) R} \hat{b}_{k^{\prime}}^{\dagger} \hat{b}_{k} \\
& =\sum_{k, k^{\prime}} A \hat{b}_{k^{\prime}}^{\dagger} \hat{b}_{k} \frac{1}{L} \sum_{R} e^{i\left(k-k^{\prime}\right) R}  \tag{B.1}\\
& =\sum_{k, k^{\prime}} A \hat{b}_{k^{\prime}}^{\dagger} \hat{b}_{k} \delta_{k, k^{\prime}}=\sum_{k} A \hat{b}_{k}^{\dagger} \hat{b}_{k} .
\end{align*}
$$

Where a representation of the delta distribution (the Kronecker delta in that case) $\delta_{k, k^{\prime}}=\frac{1}{L} \sum_{R} e^{i\left(k-k^{\prime}\right) R}$ was used in the second line.

Fourier transforming the second term leads to:

$$
\begin{aligned}
H_{2} & =B \sum_{R} \hat{b}_{R}^{2}+\left(\hat{b}_{R}^{\dagger}\right)^{2} \\
& =B \sum_{k, k^{\prime}} \frac{1}{N} \sum_{R} e^{i\left(k^{\prime}+k\right) R} \hat{b}_{k} \hat{b}_{k^{\prime}}+e^{-i\left(k^{\prime}+k\right) R} \hat{b}_{k}^{\dagger} \hat{b}_{k^{\prime}}^{\dagger} \\
& =B \sum_{k, k^{\prime}}\left(\hat{b}_{k} \hat{b}_{k^{\prime}}+\hat{b}_{k}^{\dagger} \hat{b}_{k^{\prime}}^{\dagger}\right) \delta_{k,-k^{\prime}} \\
& =B \sum_{k} \hat{b}_{k} \hat{b}_{-k}+\hat{b}_{k}^{\dagger} \hat{b}_{-k}^{\dagger}
\end{aligned}
$$

Finally the last term becomes:

$$
\begin{aligned}
H_{3} & =-t \sum_{R} \hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger} \\
& =-t \sum_{k, k^{\prime}}(e^{i k^{\prime}} \hat{b}_{k}^{\dagger} \hat{b}_{k^{\prime}}+e^{-i k} \hat{b}_{k} \hat{b}_{k^{\prime}}^{\dagger} \underbrace{\frac{1}{N} \sum_{R} e^{i\left(k-k^{\prime}\right) R}}_{\delta_{k, k^{\prime}}} \\
& =-t \sum_{k} e^{i k} \hat{b}_{k}^{\dagger} \hat{b}_{k}+e^{-i k}\left(1+\hat{b}_{k}^{\dagger} \hat{b}_{k}\right) \\
& =-t \sum_{k} e^{i k}-2 t \sum_{k} \hat{b}_{k}^{\dagger} \hat{k}_{k} \cos k
\end{aligned}
$$

Where in the third line the bosonic commutation relations were used. That the set operators $\hat{b}_{k}$ and $\hat{b}_{k}^{\dagger}$ really obey them is shown in Appendix C.

## Appendix C

## Proof of conservation of bosonic- commutation relation

The proof will be done for an expansion of operators $\hat{b}_{R}$ and $\hat{b}_{R}^{\dagger}$ in an arbitrary set of orthonormal functions $\psi_{k}(R)$ with operators $\hat{b}_{k}$ and $\hat{b}_{k}^{\dagger}$ :

$$
\begin{align*}
& \hat{b}_{R}=\sum_{k} \psi_{k}(R) \hat{b}_{k} \\
& \hat{b}_{R}^{\dagger}=\sum_{k} \psi_{k}^{*}(R) \hat{b}_{k}^{\dagger} \tag{C.1}
\end{align*}
$$

