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Bachelor's Thesis

Superfluid to Mott insulator transition in the Bose-Hubbard model

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Abstract

In this thesis, it will be considered an interacting gas of bosons on a d-dimensional cubic lattice at the temperature $T = 0$. One sees that this model exhibit a quantum phase of matter, the so-called Mott-insulating phase, which corresponds to an average integer occupation of the lattice sites and which is accompiened with a vanishing compressibility. In addition it contains a superfluid phase which indicates a phase transition between these phases. By using a mean-field approach and the non-degenerate pertubation theory, the phase diagram of the model will be determined by assuming a small transition amplitude. The analysis of the phase boundary shows, that there are points from which one can conclude a different physical mechanism leading to the transition then anywhere else on the boundary. These points are not related to a change in the average occupation number.
These results will be recapped using field-theoretical methods and afterwards effective field theories characterizing the model in the vicinity of the phase boundary will be derived. It arises two field theories which bear the two mechanisms. These are organized in different universality classes. On one hand the universality class of the so-called XY-model and on the other hand the one of the dilute bose gas. These are analysed and intepreted physically.

Zusammenfassung

In dieser Arbeit wird ein wechselwirkendes Gas von Bosonen auf einem d-dimensionalen kubischen Gitter bei der Temperatur $T = 0$ betrachtet. Man sieht, dass dieses Modell eine Quantenpahse besitzt, die sogenante Mott-Isolator Phase, welche einer mittleren, ganzzahligen Besetzung der Gitterplätze entspricht und mit einer verschwindenden Kompressibilität einhergeht. Zudem enthält es eine Suprafluide Phase, was auf einen Phasenübergang zwischen diesen Phasen schließen lässt. Durch Annahme einer kleinen Übergangsamplitude zwischen verschieden Gitterplätzen wird mit Hilfe der nicht entarteten Störungstheorie und der Molekularfeldtheorie das Phasendiagramm des Modells bestimmt. Die Analyse der Phasenübergangslinie zeigt, dass es Punkte darin gibt, die auf einen anderen physikalischen Mechanismus, der zum Phasenübegang führt, folgern lassen als im Rest der Übergangslinie. Diese Punkte sind nicht mit einem Wechsel der mittleren Besetzungszahl verbunden, wie der Rest der Übergangslinie.
Durch feldtheoretische Methoden werden diese Ergebnisse rekapituliert und die effektiven Feldttheorien hergeleitet, welche das Modell in der Nähe der Übergangslinie beschreibt. Es ergeben sich zwei Feldtheorien, die diese beiden Mechanismen in sich tragen und in verschiedene Universalitätsklassen eingeteilt werden. Einmal die Universalitätsklasse des sogenannten XY-Modells und anderseits die des verdünnten Bose Gases. Diese werden analysiert und physikalisch inerpretiert.

Contents

1 Introduction

The reductionist hypothesis does not by any means imply a "constructionist" one: The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe.
- P. W. Anderson

As Anderson elucidated, it is not possible to describe a many-body-system sytem on the basis of the fundamental laws for the individual constituents. Therefore, a shift to the methods of statistical physics allows to shed light on the physics of many-body problems.

Nowadays, ultracold atomic and molecular systems are the frontiers of modern quantum physics, and are considered to provide the most controllable systems for the study of many-body physics. It is believed that these systems will also find highly non-trivial applications in quantum information and quantum metrology and will serve as powerfull quantum simulators.

In this thesis we focus on the Bose-Hubbard model, which applies to a Bose gas in an optical lattice. It will be shown that this model contains a quantum phase of matter called the Mott-insulator phase, as first discussed by Fisher et al. [1]. Moreover, the Bose gas is predicted to undergo a quantum phase transition from the superfluid state to the Mott-insulator state as a function of the interaction potential. This quantum phase transition has recently been observed in a seminal experiment by Greiner et al. [2], and has attracted much attention. It showed that ultracold atoms in an optical lattice can be used to stimulate various lattice models of fundamental importance to condensed-matter-physics.

The phase diagramm of the model is derived using a mean-field approach combined with the non-degenerate pertubation theory. It will be looked closely at the effects that lead to the transition and at the peculiarities of the phase boundary itself.

By starting from the microscopic theory for this model and using the functional integral representation of the partition function, it will be discovered two distinced effective field theories which describe the quantum phase transition in the vicinity of the phase boundaries. Which differ only in their dynamical behaviour, one has an emergend lorentz invariance caused due to particle and hole symmetry and the other one describes the theory of a dilute Bose gas. Those will be intepreted as different physical mechanisms that lead to the transition from the Mott-insulator to the superfluid.

A Renormalization Group analysis of the field theories is only briefly discussed and stated some results. One can find a comprehensive discussion of these results for instance in Sachdev book about Quantum phase transitions [3] and in the book of Stoof et al. "Ultracold Quantum Fields" [4].

2 Theory

2.1 Functional integral representation of the partition function

From statistical physics it is known that the properties of an interacting many-body system follows from the grand-canonical partition function

$$Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right) = \sum_n \left\langle n \left| e^{-\beta(H-\mu N)} \right| n \right\rangle \tag{2.1}$$

where $\beta = 1/k_B T$, μ is the chemical potential and $\left\{ |n\rangle \right\}$ is a set of orthonormal and complete states. The goal is to evaluate this quantity by rewriting it as a **functional integral** which will allow us to go beyond the mean-field approach of the model and to use the general framework of the renormalization group. First, one has to describe the formalism of 2^{nd} **quantization**

2.1.1 2^{nd} quantization

The formalism of 2^{nd} quantization is done in many textbooks, e.g [5],[6]. This is just a short introduction of the most important aspects without prove of many relations.
Also, we will focus only on the bosonic case because it is the one used in the model of this thesis.
Working in the formalism of 2^{nd} quantization is an efficient method to characterize and manipulate many-body wavefunctions because we want to describe systems with a large number of particles which do not have to be constant. This is why use the grand-canonical partition function is used. Considering the properly symmetrized wave function for N indistinguishable bosonic particles

$$\psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_i, ..., \vec{x}_j, ..., \vec{x}_N) = +\psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_j, ..., \vec{x}_i, ..., \vec{x}_N)$$

one can expand this wavefunction into single-particle eigenstates $\phi_\alpha(\vec{x})$.

$$\psi(x_1, ..., x_N) = \sum_{\alpha_1,...,\alpha_N} c_{\alpha_1,...,\alpha_N} \frac{1}{\sqrt{N!}} \sum_{permP} \phi_{\alpha_1}(\vec{x}_{P(1)}) \cdots \phi_{\alpha_N}(\vec{x}_{P(N)}) \tag{2.2}$$

Respectively, written equivalently in a abstract form using $\phi_\alpha(\vec{x}) = \langle \vec{x} \,|\, \alpha \rangle$

$$|\alpha_1, ..., \alpha_N\rangle = \frac{1}{\sqrt{N!}} \sum_{permP} \left|\alpha_{P(1)}\right\rangle \cdots \left|\alpha_{P(N)}\right\rangle \tag{2.3}$$

where $\sqrt{N! \prod_{\alpha=0}^{\infty}(n_\alpha!)}$ normalizes the many-body wavefunction and the summation runs over all $N!$ permutations P of the set of quantum numbers $\{\alpha_1, ..., \alpha_N\}$. The underlying Hilbertspace of the N-body quantum system is

$$\mathcal{H}_N = \underbrace{\mathcal{H} \otimes ... \otimes \mathcal{H}}_{\text{N times}}$$

where $\mathcal{H}$ is a single-particle Hilbertspace which is spanned by the states $\left\{ |\alpha\rangle \right\}$. However, there are some problems arsing in this representation. As said above, it is convenient to work in the grand-canonical ensemble. Therefore, with a fluctuating number of particles, the representation of the many-body state (2.3) is a good choice to describe states with a fixed number of particles. Also, the practical computation in this language will be cumbersome. For example, in order to compute the overlap of two wavefunctions one needs no less than $(N!)^2$ different products. To overcome such problems it is possible to describe the many-body system uniquely in another representation which includes the possibility to work with a changing particle number. This leads to the **occupation number representation**, which will be briefly introduced.

Before depicting this representation, one defines operators which make it possible to create and destroy particles in the physical system.

The linear operator $a_\beta^\dagger$ creates a particle in state β:

$$a_\beta^\dagger \left|\alpha_1, ..., \alpha_N\right\rangle = \left|\beta, \alpha_1, ..., \alpha_N\right\rangle \tag{2.4}$$

and its adjoint a_β destroys a particle in state β:

$$a_\beta \left|\alpha_1, ..., \alpha_N\right\rangle = \sum_{k=1}^{N} \left\langle \beta \,|\, \alpha_k \right\rangle \left|\alpha_1, ..., (\text{no } \alpha_k), .., \alpha_N\right\rangle \tag{2.5}$$

where this relation follows from the defining equation 2.4.

Also following from 2.4 and 2.5, are the commutators:

$$\begin{aligned} \Big[a_\alpha, a_\beta\Big] &= a_\alpha a_\beta - a_\beta a_\alpha = 0 \\ \Big[a_\alpha, a_\beta^\dagger\Big] &= \delta_{\alpha,\beta} \end{aligned} \tag{2.6}$$

So far, the one particle states α and β are not specified. We could ask how the creation and annihilation operators $a_\alpha^\dagger$ and a_α change by a transformation of the basis vector $\Big\{ \left|\alpha\right\rangle \Big\}$ to some other basis $\Big\{ \left|\lambda\right\rangle \Big\}$.
It is known that this transformation can be written as

$$\left|\alpha\right\rangle = \sum_\lambda \left\langle \lambda \,|\, \alpha \right\rangle \left|\lambda\right\rangle$$

by inserting a resolution of the identity $\mathbb{1} = \sum_\lambda \left|\lambda\right\rangle\!\left\langle\lambda\right|$. Now, letting $a_\alpha^\dagger$ act on an arbitrary state $\left|\gamma_1, ..., \gamma_N\right\rangle$ one can write

$$\begin{aligned} a_\alpha^\dagger = \left|\gamma_1, ..., \gamma_N\right\rangle &= \left|\alpha, \gamma_1, ..., \gamma_N\right\rangle \\ &= \sum_\lambda \left\langle \lambda \,|\, \alpha \right\rangle \left|\lambda, \gamma_1, ..., \gamma_N\right\rangle \\ &= \sum_\lambda \left\langle \lambda \,|\, \alpha \right\rangle a_\lambda^\dagger \left|\gamma_1, ..., \gamma_N\right\rangle \end{aligned}$$

where in the second equality sign, a resolution of the identity $\mathbb{1} = \sum_\lambda \left|\lambda\right\rangle \left\langle\lambda\right|$ was inserted. Because of the fact that this holds for arbitrary $\left|\gamma_1, ..., \gamma_N\right\rangle$ one can deduce

$$\Rightarrow a_\alpha^\dagger = \sum_\lambda \left\langle \lambda \,|\, \alpha \right\rangle a_\lambda^\dagger \tag{2.7}$$

and by hermitian conjugation follows

$$\Rightarrow a_\alpha = \sum_\lambda \left\langle \alpha \,|\, \lambda \right\rangle a_\lambda \tag{2.8}$$

For instance, choosing $|\alpha\rangle = |\vec{x}\rangle$ and $|\lambda\rangle = |\vec{k}\rangle$, where $\vec{x}$ and $\vec{k}$ are continuous and discrete variables, respectively:

$$a^\dagger(\vec{x}) = \sum_{\vec{k}} \langle \vec{k}|\vec{x}\rangle \, a^\dagger_{\vec{k}} \qquad a^\dagger_{\vec{k}} = \int_{\mathbb{R}^d} \mathrm{d}^d x \; \langle \vec{x}|\vec{k}\rangle \, a^\dagger(\vec{x}) \tag{2.9}$$

and using the identity $\langle \vec{x}|\vec{k}\rangle = \frac{1}{\sqrt{V}} \exp\Big(\vec{k}\cdot\vec{x}\Big)$ this becomes

$$a^\dagger(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} \exp\Big(\vec{k}\cdot\vec{x}\Big) a^\dagger_{\vec{k}} \qquad a^\dagger_{\vec{k}} = \frac{1}{\sqrt{V}} \int_{\mathbb{R}^d} \mathrm{d}^d x \exp\Big(\vec{k}\cdot\vec{x}\Big) a^\dagger(\vec{x}) \tag{2.10}$$

Concluding that this is just the usual Fourier transformation from position space to the momentum space.