Multiplying the first line with $\psi_{k^{\prime}}^{*}$ and the second one with $\psi_{k^{\prime}}$ and summing over all $R$ leads to:

$$
\begin{align*}
& \sum_{R} \hat{b}_{R} \psi_{k^{\prime}}^{*}(R)=\sum_{k} \hat{b}_{k} \sum_{R} \psi_{k}(R) \psi_{k^{\prime}}^{*}(R)=\hat{b}_{k^{\prime}} \\
& \sum_{R} \hat{b}_{R}^{\dagger} \psi_{k^{\prime}}(R)=\sum_{k} \hat{b}_{k}^{\dagger} \underbrace{\sum_{R} \psi_{k}^{*}(R) \psi_{k^{\prime}}(R)}_{\delta_{k, k^{\prime}}}=\hat{b}_{k^{\prime}}^{\dagger} \tag{C.2}
\end{align*}
$$

Calculation now the commutator $\left[\hat{b}_{k}, \hat{b}_{k}^{\dagger}\right]$ :

$$
\begin{equation*}
\left[\hat{b}_{k}, \hat{b}_{k^{\prime}}^{\dagger}\right]=\sum_{R, R^{\prime}} \psi_{k}^{*}(R) \psi_{k^{\prime}}\left(R^{\prime}\right) \underbrace{\left[\hat{b}_{R}, \hat{b}_{R^{\prime}}^{\dagger}\right]}_{\delta_{R, R^{\prime}}}=\sum_{R} \psi_{k}^{*}(R) \psi_{k^{\prime}}(R)=\delta_{k, k^{\prime}} . \tag{C.3}
\end{equation*}
$$

That the commutators $\left[\hat{b}_{k}^{\dagger}, \hat{b}_{k^{\prime}}^{\dagger}\right]$ and $\left[\hat{b}_{k}, \hat{b}_{k^{\prime}}\right]$ vanish is trivial.
Hence it has been proven, that if the set of operators $\hat{b}_{R}$ and $\hat{b}_{R}^{\dagger}$ obey the commutation relation so do the operators $\hat{b}_{k}$ and $\hat{b}_{k}^{\dagger}$.

## Appendix D

## Calculating the $2 L \times 2 L$ matrix for the multi-mode Bogoliubov transformation

The goal is to find a matrix M which fulfills:

$$
\begin{equation*}
\left.\vec{B}^{\dagger} M \vec{B}=\sum_{R}\left[\zeta(R)\left(\hat{b}_{R}^{\dagger} \hat{b}_{R}+\hat{b}_{R} \hat{b}_{R}^{\dagger}\right)+\eta(R)\left(\hat{b}_{R}^{2}+\hat{\left(b_{R}^{\dagger}\right.}\right)^{2}\right)-\bar{t}\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R+1} \hat{b}_{R}^{\dagger}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}+\hat{b}_{R+1}^{\dagger} \hat{b}_{R}\right)\right] \tag{D.1}
\end{equation*}
$$

The product $B^{\dagger} M B$ can be rewritten as:

$$
\begin{align*}
\vec{B}^{\dagger} M \vec{B}= & \sum_{m=1}^{2 L} B_{m}^{\dagger} \sum_{n=1}^{2 L} M_{m n} B_{n}=\sum_{m=1}^{2 L} B_{m}^{\dagger}\left(\sum_{k=1}^{L} M_{m k} b_{k}+\sum_{l=L+1}^{2 L} M_{m l} b_{l}^{\dagger}\right) \\
= & \sum_{i=1}^{L} \sum_{k=1}^{L} M_{i k} b_{i}^{\dagger} b_{k}+\sum_{i=1}^{L} \sum_{l=L+1}^{2 L} M_{i l} b_{i}^{\dagger} b_{l}^{\dagger}+  \tag{D.2}\\
& \sum_{j=L+1}^{2 L} \sum_{k=1}^{L} M_{j k} b_{j} b_{k}+\sum_{j=L+1}^{2 L} \sum_{l=L+1}^{2 L} M_{j l} b_{j} b_{l}^{\dagger}
\end{align*}
$$

Because the multiplication of a Matrix with a vector is linear it is usefull to split the sum into three terms and calculate the Matrix $M_{i}$ for each of them individually.