Specifying the number of particles $n_{\alpha_i} \equiv n_i$ in each state α_i completely determines the many-body state $|\alpha_1, ..., \alpha_N\rangle$. Hence, it is possible to define

$$|n_1, n_2, ...\rangle := \frac{1}{\sqrt{n_1! n_2! \cdots}} |\underbrace{\alpha_1, ..., \alpha_1}_{n_1 \text{times}}, \underbrace{\alpha_2, ..., \alpha_2}_{n_2 \text{times}}, ...\rangle \tag{2.11}$$

These states are the so-called **Fock states**. They span the many-body Hilbert space

$$\mathcal{F} = \bigoplus_{n=0}^{N} \mathcal{H}_n \qquad \text{with} \qquad \mathcal{H}_n = \underbrace{\mathcal{H} \otimes ... \otimes \mathcal{H}}_{\text{n times}} \tag{2.12}$$

$\mathcal{H}_n$ is an n-particle Hilbert space. The state $\mathcal{H}_{n=0}$ is defined as the Hilbert space without particles. It is spanned by only one state, the vacuum state $|0\rangle$ which is defined by $a_{\alpha_i}|0\rangle := 0$ for an arbitrary state α_i. The algebra in 2.6 completely determines the structure of the Fock space. From the definition of the Fock space one can deduce how the creation and annihilation operators $a_i^\dagger$ and a_i act on a Fock state

$$a_i^\dagger |n_1, ..., n_i, ...\rangle = \sqrt{n_i + 1} \, |n_1, ..., n_i + 1, ...\rangle \tag{2.13}$$

$$a_i |n_1, ..., n_i, ...\rangle = \sqrt{n_i} \, |n_1, ..., n_i - 1, ...\rangle \tag{2.14}$$

The prefactors are normalization factors for the resulting Fock states. Using these relations one can write the Fock states in general as

$$|n_1, n_2, ...\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle \tag{2.15}$$

It is necessary to mention that in the case of bosonic particles the number of particles in a many-body state can take an arbitrary non-negative integer value, $n_i \in \{0, 1, ..., \infty\}$.
A very important operator in the occupation number representation is the occupation number operator, which is defined as

$$\hat{n}_i = a_i^\dagger a_i \tag{2.16}$$

with the property

$$\hat{n}_i |n_1, .., n_N\rangle = n_i |n_1, ..., n_N\rangle \tag{2.17}$$

resulting straightforwardly from the relations 2.13,2.14. Hence, the operator $\hat{n}_{\alpha_i} \equiv \hat{n}_i$ counts the number of particles in the state α_i.

The advantage of working with the formalism of 2^{nd} quantization is that every N-body operator can be written in terms of the creation and annihilation operators. Since only one- and two-body operators will be used for the model of this thesis, only these will be presented.

Consder a sum over one-particle operators $\hat{\mathcal{O}}_1 = \sum_{i=1}^{N} \hat{o}_i$, which is diagonal in some single particle basis $|\alpha\rangle$, with $\hat{o} = \sum_i o_{\alpha_i} |\alpha_i\rangle\langle\alpha_i|$ where $o_{\alpha_i} = \langle\alpha_i|\hat{o}|\alpha_i\rangle$. One can then write

$$\begin{aligned}\left\langle n'_{\alpha_1}, n'_{\alpha_2}, ...\middle|\hat{\mathcal{O}}_1\middle|n_{\alpha_1}, n_{\alpha_2}, ...\right\rangle &= \sum_i o_{\alpha_i} n_{\alpha_i} \left\langle n'_{\alpha_1}, n'_{\alpha_2}, ...\middle|n_{\alpha_1}, n_{\alpha_2}, ...\right\rangle \\ &= \left\langle n'_{\alpha_1}, n'_{\alpha_2}, ...\middle|\sum_i o_{\alpha_i}\hat{n}_{\alpha_i}\middle|n_{\alpha_1}, n_{\alpha_2}, ...\right\rangle\end{aligned}$$

Since the chosen occupation number states are arbitrary, one can infer the second quantized representation of the operator $\hat{\mathcal{O}}_1$,

$$\hat{\mathcal{O}}_1 = \sum_\alpha o_\alpha \hat{n}_\alpha = \sum_\alpha o_\alpha a^\dagger_\alpha a_\alpha$$

This representation is given in the diagonal basis of the operator, changing to a general basis, on obtains,

$$\hat{\mathcal{O}}_1 = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle\, a^\dagger_\mu a_\nu \tag{2.18}$$

For instance, the Hamiltonian for a free particle in an external potential in position space can be written as [5]

$$H = \int \mathrm{d}^d\vec{\mathbf{x}}\, a^\dagger(\vec{\mathbf{x}}) \left[\frac{\hat{\vec{\mathbf{p}}}^2}{2m} + V(\vec{\mathbf{x}})\right] a(\vec{\mathbf{x}}) \tag{2.19}$$

where $\hat{\vec{\mathbf{p}}} = \frac{1}{i}\boldsymbol{\nabla}$.
Eventually, a two-body operator can also be written in a second quantized form. Here, without derivation (see, [5],[6])

$$\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\lambda,\lambda',\mu,\mu'} a^\dagger_\mu a^\dagger_{\mu'} a_\lambda a_{\lambda'} \tag{2.20}$$

with $\mathcal{O}_{\lambda,\lambda',\mu,\mu'} =\equiv \langle\mu,\mu'|\mathcal{O}_2|\lambda,\lambda'\rangle$. Then a general pairwise interaction operator $\hat{U} = \frac{1}{2}\sum_{i\neq j} U(x_i - x_j)$ can be written in the second quantized representation as

$$\hat{U} = \frac{1}{2}\int \mathrm{d}^d\vec{\mathbf{x}} \int \mathrm{d}^d\vec{\mathbf{y}}\, U(\vec{\mathbf{x}} - \vec{\mathbf{y}}) a^\dagger(\vec{\mathbf{x}}) a^\dagger(\vec{\mathbf{y}}) a(\vec{\mathbf{y}}) a(\vec{\mathbf{x}}) \tag{2.21}$$

Hence, we can write a general Hamiltonian $H = \sum_{i=1}^{N}\left(\frac{-\nabla^2}{2m} + V(x_i)\right) + \frac{1}{2}\sum_{i\neq j} U(x_i - x_j)$ as

$$H = \int \mathrm{d}^d\vec{\mathbf{x}}\, a^\dagger(\vec{\mathbf{x}}) \left[\frac{\hat{\vec{\mathbf{p}}}^2}{2m} + V(\vec{\mathbf{x}})\right] a(\vec{\mathbf{x}}) + \frac{1}{2}\int \mathrm{d}^d\vec{\mathbf{x}} \int \mathrm{d}^d\vec{\mathbf{y}}\, U(\vec{\mathbf{x}} - \vec{\mathbf{y}}) a^\dagger(\vec{\mathbf{x}}) a^\dagger(\vec{\mathbf{y}}) a(\vec{\mathbf{y}}) a(\vec{\mathbf{x}}) \tag{2.22}$$

2.1.2 Coherent states

In order to be able to rewrite the partition function, one has to define the so-called **coherent states**. In this thesis one will only need bosonic coherent states because the model consists only of bosons. Their defining property is to be the eigenstate of the annihilation operator a_{α_i}, where $\alpha_i \in \{\alpha_1, ..., \alpha_N\}$ are sets of one-particle quantum numbers α_i.

$$|\psi\rangle := \exp\left(\sum_{i=1}^{N} \psi_i a_i^\dagger\right)|0\rangle \tag{2.23}$$

Letting an annihilation operator $a_{\alpha_k} \equiv a_k$ act on the coherent state 2.23 and using the commutation relation of the creation and annihilation operators $\left[a_i, a_j^\dagger\right] = \delta_{i,j}$ yield

$$\begin{aligned}
a_k|\psi\rangle &= a_k \exp\left(\sum_{i=1}^{N} \psi_i a_i^\dagger\right)|0\rangle = a_k \prod_{i=1}^{N} \exp\left(\psi_i a_i^\dagger\right) \\
&= a_k \prod_{i=1}^{N} \sum_{n_i} \frac{\psi_i^{n_i}}{n_i!}(a_i^\dagger)^{n_i}|0\rangle = a_k \sum_{n_1,...,n_N} \frac{(\psi_1 a_1^\dagger)^{n_1}}{n_1!}\frac{(\psi_2 a_1^\dagger)^{n_2}}{n_2!}\cdots\frac{(\psi_N a_N^\dagger)^{n_N}}{n_N!}|0\rangle \\
&= \prod_{i=1,i\neq k}^{N} \sum_{n_i} \left(\frac{\psi_i^{n_i}}{n_i!}(a_i^\dagger)^{n_i}\right) \sum_{n_k=0}^{\infty} \frac{\psi_k^{n_k}}{n_k!} a_k (a_k^\dagger)^{n_k}|0\rangle \\
&= \prod_{i=1,i\neq k}^{N} \sum_{n_i} \left(\frac{\psi_i^{n_i}}{n_i!}(a_i^\dagger)^{n_i}\right) \sum_{n_k=1}^{\infty} \frac{\psi_k^{n_k}}{n_k!} n_k (a^\dagger)^{n_k-1}|0\rangle \\
&= \prod_{i=1,i\neq k}^{N} \sum_{n_i} \left(\frac{\psi_i^{n_i}}{n_i!}(a_i^\dagger)^{n_i}\right) \sum_{n_k=0}^{\infty} \frac{\psi_k^{n_k+1}}{n_k!} (a^\dagger)^{n_k}|0\rangle \\
\Rightarrow a_k|\psi\rangle &= \psi_k \prod_{i=1}^{N} \sum_{n_i} \frac{\psi_i^{n_i}}{n_i!}(a_i^\dagger)^{n_i}|0\rangle = \psi_k|\psi\rangle
\end{aligned} \tag{2.24}$$

where it has been used in the second line that $\left[a_i, (a_j^\dagger)^{n_j}\right] = \delta_{i,j} n_j (a_j^\dagger)^{n_j-1}$. Hence, the state 2.23 is indeed an eigenstate of the annihilation operator a_k with eigenvalue ψ_k. Without further discussion, we list some of the most important properties of the coherent states [7][6]

(*i*) eigenstates of the creation operator $a_k^\dagger$ do not exist, but $\langle\psi| a_k^\dagger = \langle\psi|\psi_k$

(*ii*) the coherent states defined above are not orthonormal $\langle\lambda|\mu\rangle = \exp\left(\sum_i \bar{\lambda}_i \mu_i\right)$

This is a crucial property of the coherent states. They are overcomplete in the Fock space, meaning, any vector in the Fock space can be expanded in terms of coherent states. This is expressed by the closure relation following in (*iii*).

(*iii*) the resolution of identity can be written as

$$\mathbb{1} = \int \prod_{i=1}^{N} \frac{d\bar{\psi}_i d\psi_i}{2\pi i} \exp\left(-\sum_i \bar{\psi}_i \psi_i\right)|\psi\rangle\langle\psi| \tag{2.25}$$

Define for shortness the abbreviate $\prod_{i=1}^{N} \frac{d\bar{\psi}_i d\psi_i}{2\pi i} := d(\bar{\psi}, \psi)$
Then, this relation is written as

$$\mathbb{1} = \int d(\bar{\psi}, \psi) \exp\left(-\sum_i \bar{\psi}_i \psi_i\right)|\psi\rangle\langle\psi| \tag{2.26}$$

The correctness that 2.26 is indeed the resolution of $\mathbb{1}$ can be proved by showing that 2.26 commutes with the creation and annihilation operators for every state and $\langle\psi|\mathbb{1}|\psi\rangle = 1$ holds. This is done in [6].

(*iv*) The creation operator $a_k^\dagger$ acts on the coherent state $|\psi\rangle$ as

$$a_k^\dagger |\psi\rangle = \frac{\partial}{\partial \psi_k} |\psi\rangle \tag{2.27}$$

These properties will be needed to express the partition function $Z = \mathrm{Tr}(\exp(-\beta(H-\mu N)))$ as functional integral in the following.

2.1.3 Functinal integral representation

The aim is to rewrite the grand canonical partition function [7]

$$Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right) = \sum_n \left\langle n \left| e^{-\beta(H-\mu N)} \right| n \right\rangle \tag{2.28}$$

as a path integral in imaginary time $\tau = it$ with $\tau \in [0, \beta]$ in analogy to the Feynman path integral in QM. The eigenstates in which the trace operator is evaluated is chosen to be a Fock state $|n\rangle = a_1^\dagger \cdots a_n^\dagger |0\rangle$. One is able to get rid of the sum over the eigenstates $\sum_n \langle n|\cdots|n\rangle$ by inserting the closure relation for the coherent states 2.26.

$$\Rightarrow Z = \int d(\bar{\psi}, \psi) \exp\left(-\sum_i \bar{\psi}_i \psi_i\right) \sum_n \langle n|\psi\rangle \left\langle \psi \left| e^{-\beta(H-\mu N)} \right| n \right\rangle \tag{2.29}$$

Next, one can pull the factor $\langle n|\psi\rangle$ to the right, so that it is possible to use $\mathbb{1} = \sum_n |n\rangle\langle n|$ and remove the n sum from the partition function. For bosons this is easily done, since $\langle n|\psi\rangle = \langle\psi|n\rangle$[1].The partition function then becomes

$$\begin{aligned} Z &= \int d(\bar{\psi}, \psi) \exp\left(-\sum_i \bar{\psi}_i \psi_i\right) \langle\psi| e^{-\beta(H-\mu N)} \underbrace{\left(\sum_n |n\rangle\langle n|\right)}_{=\mathbb{1}} |\psi\rangle \\ &= \int d(\bar{\psi}, \psi) \exp\left(-\sum_i \bar{\psi}_i \psi_i\right) \left\langle \psi \left| e^{-\beta(H-\mu N)} \right| \psi \right\rangle \end{aligned} \tag{2.30}$$

In the next step, decompse the imaginary time intervall $[0, \beta]$ into M steps $\delta\tau = \beta/M$ so that $\delta\tau$ is small a quantity and insert 2.26 after each step. In order to be able to factorise the exponential function and to compute the matrix elements appearing in 2.30, the exponential function in $\langle ... \rangle$ has to be normal ordered. This means that every creation operator is placed to the left from all annihilation operators. The Hamiltonian can always be chosen to be normal ordered. Otherwise it would not be possible to compute the eigenvalues of the creation operators. The exponential factor $e^{-\beta(H-\mu N)}$ can not be evaluated directly because by rewriting it as $e^{-\beta(H-\mu N)} = \mathbb{1} - \frac{\beta}{2}(H-\mu N) + \beta^2(H-\mu N)^2 + ...$, it is obvious that it is not normal ordered because of the terms of second and higher orders. By

[1] For fermions, one has to be careful because this would not hold,[7] [6]. Then it would be $\langle n|\psi\rangle = \langle -\psi|n\rangle$.

splitting the imaginary time interval, one can bypass this problem

$$\begin{aligned} e^{-\beta(H-\mu N)} &= \exp\Bigg(\underbrace{-\delta\tau(H-\mu N) - ... - \delta\tau(H-\mu N)}_{\text{M times}}\Bigg) \\ &= \mathbb{1} - \delta\tau(H-\mu N) - ... - \delta\tau(H-\mu N) + \mathcal{O}(\delta\tau^2) \\ &\simeq (\mathbb{1} - \beta(H-\mu N))^M = \exp(-\delta\tau(H-\mu N))^M + \mathcal{O}(\delta\tau^2) \\ &\simeq \underbrace{e^{(-\delta\tau(H-\mu N))} \dots e^{(-\delta\tau(H-\mu N))}}_{\text{M times}} \\ \Rightarrow e^{-\beta(H-\mu N)} &\simeq e^{(-\delta\tau(H-\mu N))} \dots e^{(-\delta\tau(H-\mu N))} \end{aligned} \tag{2.31}$$

In between every exponential, which are normal ordered up to leading order in the infinitesimal time intervall $\delta\tau$, insert a resolution of the identity 2.26 and compute the matrix elements. The Hamiltonian is of the form $H = \sum_{ij} t_{ij} a_i^\dagger a_j + \sum_{ijkl} U_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$ (normal ordered) such that a general matrix element $\langle\phi|H[a^\dagger, a]|\psi\rangle$ with coherent states $|\psi\rangle, |\phi\rangle$ can be evaluated as

$$\begin{aligned} \langle\phi|H[a^\dagger, a]|\psi\rangle &= \sum_{ij} t_{ij} \langle\phi|a_i^\dagger a_j|\psi\rangle + \sum_{ijkl} U_{ijkl} \langle\phi|a_i^\dagger a_j^\dagger a_k a_l|\psi\rangle \\ &= \left(\sum_{ij} t_{ij} \bar{\phi}_i \psi_j + \sum_{ijkl} U_{ijkl} \bar{\phi}_i \bar{\phi}_j \psi_k \psi_l\right) \langle\phi|\psi\rangle \\ \Rightarrow \langle\phi|H[a^\dagger, a]|\psi\rangle &= H[\bar{\phi}, \psi] \langle\phi|\psi\rangle \end{aligned} \tag{2.32}$$

One defines the abbreviate $K = H - \mu N$ and now insert $\mathbb{1} = \int d(\bar{\psi}^{(n)}, \psi^{(n)}) \exp\Big(-\sum_i \bar{\psi}_i^{(n)} \psi_i^{(n)}\Big) \big|\psi^{(n)}\big\rangle\big\langle\psi^{(n)}\big|$ between every exponential in 2.31 where the subscript (n) counts at which time step we are $n \in [0, M]$. Transission matrix elements of the form $\Big\langle\psi^{(n+1)}\Big|e^{-\delta\tau K[a^\dagger, a]}\Big|\psi^{(n)}\Big\rangle$ between two time steps n and $n+1$ are evaluated as

$$\begin{aligned} \Big\langle\psi^{(n+1)}\Big|e^{-\delta\tau K[a^\dagger, a]}\Big|\psi^{(n)}\Big\rangle &= \Big\langle\psi^{(n+1)}\Big|\mathbb{1} - \delta\tau K[a^\dagger, a] + \mathcal{O}(\delta\tau^2)\Big|\psi^{(n)}\Big\rangle \\ &= \Big\langle\psi^{(n+1)}\Big|\mathbb{1} - \delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}] + \mathcal{O}(\delta\tau^2)\Big|\psi^{(n)}\Big\rangle \\ &= \Big\langle\psi^{(n+1)}\Big|\psi^{(n)}\Big\rangle \Big(\mathbb{1} - \delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}] + \mathcal{O}(\delta\tau^2)\Big) \\ &\simeq \exp\left(\sum_i \bar{\psi}_i^{(n+1)} \psi_i^{(n)}\right) (\mathbb{1} - \delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}]) \\ &\simeq \exp\left(\sum_i \bar{\psi}_i^{(n+1)} \psi_i^{(n)}\right) \exp\Big(-\delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}]\Big) \\ \Rightarrow \Big\langle\psi^{(n+1)}\Big|e^{-\delta\tau K[a^\dagger, a]}\Big|\psi^{(n)}\Big\rangle &\simeq \exp\left(\sum_{i=1}^{N} \bar{\psi}_i^{(n+1)} \psi_i^{(n)} - \delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}]\right) \end{aligned} \tag{2.33}$$

Finally, putting everything together the partition function becomes

$$Z = \int \prod_{n=0}^{M} d(\bar{\psi}^{(n)}, \psi^{(n)}) \exp\left(-\sum_{n=0}^{M-1} \left(\sum_{i=1}^{N} \bar{\psi}_i^{(n)} \psi_i^{(n)} - \sum_{i=1}^{N} \bar{\psi}_i^{(n+1)} \psi_i^{(n)} + \delta\tau K[\bar{\psi}^{(n+1)}, \psi^{(n)}]\right)\right) \tag{2.34}$$

with the boundary conditions $\psi^{(0)} = \psi^{(M)}$ and $\bar{\psi}^{(0)} = \bar{\psi}^{(M)}$. These arise because of the fact that it was started with $Z = \int d(\bar{\psi}, \psi) \langle\psi|...|\psi\rangle$ where the ket is evluated at the (imaginary) time $\tau = 0$ and the bra at $\tau = \beta$ in analogy to the transition matrix element of the time translation operator in QM.[7][6]

By taking the continuum limit $\delta\tau \to 0$ and using $\sum_{n=0}^{M} \tau \to \int_0^\beta$, $\psi_i^{(n)} \to \psi_i(\tau)$ and $\lim_{\delta\tau\to 0} \frac{\bar{\psi}_i^{(n)}\psi_i^{(n)} - \bar{\psi}_i^{(n+1)}\psi_i^{(n)}}{\delta\tau} = \frac{\partial\bar{\psi}_i(\tau)}{\partial\tau}\psi_i(\tau)$ with $\tau = n\delta\tau$ we arrive at

$$Z = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S[\bar{\psi},\psi]} \tag{2.35}$$

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left(\sum_{i=1}^{N} \psi_i(\tau)\partial_\tau\psi_i(\tau) + H[\bar{\psi}, \psi] - \mu N[\bar{\psi}, \psi] \right) \tag{2.36}$$

and the boundary condition $\psi(\tau = 0) = \psi(\tau = \beta)$ and equally for the complex conjugated. It has been defined $\mathcal{D}(\bar{\psi}, \psi) = \lim_{M\to\infty} \prod_{n=0}^{M} d(\bar{\psi}^{(n)}, \psi^{(n)})$ Hence, the partition function is now written as a functional integral over all possible field configurations $\bar{\psi}_i$ and ψ_i with weight $\exp(-S)$ where S is the so-called action of the system.

2.2 Hubbard Model

2.2.1 Bloch waves and Wannier functions

In this subsection it will be derived the main model of the thesis which is the Bose-Hubbard model. It is a bosonic analogue of the well known Hubbard model for electrons.
The Bose-Hubbard model is a "simple" QM lattice model for strongly interacting bosons. The derivation is from the book [4].

However, before deriving the model we say some words about band structures which state how particles act in a lattice periodic potential. The theory of band structure is developed in, e.g.[8]
The wavefunction of a free atom is a plane wave $\exp\Big(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}\Big)/\sqrt{V}$ and has an energy dispersion relation $\epsilon_{\vec{\mathbf{k}}} = \vec{\mathbf{k}}^2/2m$. Interestingly, this result does not change too much for noninteracting atoms in a periodic potential. The relevant wavefunctions are now called Bloch waves and the dispersion develops a band structure. Indeed, the wavefunction can be written as a product of a plane wave and lattice periodic function $u_{n,\vec{\mathbf{k}}}(\vec{\mathbf{x}})$,i.e.

$$\psi_{n,\vec{\mathbf{k}}}(\vec{\mathbf{x}}) = \exp\Big(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}\Big)u_{n,\vec{\mathbf{k}}}(\vec{\mathbf{x}})$$

where n is the band index and $\hbar\vec{\mathbf{k}}$ is the quasi-momentum which takes on values within the first Brillouin zone. This is the well-known result from Bloch's theorem,[8]. Accordingly, the dispersion relation is no longer quadratic with the momentum, but develops gaps at specific locations determined by the lattice structure.

Considering now an atom in a lattice with minima located at the lattice sites $\vec{\mathbf{x}}_i$. It can be shown that for each band a set of Wannier functions $w_n(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)$ exists, such that the exact Bloch wavefunctions can be written [8] as

$$\psi_{n,\vec{\mathbf{k}}}(\vec{\mathbf{x}}) = \sum_i \exp\Big(i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}\Big)w_n(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)$$

The Wannier functions are orthogonal for different bands n as well as for different i. They are localized at positions $\vec{\mathbf{x}}_i$ and decay exponentially away from $\vec{\mathbf{x}}_i$ but also oscillate such that their average vanishes.

2.2.2 Derivation of the Hubbard model

The action that describes a gas of atoms in a periodic potential is given by

$$\begin{aligned} S[\bar{\psi},\psi] = &\int_0^\beta d\tau \int \mathrm{d}^d x\, \bar{\psi}(\vec{\mathbf{x}},\tau)\left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2m} + V_{\mathrm{ex}}(\vec{\mathbf{x}}) - \mu\right)\psi(\vec{\mathbf{x}},\tau) \\ &+\frac{1}{2}\int_0^\beta d\tau \int \mathrm{d}^d\vec{\mathbf{x}} \int \mathrm{d}^d\vec{\mathbf{x}}'\, \bar{\psi}(\vec{\mathbf{x}},\tau)\bar{\psi}(\vec{\mathbf{x}}',\tau)V(\vec{\mathbf{x}}-\vec{\mathbf{x}}')\psi(\vec{\mathbf{x}}',\tau)\psi(\vec{\mathbf{x}},\tau) \end{aligned} \tag{2.37}$$

where $V_e x(\vec{\mathbf{x}})$ is a lattice periodic function, $V(\vec{\mathbf{x}}-\vec{\mathbf{x}}')$ is a two-body interaction term and μ is the chemical potential which is inserted to be able to fix the particle number. Assume that the gas is dilute enough, i.e. the spatial spacing is larger than the interaction range, and that the temperature is sufficiently small so that it is possible to neglect more than two-body interactions. Using the Wannier functions introduced before, we can axpand the field operators $\psi, \bar{\psi}$ as

$$\psi(\vec{\mathbf{x}},\tau) = \sum_{n,i} a_{n,i}(\tau)w_n(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i) \tag{2.38}$$

where the expansion coefficients $\bar{a}_{n,i}(\tau)$ and $a_{n,i}(\tau)$ correspond to the creation and annihilation operator respectively of a particle in the Wannier state $w_n(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)$ at site i. It is worth to mention that in the action these are not operators but rather the eigenvalues of the annihilation operator in the coherent states.
In the tight-binding limit the Wannier functions of the lattice are replaced by harmonic oscillator states on each site, which depend on the band index n. At sufficiently low temperatures and for sufficiently small interaction energies, the particles only occupy the lowest $n=0$ state of the lattice. As a result, the expansion leads the lattice action