The first term of D. 1 leads to:

$$
\begin{equation*}
\vec{B}^{\dagger} M_{1} \vec{B} \stackrel{!}{=} \sum_{R} \zeta(R)\left(\hat{b}_{R}^{\dagger} \hat{b}_{R}+\hat{b}_{R} \hat{b}_{R}^{\dagger}\right) \tag{D.3}
\end{equation*}
$$

With the last line of equation D. 2 it can be seen, that $M_{1}$ has to fulfill:

$$
M_{1, i j}= \begin{cases}\zeta(i) \cdot \delta_{i, j}, & \forall \mathrm{i}, \mathrm{j} \in[1, L]  \tag{D.4}\\ \zeta(i-L) \cdot \delta_{i, j}, & \forall \mathrm{i}, \mathrm{j} \in[L+1,2 L] \\ 0, \text { else } & \end{cases}
$$

The matrix $M_{2}$ has to satisfy:

$$
\begin{equation*}
\vec{B}^{\dagger} M_{2} \vec{B}=\sum_{R} \eta(R)\left(\hat{b}_{R}^{2}+\hat{\left(b_{R}^{\dagger}\right)^{2}}\right) \tag{D.5}
\end{equation*}
$$

Equating coefficients from D. 2 gives the matrix $M_{2}$ :

$$
M_{2, i j}=\left\{\begin{array}{l}
\eta(i) \cdot \delta_{i+L, j}, \forall \mathrm{i} \in[1, L], j \in[L+1,2 L]  \tag{D.6}\\
\eta(i) \cdot \delta_{i, j+L}, \forall \mathrm{i} \in[L+1,2 L], j \in[1, L] \\
0, \text { else }
\end{array}\right.
$$

$M_{3}$ finally has to fulfill:

$$
\begin{equation*}
\vec{B}^{\dagger} M_{3} \vec{B}=\sum_{R}-\bar{t}\left(\hat{b}_{R}^{\dagger} \hat{b}_{R+1}+\hat{b}_{R+1} \hat{b}_{R}^{\dagger}+\hat{b}_{R} \hat{b}_{R+1}^{\dagger}+\hat{b}_{R+1}^{\dagger} \hat{b}_{R}\right) \tag{D.7}
\end{equation*}
$$

so that:

$$
M_{3, i j}=\left\{\begin{array}{l}
-\bar{t} \cdot \delta_{i+1, j} \forall i \in[1, L-1]  \tag{D.8}\\
-\bar{t} \cdot \delta_{i, j+1} \forall j \in[1, L-1] \\
-\bar{t} \cdot \delta_{i+1, j} \forall i \in[L+1,2 L-1] \\
-\bar{t} \cdot \delta_{i, j+1} \forall j \in[L+1,2 L-1] \\
-\bar{t} \text { for } i=L \text { and } j=1 \\
-\bar{t} \text { for } i=1 \text { and } j=L \\
-\bar{t} \text { for } i=2 L \text { and } j=L \\
-\bar{t} \text { for } i=L \text { and } j=2 L \\
0, \text { else }
\end{array}\right.
$$

This complicated expression means, that if $M_{3}$ is divided into four sectors, like it is done in 2.31 , it is an matrix with the element $-\bar{t}$ above and under the main diagonal of the upper left and lower right sector. In addition to this there are four extra entries at the corners of these sectors because of the periodic boundary condition.

The whole matrix M is then simply given by the sum of all of these 3 matrices, what proofs 2.31.

## Appendix E

## Derivation of the condition for the commutation relations for the multi-mode Bogoliubov transformation

The goal to derivate that if $\vec{B}=U \vec{P}$ then:

$$
\begin{equation*}
\left[\vec{B}, \vec{B}^{\dagger}\right]=U\left[\vec{P}, \vec{P}^{\dagger}\right] U^{\dagger} \tag{E.1}
\end{equation*}
$$

will be achieved in matrix notation. Therefore it is important first to define what actually the commutator of two vectors is. The simple expression $\left[\vec{B}, \vec{B}^{\dagger}\right]=\vec{B} \vec{B}^{\dagger}-\vec{B}^{\dagger} \vec{B}$ is in fact not even defined, since the $\vec{B} \vec{B}^{\dagger}$ is a matrix of operators and $\vec{B}^{\dagger} \vec{B}$ is a scalar operator. ${ }^{1}$