$$\begin{aligned} S[\bar{a},a] = \int_0^\beta d\tau \Big\{ & \sum_{ij} \bar{a}_i(\tau)\frac{\partial}{\partial\tau}a_j(\tau)\int \mathrm{d}^d x\, \bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_j) \\ & + \sum_{ij}\bar{a}_i(\tau)a_j(\tau)\int \mathrm{d}^d x\, \bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\left(-\frac{\nabla^2}{2m}+V_{\mathrm{ex}}(\vec{\mathbf{x}})-\mu\right)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_j) \\ & + \frac{1}{2}\sum_{ii'jj'}\bar{a}_i(\tau)\bar{a}_{i'}(\tau)a_j(\tau)a_{j'}(\tau) \\ & \times \int \mathrm{d}^d\vec{\mathbf{x}}\,\mathrm{d}^d\vec{\mathbf{x}}'\,\bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\bar{w}_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_{i'})V(\vec{\mathbf{x}}-\vec{\mathbf{x}}')w_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_j)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_{j'})\Big\} \end{aligned} \tag{2.39}$$

where for notational convenience the now redundant band index of the particle fields is omitted. Rewriting the above action more compactly as

$$S[\bar{a},a] = S_0[\bar{a},a] + S_{\mathrm{int}}[\bar{a},a] \tag{2.40}$$

with the non-interacting part given by

$$S_0[\bar{a},a] = \int_0^\beta d\tau\Big\{\sum_i \bar{a}_i(\tau)\left(\frac{\partial}{\partial\tau}+\epsilon_i-\mu\right)a_i(\tau) - \sum_{i\neq j}\bar{a}_i(\tau)t_{i,j}a_j(\tau)\Big\} \tag{2.41}$$

where the orthonormality of the Wannier functions in the same band has been used, i.e. $\int \mathrm{d}^d x\, \bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_j)=\delta_{i,j}$. We have also introduced the on-site energy

$$\epsilon_i = \int \mathrm{d}^d x\, \bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\Big\{-\frac{\nabla^2}{2m}+V_{\mathrm{ex}}(\vec{\mathbf{x}})\Big\}w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i) \tag{2.42}$$

and the tunneling or hopping amplitude between sites i abd j

$$t_{i,j} = -\int \mathrm{d}^d x\, \bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\Big\{-\frac{\nabla^2}{2m}+V_{\mathrm{ex}}(\vec{\mathbf{x}})\Big\}w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_j) \tag{2.43}$$

The double summation in the tunneling term in 2.41 is over all combinations i,j for which $i\neq j$. For a deep lattice, the hopping energy $t_{i,j}$ will be exponentially suppressed for all sites that are not nearest neighbors. Therefore, restrict the summation to nearest neighbors only, where the corresponding summation is denoted by $\sum_{\langle i,j\rangle}$, while the nearest-neighbor hopping amplitude is denoted by t.

The interactions between the particles are determined by the matrix elements

$$\int \mathrm{d}^d\vec{\mathbf{x}}\,\mathrm{d}^d\vec{\mathbf{x}}'\,\bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\bar{w}_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_{i'})V(\vec{\mathbf{x}}-\vec{\mathbf{x}}')w_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_j)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_{j'})$$

which not only include on-site interactions but also interactions between atoms that are on remote sites. However, the latter interactions are typically exponentially suppressed. For practical purposes it usually suffices to take only the on-site interactions into account. One then gets

$$S_{\mathrm{int}}[\bar{a},a] = \int_0^\beta d\tau \frac{U}{2}\sum_i \bar{a}_i(\tau)\bar{a}_i(\tau)a_i(\tau)a_i(\tau) \tag{2.44}$$

where we have defined the on-site interaction strength U as

$$U = \int \mathrm{d}^d\vec{\mathbf{x}}\,\mathrm{d}^d\vec{\mathbf{x}}'\,\bar{w}_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i)\bar{w}_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_i)V(\vec{\mathbf{x}}-\vec{\mathbf{x}}')w_0(\vec{\mathbf{x}}'-\vec{\mathbf{x}}_i)w_0(\vec{\mathbf{x}}-\vec{\mathbf{x}}_i). \tag{2.45}$$

For bosons, the corresponding Hamiltonian to the action in 2.40 is known as the **Bose-Hubbard model** and is given by

$$H = -t\sum_{\langle i,j\rangle} a_i^\dagger a_j + \sum_i(\epsilon_i-\mu)a_i^\dagger a_i + \frac{U}{2}\sum_i a_i^\dagger a_i^\dagger a_i a_i \tag{2.46}$$

or using the commutation relation for bosons $\left[a_i, a_j^\dagger\right] = \delta_{i,j}$ this can be written equivalently as

$$H = -t\sum_{\langle i,j\rangle} a_i^\dagger a_j + \sum_i(\epsilon_i-\mu)\hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i-1) \tag{2.47}$$

where $\hat{n}_i = a_i^\dagger a_i$ is the occupation number on site i. This is the model that will be analyzed in this thesis. In the following discussion the on-site energy ϵ_i will be assumed to be the same on all sites and therefore set to zero for simplicity. This may be done because it simply gives an energy offset on every site.

3 Phase diagram of the Bose-Hubbard model

The Bose-Hubbard model describes a Mott-insulator-Superfluid transition. This model can be described by the following Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \tag{3.1}$$

with $U > 0$ for a repulsive on-site interaction and μ the chemical potential, included to be able to fix the particle number. The creation and annihilation operators $a_i^\dagger$ and a_i fulfill the commutator relation $\left[a_i, a_j^\dagger\right] = \delta_{i,j}$ and hence describe spinless bosonic particles. $\hat{n}_i = a_i^\dagger a_i$ is the occupation number operator for lattice site i. It will be considered a hypercubic lattice in $d \geq 2$ and the lattice spacing taken to be of unit length. The first term of the Hamiltonian describes the dynamics of the system, a_j destroys one particle on site j and $a_i^\dagger$ creates one on another site i, where the sites i, j have to be next nearest neighbors ($\langle i, j \rangle$ represents nearest neighbor pairs). t is the hopping amplitude by which this process happens. The third term (interaction term) describes the on-site repulsion of two or more particles at the same lattice site. For none or one particle at the same site there is no interaction.
The phase diagramm of the model for $T = 0$ will be studied.
By considering the cases where $t/U \to 0$ and $U/t \to 0$ we will see that the system is in completely different phases of matter for the two possibilities. Assuming that there is one boson on average ($\bar{n} = 1$), in the limit $t/U \to 0$ there must be one boson on each lattice site. Moving a particle would create an empty and a doubly-occupied lattice site which requires a very large energy (U) with respect to the gain in kinetic energy (t). Hence, it is very unlikely for this to happen. Therefore, for an integer density of particles, the bosons will be suppressed to move from one site to another and the system is in an insulating state. In the opposite limit where $U/t \to 0$, the system becomes **superfluid**. In this state the particles can move without resistance through the system. Thus, as the ratio t/U increases we expect a phase transition between an insulating ground state (known as a **Mott-insulating phase**) and a superfluid ground state. As it appears only at $T = 0$, it is called a quantum phase transition[2],[3].
Now, suppose that some particles are added to the system so that the average density of bosons per lattice site $\langle n \rangle$ is slightly larger than unity. Then the excess bosons could move through the system without changing the average density so that one could expect that the system is in the superfluid state even for $t/U \to 0$. More general, for any incommensurate density $\langle n \rangle = n_0 + \delta n$ in the small t/U limit where n_0 is a commensurate (integer) density one can view the excess particles as a dilute gas of delocalized particles responsible for the superfluidity of the system.

Additionally, it is important to mention that this Hamiltonian has a global $U(1)$-symmetry. H is invariant under the transformation $a_i^\dagger \to a_i^\dagger e^{-i\theta}$ and similar for the hermitian conjugate, where $\theta \in \mathbb{R}$. The transformation is independent of the lattice site.

[2]In the usual case the phase transition is driven by thermal fluctuations. That is not possible for $T = 0$, the fluctuations are of quantum nature. They appear because of the Heisenberg uncertainty principle and become so strong that phase transitions can happen. Therefore, they are called quantum phase transitions.

3.1 Superfluid phase

For the limit $U/t << 1$ one can set $U = 0$ for simplicity. The Hamiltonian then becomes

$$H_{U=0} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \mu \sum_i a_i^\dagger a_i \tag{3.2}$$

This Hamiltonian can be diagonalized by Fourier transforming the apperaring creation and annihilation operators. Inserting $a_j = \frac{1}{\sqrt{N}} \sum_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_j} a_{\vec{\mathbf{k}}}$ and $a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{\mathbf{k}}} e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_j} a_{\vec{\mathbf{k}}}^\dagger$ into $H_{U=0}$ yield

$$H_{U=0} = \sum_{\vec{\mathbf{k}}} (\epsilon_{\vec{\mathbf{k}}} - \mu) a_{\vec{\mathbf{k}}}^\dagger a_{\vec{\mathbf{k}}} \tag{3.3}$$

with $\epsilon_{\vec{\mathbf{k}}} = -2t \sum_{\alpha=1,\ldots,d} \cos(k_\alpha)$ and where the lattice spacing a between neighboring lattice sites was set to one. The resulting Hamiltonian in this limit describes a free Bose gas. The quantum statistical description of the non-interactig Bose gas is a popular subject described in many text books, see for instance [5] [4], [9]. The free Bose gas provides the simplest realization of a free Bose-Einstein condensation. The Bose-Einstein condensate is a state of matter that bosonic systems can reach under a critical tempereture. The statistic of bosons allows an arbitrary number of particles to be in a quantum state. For small temperatures the particles tend to be in the state with the lowest energy. Hence, due to the statistic the majority of the bosons will be in the state of lowest energy for a sufficiently small temperature.

In the present case where $T = 0$ all the bosons will occupy the state where $\vec{\mathbf{k}} = 0$ which is obviously the one with the lowest energy. The ground-state ket of the system for a fixed particle number N is, however

$$|\Omega\rangle = \left(a_{\vec{\mathbf{k}}=0}^\dagger\right)^N |0\rangle = \left(\frac{1}{\sqrt{N}} \sum_{i=1}^M a_i^\dagger\right)^N |0\rangle \,. \tag{3.4}$$

This means that all bosons are maximally delocalized with probability $\sim 1/N$ to be found on an arbitrary lattice site. So the wavefunction of every boson is spread over the whole lattice which indicates the superfluid state where all bosons can move freely over the whole lattice. This gound state holds in canonical ensemble where the number of particles is fixed at N. If one fixes the average densiy of particles on the lattice at $\left\langle a_i^\dagger a_i \right\rangle = \frac{N}{M} = n$ and compute the ground-state ket in grand-canonical ensemble, [7]

$$|\Omega\rangle = e^{\sqrt{N} a_{\vec{\mathbf{k}}=0}^\dagger} |0\rangle = \prod_{i=1}^M \left(e^{\sqrt{N/M} a_i^\dagger}\right) |0\rangle \tag{3.5}$$

This is a product of coherent states at each lattice site, which has the same intepretation as the ground-state in the canonical state. The expectation value $\langle a_i \rangle$ is the order parameter of the superfluid state. The non-vanishing of this order parameter indicates that the sytem is in a suerfluid state,[9]. In the grand-canonical ensemble, the expectation value $\langle a_i \rangle = \frac{\langle \Omega | a_i | \Omega \rangle}{\langle \Omega | \Omega \rangle}$ ca be computed to be, [7]

$$\langle a_i \rangle = \frac{\langle \Omega | a_i | \Omega \rangle}{\langle \Omega | \Omega \rangle} = \sqrt{N/M} \tag{3.6}$$

which is indeed non-vanishing. Therefore the system is in the superfluid state for the case of a free Bose gas.

3.2 Mott-insulating phase

First, it will be considered the strong coupling limit without hopping $t = 0$ and $U \gg 1$. The Hamiltonian becomes

$$H_{t=0} = \sum_{i=1}^{M} \left(\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right) \tag{3.7}$$

where M is the number of lattice sites. This Hamiltonian is local and therefore the same on all lattice sites. Hence, on can focus on the local Hamiltonian

$$H_{\text{loc}} = \frac{U}{2} \hat{n}(\hat{n} - 1) - \mu \hat{n} \tag{3.8}$$

which is diagonal in the occupation number state $|n\rangle$. This follows from the fact that H_{loc} commutes with $\hat{n}$. According to the chapter about 2^{nd} quantization, the state $|n\rangle$ has the following properties

$$\hat{n} |n\rangle = n |n\rangle \quad a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad a |n\rangle = \sqrt{n} |n-1\rangle \tag{3.9}$$

where n is the number of particles on a site.
Computing the eigenvalues of H_{loc} in its eigenbase, one obtains

$$\epsilon_n := \langle n | H_{\text{loc}} | n \rangle = \frac{U}{2} n(n-1) - \mu n \tag{3.10}$$

One wants to find the local occupation $n_0(\mu, U)$ of the insulating ground state which minimizes the energy.
The ground state $|n_0\rangle$ is defined as the eigenstate of $\epsilon_{n_0} = \min_n \epsilon_n$, where the number n can only be an integer or zero. In order to get the occupation $n_0(\mu, U)$, it is possible to proceed in the following way. It is known that the ground state is a Mott-insulator. The most stable state is when there is the same number of particles on all sites. By calculating the energy cost to add or remove one particle to the system, one can conclude the integer values of $n_0(\mu, U)$. Assuming that ϵ_{n_0} is the ground state energy. Then the energy cost to add one particle to the stystem is

$$\epsilon_{n_0} < \epsilon_{n_0+1} = \frac{U}{2}(n_0+1)n_0 - \mu(n_0+1) = \epsilon_{n_0} + U n_0 - \mu \tag{3.11}$$

from this one can deduce the condition $n_0 > \dfrac{\mu}{U}$. For the cost to remove a particle

$$\epsilon_{n_0} < \epsilon_{n_0-1} = \frac{U}{2}(n_0-1)(n_0-2) - \mu n_0 = \mu = \epsilon_{n_0} + U(1-n_0) + \mu \tag{3.12}$$

and from this relation follows $\frac{\mu}{U} > n_0 - 1$. Summarizing both conditions, one can conclude the dependence of n_0 on μ/U.

$$\Rightarrow n_0 > \mu/U > n_0 - 1 \tag{3.13}$$

If initially there was no particle in the state ($n_0 = 0$), one only has the condition $\mu/U < n_0 = 0$. Hence, the occupation number in the ground state depending on μ/U is

$$n_0 = \begin{cases} 0, & \text{for } \mu/U < 0 \\ 1, & \text{for } 0 < \mu/U < 1 \\ 2, & \text{for } 1 < \mu/U < 2 \\ \vdots & \\ n, & \text{for } n-1 < \mu/U < n \end{cases} \tag{3.14}$$

Further, asking what energy is needed to excite one boson from one site to another, which leaves a site with occupancy $n-1$ and creates one with $n+1$, leads to the so-called excitation gap of the Mott insulator. A non-vanishing excitation gap is a characteristic property of the insulating phase.The excitation gap for $t = 0$ is the sum of the energy cost needed to add and to remove one particle from the system and will be denoted as Δ_0.

$$\Delta_0 = (\epsilon_{n_0+1} - \epsilon_{n_0}) = (\epsilon_{n_0-1} - \epsilon_{n_0}) = U \tag{3.15}$$

The excitation spectrum of the superfluid phase is gapless.[3]
The states where μ/U takes an integer value are doubly degenerate on every site. Hence, one has a 2^M fold degeneracy on the whole lattice in these cases. This degeneracy will be lifted by a non-zero t. One can derive the ground state of the insulating phase by a variational ansatz for this state which minimizes the expectation value of the Hamiltonian $H_{t=0}$ and which is normalized, [10]. The ground state is

$$|\Omega\rangle = \prod_{i=1}^{M} \frac{1}{\sqrt{n_0}} (b_i^\dagger)^{n_0} |0\rangle \tag{3.16}$$

However, the ground state is just a Fock state with the same number of particles n_0 (occupancy for minimal energy) on each site of the lattice.

[3]These are gapless phonon modes according to the Goldstone theorem

3.3 Mean-field theory

It is not possible to find a transition from the superfluid to the Mott-insulating state, known from the Bogoljubov theory for a weakly interacting bosonic gas. This theory would describe the transition between a normal gas and the superfluid state,[4]. One has to start from the other limit. One supposes that the model is initially in the Mott-insulating state. One can take the hopping amplitude $t > 0$ and perform a mean field decoupling in the hopping term of the Hamiltonian 3.1. This leads to the quantitatively right description of the phase transition. In this proceeding, it is necessary to compute corrections to the ground state energy in the usual non-degenerate Schrödinger-perturbation theory up to fourth order.
One has to start again with the Hamiltonian of the Bose Hubbard model

$$H = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \tag{3.17}$$

and decouple the hopping term by assuming that the expectation value $\langle a_i \rangle \equiv \phi \in \mathbb{C}$ is non-zero but small and the same on all sites. ϕ is in analogy the Bogoljubov theory the order parameter of the superfluid state. Expand the creation and annihilation operator in the hopping term around their expectation values plus small fluctuations $a_i = \phi + \delta a_i$, so that the product $a_i^\dagger a_j$ can be written as

$$a_i^\dagger a_j = \phi a_i^\dagger + \bar{\phi} a_j - |\phi|^2$$

In this approximation the Hamiltonian becomes

$$H_{\text{eff}} = \sum_i \left(\frac{U}{2} \hat{n}_i(\hat{n}_i) - \mu \hat{n}_i \right) - t \sum_{\langle i,j \rangle} \left(\phi a_i^\dagger + \bar{\phi} a_j - |\phi|^2 \right) \tag{3.18}$$

The sum in the second term can be carried out in one index

$$H_{\text{eff}} = \sum_i \left(\frac{U}{2} \hat{n}_i(\hat{n}_i) - \mu \hat{n}_i + tz|\phi|^2 \right) - tz \sum_i \left(\phi a_i^\dagger + \bar{\phi} a_i \right) \tag{3.19}$$

$$\equiv \sum_i \left(h_i^{(0)} + V_i^{\text{t}} \right) \tag{3.20}$$

where z is the coordination number, counting the number of next nearest neighbors. $V^{\text{t}} = -tz \left(\phi a_i^\dagger + \bar{\phi} a_i \right)$ will be treated as a weak perturbation to the unperturbed Hamiltonian $h_i^{(0)}$ where we consider that $\phi, \bar{\phi}$ are small expansion parameters. The approximated effective Hamiltonian is now local, so one can focus again on one lattice site. Therefore, the lattice index will be suppressed.

$$H_{\text{loc}} = h^{(0)} + V^{\text{t}} \tag{3.21}$$

The eigenstates of the unperturbed Hamiltonian $\sum_i h^{(0)}$ are the same as previous

$$|\Omega\rangle = \prod_{i=1}^{M} \frac{1}{\sqrt{n_0}} (b_i^\dagger)^{n_0} |0\rangle \tag{3.22}$$

but now with the eigenergies

$$E_{n_0}^{(0)} = \frac{U}{2} n_0(n_0 - 1) - \mu n_0 + tz|\phi|^2 \tag{3.23}$$

The occupation number n_0 is also as before

$$n_0 = \begin{cases} 0, & \text{for } \mu/U < 0 \\ 1, & \text{for } 0 < \mu/U < 1 \\ 2, & \text{for } 1 < \mu/U < 2 \\ \vdots & \\ n, & \text{for } n-1 < \mu/U < n \end{cases} \tag{3.24}$$

The next step is to compute the energy- and state corrections. The state correction to p-th order can be computed using the well known formula

$$\left|n_0^{(p)}\right\rangle = \sum_{m\neq n} \left|m_0^{(0)}\right\rangle \frac{\left\langle m_0^{(0)}\middle|V^{\mathrm{t}}\middle|n_0^{(p-1)}\right\rangle}{E_{n_0}^{(0)} - E^{(m_0)}} - \sum_{i=1}^{p} E_{n_0}^{(j)} \sum_{m\neq n} \left|m_0^{(0)}\right\rangle \frac{\left\langle m_0^{(0)}\middle|n^{(p-j)}\right\rangle}{E_{n_0}^{(0)} - E_{m_0}^{(0)}} \tag{3.25}$$

The energy correction to p-th order takes a simpler form

$$E_{n_0}^{(p)} = \left\langle n_0^{(0)}\middle|V^{\mathrm{t}}\middle|n_0^{(p-1)}\right\rangle \tag{3.26}$$

The unperturbed state is the occupation number basis $\left|n_0^{(0)}\right\rangle = \frac{1}{\sqrt{n_0}}\left(a^\dagger\right)^{n_0}|0\rangle$ which is the eigenbasis of the gound state.[4] Due to the fact that the pertubation V^{t} is linear in the creation and annihilation operator, all corrections of an odd order to the the energy will vanish in the occupation number basis. We will from now denote the unperturbed state $\left|n_0^{(0)}\right\rangle \equiv |n_0\rangle$ to simplify the notation.
For instance, the first order correction to the energy is

$$\begin{aligned} E_{n_0}^{(1)} &= \langle n_0|V^{\mathrm{t}}|n_0\rangle = -tz\,\langle n_0|\left(\phi a^\dagger + \bar{\phi}a\right)|n_0\rangle \\ &= -tz\left(\phi\sqrt{n_0+1}\underbrace{\langle n_0|n_0+1\rangle}_{\delta_{n_0,n_0+1}=0} + \bar{\phi}\sqrt{n_0}\underbrace{\langle n_0|n-1\rangle}_{\delta_{n_0,n_0-1}=0}\right) \\ \Rightarrow E_{n_0}^{(1)} &= 0 \end{aligned} \tag{3.27}$$

This follows from the orthonormality of the occupation number basis. Using 3.25, we can calculate the first order correction to the state

$$\begin{aligned} \left|n_0^{(1)}\right\rangle &= \sum_{m\neq n} |m_0\rangle \frac{\langle m_0|-tz\left(\phi a^\dagger + \bar{\phi}a\right)|n_0\rangle}{E_{n_0}^{(0)} - E^{(m_0)}} - E_{n_0}^{(1)} \sum_{m\neq n} |m_0\rangle \frac{\delta_{n_0,m_0}}{E_{n_0}^{(0)} - E_{m_0}^{(0)}} \\ &\overset{(3.27)}{=} \sum_{m\neq n} |m_0\rangle \frac{-tz\left(\phi\sqrt{n_0+1}\delta_{m_0,n_0+1} + \bar{\phi}\sqrt{n_0}\delta_{m_0,n_0-1}\right)}{E_{n_0}^{(0)} - E_{m_0}^{(0)}} \\ &= -tz\left(\frac{\phi\sqrt{n_0+1}\,|n_0+1\rangle}{E_{n_0}^{(0)} - E_{n_0+1}^{(0)}} + \frac{\bar{\phi}\sqrt{n_0}\,|n_0-1\rangle}{E_{n_0}^{(0)} - E_{n_0-1}^{(0)}}\right) \end{aligned}$$

where $E_{n_0}^{(0)} - E_{n_0+1}^{(0)} = \mu - Un_0$ and $E_{n_0}^{(0)} - E_{n_0-1}^{(0)} = U(n_0-1) - \mu$ as previously calculated. Hence, one gets

$$\left|n_0^{(1)}\right\rangle = -tz\left(\frac{\phi\sqrt{n_0+1}\,|n_0+1\rangle}{\mu - Un_0} + \frac{\bar{\phi}\sqrt{n_0}\,|n_0-1\rangle}{U(n_0-1)-\mu}\right) \tag{3.28}$$

[4] Focussing on the ground state per site, because the Hamiltonian is local.