Because the commutator just makes sense for single elements of these vectors

[^8]like in 2.32 we can see that:
\[

$$
\begin{equation*}
\left[\vec{B}, \vec{B}^{\dagger}\right]=\vec{B} \vec{B}^{\dagger}-\left(\left(\vec{B}^{\dagger}\right)^{T}(\vec{B})^{T}\right)^{\dagger} \tag{E.2}
\end{equation*}
$$

\]

leads to the desired matrix S. Unlike in matrices with scalar entries it's not allowed to simplify $\left(\vec{B}^{\dagger}\right)^{T}(\vec{B})^{T}$ to $\left(\vec{B} \vec{B}^{\dagger}\right)^{T}$, because the operators doesn't commute. This can be recognized by just looking on the first diagonal entries of both expressions.
With the commutator defined it is possible to plug in the multi mode Bogoliubov transformation $\vec{B}=U \vec{P}$ :

$$
\begin{aligned}
{\left[\vec{B}, \vec{B}^{\dagger}\right] } & =U \vec{P} \vec{P}^{\dagger} U^{\dagger}-\left(\left(\vec{P}^{\dagger} U^{\dagger}\right)^{T}(U \vec{P})^{T}\right)^{\dagger} \\
& =U \vec{P} \vec{P}^{\dagger} U^{\dagger}-\left(\left(U^{\dagger}\right)^{T} \overrightarrow{\left.\left(P^{\dagger}\right)^{T} \vec{P}^{T} U^{T}\right)^{\dagger}}\right. \\
& =U \vec{P} \vec{P}^{\dagger} U^{\dagger}-\left(U^{T}\right)^{\dagger}\left(\left(\vec{P}^{\dagger}\right)^{T}(\vec{P})^{T}\right)^{\dagger} U^{T} \\
& =U\left[\vec{P}, \vec{P}^{\dagger}\right] U^{\dagger}
\end{aligned}
$$

The last line is only correct if U is assumed to be a real transformation (all entries are real).
Note that in the second line instead of $\left(\vec{P}^{\dagger} U^{\dagger}\right)^{T}$ the expression $\left(U^{\dagger}\right)^{T} \overrightarrow{\left(P^{\dagger}\right)^{T}}$ can be written, because the multiplication of an operator from $\vec{P}^{\dagger}$ with a scalar element of U commutes.

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[^0]:    ${ }^{1}$ See Appendix A for detailed calculation.

[^1]:    ${ }^{2}$ See Appendix B for detailed calculation.

[^2]:    ${ }^{3} v_{-k}=v_{k}, u_{-k}=u_{k}$ and $\cos (-k)=\cos k$

[^3]:    ${ }^{4}$ The average values $\phi(R)$ were calculated with the GPE 2.6 , hence terms linear in the fluctuation operators have already vanished. Terms of third or higher order in the fluctuation operators are neglected

[^4]:    ${ }^{5}$ All not listed entries are zero.

[^5]:    ${ }^{6} S \circ S=I$ or $S=S^{-1}$
    ${ }^{7}$ See Appendix E for a derivation for this formula.

[^6]:    ${ }^{8}$ Eigenvectors to degenerate eigenvalues were already chosen orthogonal.

[^7]:    ${ }^{1}$ The last row in the Jacobi matrix used in the Newton algorithm came from the normalization 3.6. The last column from the derivations of the GPE regarding the chemical potential.
    ${ }^{2}$ In this case I mean with potential energy just the contribution of the external potential $\mathrm{V}(\mathrm{R})$, although the energy from the interaction term $U|\phi(R)|^{2}$ would also count as potential energy.

[^8]:    ${ }^{1} \vec{B}$ is a column vector and $\vec{B}^{\dagger}$ a row vector.