With this result, the second order correction to the energy can be computed

$$E_{n_0}^{(2)} = \left\langle n_0 \middle| V^{\mathrm{t}} \middle| n_0^{(1)} \right\rangle = (tz)^2 \left[\langle n_0 | \left(\phi a^\dagger + \bar{\phi} a\right) \left(\frac{\phi\sqrt{n_0+1}\,|n_0+1\rangle}{\mu - Un_0} + \frac{\bar{\phi}\sqrt{n_0}\,|n_0-1\rangle}{U(n_0-1)-\mu} \right) \right]$$
$$= (tz)^2 \left[|\phi|^2 \frac{n_0+1}{\mu - Un_0} + |\phi|^2 \frac{n_0}{U(n_0-1)-\mu} \right]$$

$$\Rightarrow E_{n_0}^{(2)} = \left[(tz)^2 \left(\frac{n_0+1}{\mu - Un_0} + \frac{n_0}{U(n_0-1)-\mu} \right) \right] |\phi|^2 \tag{3.29}$$

The calculation of the correction to the energy up to fourth order is very tedious.
It will come out to the fact that the Landau theory of phase transitions can be used to argue where the phase transition appear. Hence, one ignores the state corrections and state only the energy correction of fourth order

$$E_{n_0}^{(4)} = (tz)^4 |\phi|^4 \left[\frac{(n_0+1)(n_0+2)}{(\mu - Un_0)^2(2\mu - U(2n_0+1))} + \frac{n_0(n_0-1)}{(U(n_0-1)\mu)^2(U(2n_0-3)-2\mu)} \right. \tag{3.30}$$
$$\left. - \left(\frac{n_0}{U(n_0-1)-\mu} + \frac{n_0+1}{\mu - Un_0} \right) \left(\frac{n_0}{(U(n_0-1)-\mu)^2} + \frac{n_0+1}{(\mu - Un_0)^2} \right) \right] \tag{3.31}$$

Now, summarizing all terms of the calculation the energy of the perturbed system is

$$E(\phi, \bar{\phi}) = a_0 + a_2 |\phi|^2 + a_4 |\phi|^4 + \mathcal{O}(|\phi|^6) \tag{3.32}$$

with

$$a_0 = \frac{U}{2} n_0(n_0-1) - \mu n_0 \quad \text{(unpertubated ground state energy)} \tag{3.33}$$

$$a_2 = tz + (tz)^2 \left(\frac{n_0+1}{\mu - Un_0} + \frac{n_0}{U(n_0-1)-\mu} \right) \tag{3.34}$$

$$a_4 = (tz)^4 \left[\frac{(n_0+1)(n_0+2)}{(\mu - Un_0)^2(2\mu - U(2n_0+1))} + \frac{n_0(n_0-1)}{(U(n_0-1)\mu)^2(U(2n_0-3)-2\mu)} \right. \tag{3.35}$$
$$\left. - \left(\frac{n_0}{U(n_0-1)-\mu} + \frac{n_0+1}{\mu - Un_0} \right) \left(\frac{n_0}{(U(n_0-1)-\mu)^2} + \frac{n_0+1}{(\mu - Un_0)^2} \right) \right] \tag{3.36}$$

It is obvious that the global $U(1)$-symmetry of the initial Hamiltonian is preserved. The energy 3.32 can be identified as the expansion of a thermodynamic potential in powers of a order parameter. According to the phenomenological Landau theory of phase transitions the phase transition will happen when the expansion coefficient a_2 vanishes if the coefficient a_4 is positive, otherwise $E(\phi, \bar{\phi})$ would be unbound from below. Indeed, a_4 is positive, which can be shown,[4].
Following Landau's theory minimizing the energy functional with respect to $\bar{\phi}$ leads to

$$\frac{\partial E(\phi, \bar{\phi})}{\partial \bar{\phi}} = a_2 \phi + 2a_4 |\phi|^2 \phi \stackrel{!}{=} 0 \tag{3.37}$$

$$\Rightarrow \phi_0 = 0 \quad \text{or} \quad |\phi_\pm|^2 = \frac{-a_2}{2a_4} \tag{3.38}$$

The solution that minimizes the energy is the one for which the second derivative is positive. This will depend on the sign of a_2.

$$\frac{\partial^2 E}{\partial \phi \partial \bar{\phi}} = a_2 + 4a_4 |\phi|^2 \stackrel{!}{>} 0 \tag{3.39}$$

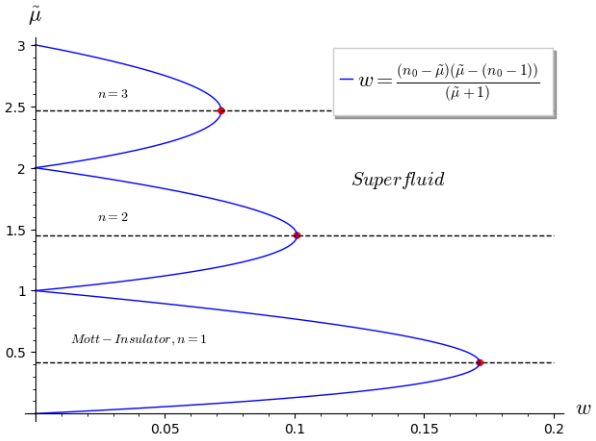

Figure 1: Mean-field phase diagram of the Bose-Hubbard model showing the first three Mott-lobes and the superfluid phase. The transition line $\tilde{\mu}(w)$ is given by 3.44 for a given Mott-lobe with n_0 per lattice site. The straight dotted line describes states with an integer-average boson density $\langle n \rangle$ per lattice site

From this condition follows

$$|\phi| = \begin{cases} 0 & \text{for } a_2 > 0 \\ \sqrt{\dfrac{-a_2}{2a_4}} & \text{for } a_2 < 0 \end{cases} \tag{3.40}$$

The solution for $a_2 < 0$ corresponds to a continuum of points, namely the boundary of a circle with radius of $\sqrt{\frac{-a_2}{2a_4}}$. The ground state will choose one of the points spontaneously. This leads to a gapless Goldstone mode which corresponds to phonon excitations in the superfluid state.
Due to the fact that the order parameter ϕ is non-zero for $a_2 < 0$ and zero for $a_2 > 0$, there has to be a phase transition of second order for $a_2 = 0$. The order parameter ϕ characterizes the superfluid phase. Hence, one expects that the Mott-insulating phase is stable for $a_2 > 0$ where for $a_2 < 0$ the superfluid occurs. Now, the condition $a_2 = 0$ yields

$$a_2 = tz + (tz)^2 \left(\frac{n_0 + 1}{\mu - U n_0} + \frac{n_0}{U(n_0 - 1) - \mu} \right) \stackrel{!}{=} 0 \tag{3.41}$$

Define new variables $\tilde{\mu} \equiv \mu/U$ and $w \equiv tz/U$. Solving for w leads to the expression

$$w = \frac{(n_0 - \tilde{\mu})(\tilde{\mu} - (n_0 - 1))}{\tilde{\mu} + 1} \tag{3.42}$$

3.42 states when the Superfluid-Mott-insulator transition appears. Going back to the cases where the ground state energy of the system is degenerate, $\mu = U n_0$ or $\mu = U(n_0 - 1)$. At this special points is $w = 0$, which can be seen from 3.42 by inserting $\mu = U n_0$ or $\mu = U(n_0 - 1)$. These correspond to the intersection points with the $\tilde{\mu}$-axis between two so-called "Mott-lobes", see figure 1 above. This means that the phase boundary extends down to $t = 0$. However, the system will be for all $t > 0$ in superfluid state even for $U \to \infty$ $\left(w = \dfrac{tz}{U} \underset{U \to \infty}{\to} 0^+ \right)$.
Solving 3.42 for $\tilde{\mu}$ leads to the quadratic equation

$$\tilde{\mu}^2 - \tilde{\mu}(2n_0 - 1 - w) + w + n_0(n_0 - 1) = 0 \tag{3.43}$$

which admits two solutions

$$\tilde{\mu}_\pm = n_0 - 1/2 - w/2 \pm \sqrt{w^2 - 4w(n_0 + 1/2) + 1} \tag{3.44}$$

for given values of n_0 provided that $w^2 - 4w(n_0 + 1/2) + 1 > 0$. The relation $\tilde{\mu}_\pm = \tilde{\mu}_\pm(w)$ defines the transition line for the Mott-lobes with a given integer value n_0. $\tilde{\mu}_+$ corresponds to the upper branch of a lobe and $\tilde{\mu}_-$ to the lower one.
The solutions merge for $w^2 - 4w(n_0 + 1/2) + 1 = 0$. Tese points correspond to the tips of the Mott-lobes and are indicated by dots at the tips in figure 1. Solving this condition for w gives the critical values for w and μ where the phase transition happens at the tips of the Mott-lobes[5]

$$w_c = 2n_0 + 1 - 2\sqrt{n_0^2 + n_0} \tag{3.45}$$

and inserted in 3.44 to

$$\tilde{\mu}_c = n_0 - 1/2 - w_c/2 = -1 + \sqrt{n_0^2 + n_0} \tag{3.46}$$

For instance, the critical value for $n_0 = 1$ is

$$w_c = \left(\frac{tz}{U}\right)_c \simeq 0.172$$

The initial Hamiltonian analyzed in the decoupling procedure is written in a "gran-canonical" form. The $-\mu\hat{n}$ is included because one wants to work with a varying particle number and therefore operate in the gran-canonical ensemble. Tthe ground-state energy 3.32 is recognized as the gran-canonical potential. Thus it is possible to calculate the average particle number per lattice site[6] by the well-known thermodynamic relation

$$\langle n \rangle = -\frac{\partial E(\phi, \bar{\phi})}{\partial \mu} \tag{3.47}$$

Insertion of 3.32 yields

$$\begin{aligned} \langle n \rangle &= -\frac{\partial}{\partial \mu} a_0 - \frac{\partial}{\partial \mu}\left(a_2|\phi|^2\right) - \frac{\partial}{\partial \mu}\left(a_4|\phi|^4\right) \\ &\overset{3.33}{=} n_0 - \frac{\partial}{\partial \mu}\left(a_2|\phi|^2 + a_4|\phi|^4\right) \end{aligned} \tag{3.48}$$

In the Mott-insulating state where $\phi = 0$, this becomes

$$\langle n \rangle = n_0 \tag{3.49}$$

which indeed shows that the average particle number per site in the insulating state is equal to the number of particles per site minimizing the the energy. This holds within a Mott-lobe for a given n_0. For the superfluid phase ϕ is non-zero and takes the value $|\phi|^2 = \dfrac{-a_2}{2a_4}$, consequently the average density becomes

$$\langle n \rangle = n_0 + \frac{\partial}{\partial \mu}\left(\frac{a_2^2}{4a_4}\right) \tag{3.50}$$

$$= n_0 + \frac{a_2}{2a_4}\frac{\partial a_2}{\partial \mu} - \frac{a_2^2}{4a_4^2}\frac{\partial a_4}{\partial \mu}, \tag{3.51}$$

and the superfluid has a density $\langle n \rangle = n_0$ if

$$\frac{a_2}{2a_4}\frac{\partial a_2}{\partial \mu} - \frac{a_2^2}{4a_4^2}\frac{\partial a_4}{\partial \mu} = 0. \tag{3.52}$$

[5]The other solution of the quadratic equation would lead to $\tilde{\mu}_c < 0$ and therefore to a vanishing occupation number.3.24

[6]3.32 is the ground state energy per site because the underlying Hamiltonian 3.21 is local

Right at the tips of the Mott-lobes, the relation $\frac{\partial a_2}{\partial \mu} = 0$ is satisfied. Thus, the phase transition at the tips happens at fixed constant integer density $\langle n \rangle = {n_0}^7$ while anywhere else on the transition line, the transition is accompanied by a density change. The areas of constant average integer density in the $(\tilde{\mu}, w)$-plane are depicted by the straight dotted lines in figure 1.

Additionally, it is interesting to look at the compressibility of the two phases. Again, from thermodynamics it is known that the compressibility κ can be computed using the relation

$$\kappa = \langle n \rangle^{-2} \frac{\partial \langle n \rangle}{\partial \mu} \tag{3.53}$$

Because of the fact that the average density of the Mott-insulating phase is constant, however, the compressibility vanishes in this state. The system is incompressible within a Mott-lobe with fixed average integer density. This is a defining property of the Mott-insulator.

For the superfluid state the compressibility is non-vanishing

$$\kappa = \langle n \rangle^{-2} \partial_\mu^2 \left(\frac{a_2^2}{4a_4} \right). \tag{3.54}$$

[7] It is possible to ignore the second term in 3.52 because it is less singular as a_2 approaches zero.

4 Field theoretical insight into the Bose-Hubbard model

In this section the functional integral representation of the partition function will be used to re-derive the mean-field results from the previous and to go beyond them. Then the effecive field theory that describes the phase transition in the vicinity of the phase boundary will be derived. This section is leaned on the chapter about optical lattices in [4], on the chapter about the Bose-Hubbard model in [3] and on the paper [11].

4.1 Hubbard-Stratonovich transformation

According to the section 2.1.3, the grand canonical partition function of the Bose-Hubbard model can be written as

$$Z = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S[\bar{\psi},\psi]} \tag{4.1}$$

with

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left(\sum_{i=1}^N \bar{\psi}_i(\tau)\partial_\tau \psi_i(\tau) + H_{BH}[\bar{\psi}, \psi] \right) \tag{4.2}$$

$$H_{HB} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \tag{4.3}$$

H_{HB} has to be normal ordered in order to be able to exchange the operators a_i and $a_i^\dagger$ with their eigenvalues ψ_i and $\bar{\psi}_i$, respectively, in the coherent states. This can be accomplished by rewriting the interaction term which is the only term not normal ordered, using $\hat{n}_i = a_i^\dagger a_i$

$$\hat{n}_i(\hat{n}_i - 1) = a_i^\dagger a_i (a_i^\dagger a_i - 1) \tag{4.4}$$

$$= a_i^\dagger (1 + a_i^\dagger a_i) a_i - a_i^\dagger a_i \tag{4.5}$$

$$= a_i^\dagger a_i^\dagger a_i a_i. \tag{4.6}$$

Then, the action becomes

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left[\sum_{i=1}^N \left(\bar{\psi}_i(\tau)(\partial_\tau - \mu)\psi_i(\tau) + \frac{U}{2} \bar{\psi}_i \bar{\psi}_i \psi_i \psi_i \right) - t \sum_{\langle i,j \rangle} \bar{\psi}_i \psi_j \right] \tag{4.7}$$

Next, define $t_{i,j} := \sum_{\alpha,k} t\delta_{i,j+\alpha\vec{\mathbf{a}}_k}$ where $\alpha = \pm 1$ and $\vec{\mathbf{a}}_k$ are basis lattice vectors with $k = \{1, .., d\}$. Therefore, the kinetic term of the action can be written as $S_{\text{kin}}[\bar{\psi}, \psi] = \int_0^\beta d\tau \left(- \sum_{i,j} \bar{\psi}_i t_{i,j} \psi_j \right)$. Hence, the action is

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left[\sum_{i=1}^N \left(\bar{\psi}_i(\tau)(\partial_\tau - \mu)\psi_i(\tau) + \frac{U}{2} \bar{\psi}_i \bar{\psi}_i \psi_i \psi_i \right) - \sum_{i,j} \bar{\psi}_i t_{i,j} \psi_j \right] \tag{4.8}$$

From field theroretical framework, as in the mean-field case, one has to start from the strong-coupling limit, $U/t >> 1$. In the weak coupling limit one would describe the usual superfluid to normal fluid transition, which we are not interested in.

To continue, it will be performed a so-called Hubbard-Stratonovich transformation by inserting a $\mathbb{1}$ in the form[8]

$$\mathbb{1} = \int \mathcal{D}[\bar{\phi}, \phi] \exp\left(- \int_0^\beta d\tau \sum_{i,j} \bar{\phi}_i t_{ij}^{-1} \phi_j \right) \tag{4.9}$$

and shift the variable ϕ and $\bar{\phi}$ in order to decouple the hopping term. [9]

$$\phi_j \to \phi_j + \sum_k t_{j,k} \psi \tag{4.10}$$

$$\Rightarrow \sum_{i,j} (\bar{\phi}_i + \sum_k t_{i,k} \bar{\psi}_k) t_{i,j}^{-1} (\phi_j + \sum_l t_{j,l} \psi) = \tag{4.11}$$

$$\sum_{i,j} \bar{\phi}_i t_{i,j}^{-1} \phi_j + \sum_i (\bar{\psi}_i \phi_i + \bar{\phi}_i \psi_i) + \sum_{i,j} \bar{\psi}_i t_{i,j} \psi_j \tag{4.12}$$

In the calculation it has been used that $\sum_i t_{i,k} t_{i,j}^{-1} = \delta_{k,j}$.

After this transformation, the initial partition function and action becomes

$$Z = \int \mathcal{D}[\bar{\psi}, \psi, \bar{\phi}, \phi] e^{-S[\bar{\psi}, \psi, \bar{\phi}, \phi]} \tag{4.13}$$

$$S[\bar{\psi}, \psi, \bar{\phi}, \phi] = \int_0^\beta \left[\sum_{i=1}^N \left(\bar{\psi}_i (\partial_\tau - \mu) \psi_i + \frac{U}{2} \bar{\psi}_i \bar{\psi}_i \psi_i \psi_i \right) + \sum_{i=1}^N (\bar{\psi}_i \phi_i + h.c.) + \sum_{i,j} \bar{\phi}_i t_{i,j}^{-1} \phi_j \right] \tag{4.14}$$

with a new auxilliary field ϕ. The next step would be to integrate out the bosonis fields $\psi, \bar{\psi}$, to get a effective theory for the auxilliary fields $\phi, \bar{\phi}$. This is not directly possible because the argument of the exponential function in the integrand is quartic in the fields ψ. But it is possible to get the effective theory perturbatively.

Define $S_{\text{loc}}[\bar{\psi}, \psi] = \int_0^\beta d\tau \sum_{i=1}^N \left(\bar{\psi}_i (\partial_\tau - \mu) \psi_i + \frac{U}{2} \bar{\psi}_i \bar{\psi}_i \psi_i \psi_i \right)$ for the local action that was solved exactly in section 3.2.

Assume that by integrating out the fields $\psi, \bar{\psi}$ the result is of the form

$$\Rightarrow e^{-S_{\text{eff}}[\bar{\phi}, \phi]} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-S[\bar{\psi}, \psi, \bar{\phi}, \phi]}. \tag{4.15}$$

$S_{\text{eff}}[\bar{\phi}, \phi]$ is the effective action for the auxilliary field ϕ which is of interest. 4.15 can be further rewritten with

$$S[\bar{\psi}, \psi, \bar{\phi}, \phi] = S_{\text{loc}}[\bar{\psi}, \psi] + \int_0^\beta d\tau \left(\sum_{i,j} \bar{\phi}_i t_{i,j}^{-1} \phi_j + \sum_i (\bar{\psi}_i \phi_i + \bar{\phi}_i \psi_i) \right) \tag{4.16}$$

as

$$\Rightarrow e^{-S_{\text{eff}}[\bar{\phi}, \phi]} = e^{-\int_0^\beta d\tau \sum_{i,j} \bar{\phi}_i t_{i,j}^{-1} \phi_j} \int \mathcal{D}[\bar{\psi}, \psi] e^{-\int_0^\beta d\tau \sum_i (\bar{\psi}_i \phi_i + \bar{\phi}_i \psi_i)} e^{-S_{\text{loc}}[\bar{\psi}, \psi]} \tag{4.17}$$

$$= Z_{\text{loc}} e^{-\int_0^\beta d\tau \sum_{i,j} \bar{\phi}_i t_{i,j}^{-1} \phi_j} \left\langle e^{-\int_0^\beta d\tau \sum_i (\bar{\psi}_i \phi_i + \bar{\phi}_i \psi_i)} \right\rangle_{\text{loc}}. \tag{4.18}$$

It has been defined that

$$\langle (...) \rangle_{\text{loc}} = \frac{1}{Z_{\text{loc}}} \int \mathcal{D}[\bar{\psi}, \psi] (...) e^{-S_{\text{loc}}[\bar{\psi}, \psi]} \tag{4.19}$$

[8] The normalization constant is absorbed into the definition of the integration measure $\mathcal{D}[\bar{\phi}, \phi]$

[9] This is possible because the functional integral in 4.9 is translationally invariant.

So, the average $\left\langle e^{-\int_0^\beta d\tau \sum_i (\bar{\psi}_i\phi_i + \bar{\phi}_i\psi_i)} \right\rangle_{\text{loc}}$ has to be calculated in the limit $T \to 0$.[10] This will be done pertubativaley by assuming that ϕ is small which is justified in the vicinity of the phase boundary. The average can be approximated by a cummulant expansion $\langle e^{-x} \rangle \simeq e^{-\langle x \rangle - (\langle x^2 \rangle - \langle x \rangle^2)/2}$ for small x.

The averages will not be calculated in the fuctional integral representation 4.19 because the action S_{loc} is quartic in the fileds and therefore not calcuable. It will instead be evaluated in the classical thermodynamic average weighted with the grand-canonical density operator.

$$\langle (...) \rangle_{\text{loc}} = \frac{1}{Z_{\text{loc}}} \text{Tr}\Big((...) e^{-\beta H_{\text{loc}}} \Big) \quad \text{with} \quad Z_{\text{loc}} = \text{Tr}\Big(e^{-\beta H_{\text{loc}}} \Big) \tag{4.20}$$

$$\text{and} \quad H_{\text{loc}} = \sum_{i=1}^{N} \left(\bar{\psi}_i (\partial_\tau - \mu) \psi_i + \frac{U}{2} \bar{\psi}_i \bar{\psi}_i \psi_i \psi_i \right) \tag{4.21}$$

In this representation the averages can be calculated by evaluating the trace in the eigenbase of H_{loc}. This Hamiltonian was solved exactly in section 3.2.

The first order cummulant $\left\langle -\int_0^\beta \sum_i (\bar{\phi}_i \psi_i + \bar{\psi}_i \phi_i) \right\rangle_{\text{loc}} = -\int_0^\beta \sum_i \left(\bar{\phi}_i \langle \psi_i \rangle_{\text{loc}} + \phi_i \left\langle \psi_i^\dagger \right\rangle_{\text{loc}} \right)$ is linear in the creation and annihilation operators $\psi^\dagger$ and ψ. It will therefore vanish when the trace is evaluated in the particle number basis 3.9. For instance[11]

$$\begin{aligned} \langle \psi_i(\tau) \rangle_{\text{loc}} = \text{Tr}\Big(\psi_i(\tau) e^{-\beta H_{\text{loc}}} \Big) &= \sum_n \langle n | \psi_i(\tau) e^{-\beta \epsilon_n} | n \rangle \\ &= \sum_n \langle n | e^{\tau \epsilon_n} \psi_i e^{-\beta \epsilon_n} e^{-\tau \epsilon_n} | n \rangle \\ &= \sum_n e^{-\beta \epsilon_n} \underbrace{\langle n | \psi_i | n \rangle}_{= \sqrt{n} \delta_{n,n-1}} \\ &= 0, \end{aligned} \tag{4.22}$$

and analogously for $\left\langle \psi_i^\dagger \right\rangle_{\text{loc}}$.

Hence, only the second cummulant is left to calculate in

$$\left\langle e^{-\int_0^\beta d\tau \sum_i (\bar{\psi}_i \phi_i + \bar{\phi}_i \psi_i)} \right\rangle_{\text{loc}} = e^{-\left\langle \left(\int_0^\beta d\tau \sum_i (\bar{\phi}_i \psi_i + \bar{\psi}_i \phi_i) \right)^2 \right\rangle_{\text{loc}} / 2}. \tag{4.23}$$

$$\begin{aligned} &\Rightarrow \frac{1}{2} \left\langle \left(\int_0^\beta d\tau \sum_i (\bar{\phi}_i \psi_i + \bar{\psi}_i \phi_i) \right)^2 \right\rangle_{\text{loc}} = \\ &\frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{i,j} \left\langle \bar{\phi}_i(\tau) \phi_j(\tau') \psi_i(\tau) \bar{\psi}_j(\tau') + \bar{\phi}_j(\tau') \phi_i(\tau) \bar{\psi}_i(\tau) \psi_j(\tau') \right\rangle_{\text{loc}} \end{aligned} \tag{4.24}$$

To translate the expectation value of the fields into the expectation value of operators, one has to introduce the imaginary time ordering operator T.

$$\left\langle \psi_i(\tau) \bar{\psi}_j(\tau') \right\rangle_{\text{loc}} = \left\langle T_\tau \left[\psi_i(\tau) \psi_j^\dagger(\tau') \right] \right\rangle_{\text{loc}} \tag{4.25}$$

[10] The quantum phase transition happens at $T = 0$.

[11] The Hamiltonian is local for which reason the on-site average is taken

In addition, the averages are taken on a single site, which means they are only non-zero on the same site.

$$\left\langle T_\tau \left[\psi_i(\tau)\psi_j^\dagger(\tau')\right]\right\rangle_{\text{loc}} = \delta_{i,j}\left\langle T_\tau \left[\psi_i(\tau)\psi_i^\dagger(\tau')\right]\right\rangle_{\text{loc}} \tag{4.26}$$

4.24 becomes then

$$\begin{aligned} 4.24 &= \frac{1}{2}\int_0^\beta d\tau d\tau' \sum_{i,j} \bar{\phi}_i(\tau) 2\delta_{i,j}\left\langle T_\tau \left[\psi_i(\tau)\psi_j^\dagger(\tau')\right]\right\rangle_{\text{loc}} \phi_j \\ &= \int d\tau d\tau' \sum_i \bar{\phi}_i(\tau)\left\langle T_\tau \left[\psi_i(\tau)\psi_j^\dagger(\tau')\right]\right\rangle_{\text{loc}} \phi_i(\tau') \\ &= -\int d\tau d\tau' \sum_i \bar{\phi}_i(\tau) G(\tau-\tau')\phi_i(\tau') \end{aligned} \tag{4.27}$$

The on-site propagator $G(\tau-\tau')$ has previously been defined as

$$G(\tau-\tau') = -\left\langle T_\tau(\psi_i(\tau)\psi_i^\dagger(\tau'))\right\rangle.$$

It characterizes the propagation of bosonic field form a site i at time τ' to the same site i at another time τ. As the system is time translationally invariant, it is sufficient to calculate $G(\tau)$

$$G(\tau) = -\left\langle T_\tau(\psi_i(\tau)\psi_i^\dagger(0))\right\rangle = -\left\langle \psi_i(\tau)\psi_i^\dagger(0)\right\rangle \tag{4.28}$$

$$= -\frac{1}{Z_{\text{loc}}}\sum_n (n+1)e^{-(\beta-\tau)\epsilon_n - \tau\epsilon_{n+1}} \tag{4.29}$$

Also, it will be useful to determine the propagator in Fourier space

$$G(i\omega) = \int_0^\beta G(\tau)e^{i\omega\tau} \tag{4.30}$$

$$= -\frac{1}{Z_{\text{loc}}}\sum_{n=0}^{\infty}(n+1)\frac{e^{-\beta\epsilon_{n+1}} - e^{-\beta\epsilon_n}}{i\omega + \epsilon_n - \epsilon_{n+1}} \tag{4.31}$$

Finally, taking the limit $T \to 0 (\beta \to \infty)$ leads to

$$G(i\omega) = \frac{n_0+1}{i\omega + \epsilon_{n_0} - \epsilon_{n_0+1}} - \frac{n_0}{i\omega + \epsilon_{n_0-1} - \epsilon_{n_0}} \tag{4.32}$$

where ϵ_{n_0} is the grond state energy 3.10. It has been used that $Z_{\text{loc}} \to e^{-\beta\epsilon_{n_0}}$ for $T \to 0$. From section 3.2 it is known that

$$\begin{aligned} \epsilon_{n+1} - \epsilon_n &= Un - \mu \\ \epsilon_{n-1} - \epsilon_n &= \mu - U(n-1). \end{aligned}$$

$$G(i\omega) = \frac{n+1}{i\omega + \mu - Un} - \frac{n}{i\omega + \mu - U(n-1)} \tag{4.33}$$

Going back to 4.23, it becomes

$$\left\langle e^{-\int_0^\beta d\tau \sum_i (\bar{\psi}_i\phi_i + \bar{\phi}_i\psi_i)}\right\rangle_{\text{loc}} \simeq e^{-\int_0^{beta} d\tau d\tau' \sum_i \bar{\phi}_i(\tau)G(\tau-\tau')\phi_i(\tau')} \tag{4.34}$$

and the integrand of the initial functional integral 4.15 is

$$e^{-S_{\text{eff}}[\bar{\phi},\phi]} = Z_{\text{loc}} e^{-\int_0^\beta d\tau d\tau' \sum_{i,j} \bar{\phi}_i(\tau)\left(t_{i,j}^{-1}\delta(\tau-\tau')+G(\tau-\tau')\delta_{i,j}\right)\phi_j(\tau')} \tag{4.35}$$

and the partition function can be written as

$$Z = Z_{\text{loc}} \int \mathcal{D}[\bar{\phi},\phi] e^{-S_{\text{eff}}[\bar{\phi},\phi]}. \tag{4.36}$$

From 4.36 one can recognize S_{eff} to be

$$\begin{aligned} S_{\text{eff}}[\bar{\phi},\phi] &= \int_0^\beta d\tau d\tau' \sum_{i,j} \bar{\phi}_i(\tau)\left(t_{i,j}^{-1}\delta(\tau-\tau') + G(\tau-\tau')\delta_{i,j}\right)\phi_j(\tau') \\ &:= \int_0^\beta d\tau d\tau' \sum_{i,j} \bar{\phi}_i(\tau)\mathcal{G}_{i,j}^{-1}(\tau-\tau')\phi_j(\tau') \end{aligned} \tag{4.37}$$

where the propagator $\mathcal{G}_{i,j}(\tau-\tau') = t_{i,j}^{-1}\delta(\tau-\tau') + G(\tau-\tau')\delta_{i,j}$ for the auxiliary field was deduced for practical reasons.

It will be very useful to Fourier transform the effective action by transforming the fields ϕ and $\bar{\phi}$

$$\phi_j(\tau) = \frac{1}{\sqrt{M\beta}} \sum_{\vec{\mathbf{q}},\omega} \phi_q e^{-i\omega\tau - i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_j} \quad \text{with} \quad q = (i\omega, \vec{\mathbf{q}}).$$

4.37 becomes then

$$\begin{aligned} S_{\text{eff}} &= \sum_q \bar{\phi}_q \left(-t_{\vec{\mathbf{q}}}^{-1} + G(i\omega)\right)\phi_q \\ &= -\sum_q \bar{\phi}_q \left(\mathcal{G}^{-1}(\vec{\mathbf{q}}, i\omega)\right)\phi_q \end{aligned} \tag{4.38}$$

with $t_{\vec{\mathbf{q}}} = -2t\sum_{l=1}^d \cos(q_l)$ and $G(i\omega) = 4.33$ from before. The inverse propagator $\mathcal{G}^{-1}(\vec{\mathbf{q}}, i\omega)$ for the auxiallary field ϕ in momentum and frequency space is given by

$$\mathcal{G}^{-1}(q) = t_{\vec{\mathbf{q}}}^{-1} - \frac{n+1}{i\omega+\mu-Un} - \frac{n}{i\omega+\mu-U(n-1)} \tag{4.39}$$

Analyzing the static limit $q=0 \quad q=(\vec{\mathbf{q}}, i\omega)$

$$\mathcal{G}^{-1}(0) = t_{\vec{\mathbf{q}}=0}^{-1} - \frac{n+1}{\mu-Un} - \frac{n}{\mu-U(n-1)} \quad \text{with} \quad t_{\vec{\mathbf{q}}=0} = -2td \tag{4.40}$$

and comparing with 4.36 one can see that the path integral is unstable for $\mathcal{G}^{-1}(\vec{\mathbf{q}}=0)$ and stable otherwise[12]. Therefore one expects that the transition line is obtained from the criterion

$$\mathcal{G}^{-1}(\vec{\mathbf{q}}=0) = 0 = t_{\vec{\mathbf{q}}=0}^{-1} - G(\imath\omega=0) \tag{4.41}$$

$$= -\frac{1}{2td} - \frac{n+1}{\mu-Un} - \frac{n}{\mu-U(n-1)} \tag{4.42}$$

Hence, this yields the equation

$$\frac{U}{2td} = -\frac{n+1}{\mu-Un} + \frac{n}{\mu-U(n-1)} \tag{4.43}$$

which is the same result as in the mean-field case 3.41 for $z=2d$, with z as the coordination number.

As an outlook, one could analayze the poles of the frequency and momentum dependent propagator, which yields the excitation spectrum of quasiparticles and quasiholes in the Mott-unsulating state.

[12] A Gaussian integral $\int dx e^{-ax^2}$ is only divergent for $a > 0$.

4.2 Effective theory

To derive the effective theory in the vicinity of the phase transition it is possible to expand the propagator $\mathcal{G}^{-1}(q)$ in 4.38 for small momenta and frequencies. This expansion yields

$$\mathcal{G}^{-1}(q) \simeq \mathcal{G}^{-1}(0,0) + \frac{\partial \mathcal{G}^{-1}(0,0)}{\partial \mu} i\omega + \frac{1}{4d^2 t}\vec{\mathbf{q}}^2 - \frac{1}{2}\frac{\partial^2 \mathcal{G}^{-1}(0,0)}{\partial \mu^2} \tag{4.44}$$

where $\frac{\partial \mathcal{G}^{-1}(0,0)}{\partial i\omega} = \frac{\partial \mathcal{G}^{-1}(0,0)}{\partial \mu}$ has been used. Terms higher than second order has been ignored. Hence, the effective action is

$$S_{\text{eff}}[\bar{\phi}, \phi] = \sum_{\vec{\mathbf{q}}, i\omega} \left(r|\phi|^2 - \frac{1}{2}\omega^2 \frac{\partial^2 r}{\partial \mu^2}|\phi| - \frac{\vec{\mathbf{q}}^2}{4d^2 t}|\phi|^2 + \frac{\partial r}{\partial \mu} i\omega |\phi|^2 \right). \tag{4.45}$$

where it has been defined $\mathcal{G}^{-1}(0,0) = -a_2(zt)^2 \equiv -r$ and a_2 corresponds to 3.41. Going back to the space and time representation this can be written as

$$S_{\text{eff}}[\bar{\phi}, \phi] = \int \mathrm{d}^d x \int d\tau \left(r|\phi|^2 - \frac{1}{2}\frac{\partial^2 r}{\partial \mu^2}|\partial_\tau \phi| - \frac{1}{4d^2 t}|\boldsymbol{\nabla}\phi|^2 - \frac{\partial r}{\partial \mu}\bar{\phi}\partial_\tau \phi \right). \tag{4.46}$$

Now, in this action there are two different cases to distinguish. The parameter r in the first term is proportional to a_2, the quantitity that describes the phase bouandary in figure 1. Note that the derivative $\frac{\partial r}{\partial \mu}$ vanishes when r is $\mu-$independent. However, this is precisely the condition in which the Mott insulator-superfluid phase boundary in figure 1 has a vertical tangent. This means that the linear term in the frequency ω vanishes at the tips of the Mott-lobes. Hence, the two cases are when $\frac{\partial r}{\partial \mu} \neq 0$ and $\frac{\partial r}{\partial \mu} = 0$.

Lookin first at the case where $\frac{\partial r}{\partial \mu} \neq 0$ holds. Oone can set $r = -\tilde{r}$. In this case the quadratic time derivative term can be neglected because it is dominated by the linear one.

$$S_{\text{eff}}[\bar{\phi}, \phi] = \left(\frac{\partial \tilde{r}}{\partial \mu}\bar{\phi}\partial_\tau \phi - \frac{1}{2m^*}|\boldsymbol{\nabla}\phi|^2 - \tilde{r}|\phi|^2 \right) \tag{4.47}$$

In this equation it has been defined that $m^* \equiv 2d^2 t$ Now, one can rescale the fields so that the time derivative term does not have a prefactor.

$$\phi \to \sqrt{\frac{\partial \tilde{r}}{\partial \mu}}\phi \tag{4.48}$$

$$\Rightarrow S_{\text{eff}}[\bar{\phi}, \phi] = \int \mathrm{d}^d x \int d\tau \left[\bar{\phi}\partial_\tau \phi - \frac{1}{2m}|\boldsymbol{\nabla}\phi|^2 - \tilde{\mu}|\phi|^2 \right] \tag{4.49}$$

The new prefactors are defined as

$$m \equiv -m^* \frac{\partial \tilde{r}}{\partial \mu} \quad \text{and} \quad \tilde{\mu} \equiv -\tilde{r}\frac{1}{\frac{\partial \tilde{r}}{\partial \mu}}.$$

This action describes only the free motion of the fields, it is the free non-interacting part of the action. In order to get an interacting theory, one has to include an interaction term. The initial Hamiltonian 3.1 has a global $U(1)-$symmetry, however this symmetry should be kept in the effective action. The free action, that was derived from a microscopic theory, has this symmetry. The next lowest order term which preserves this symmetry is of fourth order $\sim |\phi|^4$. Hence, the interacting effective action is

$$S_{\text{eff}}[\bar{\phi}, \phi] = \int \mathrm{d}^d x \int d\tau \left[\bar{\phi}\partial_\tau \phi + \frac{1}{2m}|\boldsymbol{\nabla}\phi|^2 + \tilde{\mu}|\phi|^2 + \frac{u}{4!}\left(|\phi|^2\right)^2 \right] \tag{4.50}$$

Later it will be argued that the quadratic term can be neglected because the coupling-constant $\tilde{\mu}$ is a so-called irrelevant variable for the quantum phase transition. The final effective action is

$$S_{\text{eff}}[\bar{\phi},\phi] = \int \mathrm{d}^d x \int d\tau \left[\bar{\phi}\left(\partial_\tau - \frac{\nabla^2}{2m}\right)\phi + \frac{u}{4!}\left(|\phi|^2\right)^2\right] \tag{4.51}$$

This is the critical theory of a dilute Bose gas,[3]. This result can be interpreted as follows. In the end of section 3.3 it has been seen that the phase transition is accompanied with a small density change away from integer filling anywhere on the phase boundary except at the tips of the Mott-lobes. The excess particles that arise would not change the average density and could move freely over the whole lattice, because the chemical potential becomes large or small enough so that particles that got added or removed can overcome the potential energy by the gain of kinetic energy. This free moving particles can be viewed as a free Bose gas.

Now, looking at the case where $\frac{\partial r}{\partial \mu} = 0$, one can see that the first order time derivative term vanishes and one gets

$$S_{\text{eff}}[\bar{\phi},\phi] = \int \mathrm{d}^d x \int d\tau \left(r|\phi|^2 - \frac{1}{2}\frac{\partial^2 r}{\partial \mu^2}|\partial_\tau \phi|^2 - \frac{1}{2m^*}|\boldsymbol{\nabla}\phi|^2 + u_0\left(|\phi|^2\right)^2\right) \tag{4.52}$$

where again $m = 2d^2 t$ an interaction term with coupling-constant u_0 was included. Next, one redefines $r = -\tilde{r}$ and rescales the fields $\phi \to \sqrt{\frac{\partial^2 \tilde{r}}{\partial \mu^2}}\phi$. The effective action becomes

$$\begin{aligned} S_{\text{eff}}[\bar{\phi},\phi] &= \int \mathrm{d}^d x \int d\tau \left(\frac{1}{2}|\partial_\tau \phi|^2 - \frac{1}{2m\,\partial^2\tilde{r}/\partial\mu^2}|\boldsymbol{\nabla}\phi|^2 - \frac{\tilde{r}}{\partial^2\tilde{r}/\partial\mu^2}|\phi|^2 + \frac{u_0}{\partial^2\tilde{r}/\partial\mu^2}\left(|\phi|^2\right)^2\right) \\ &\underset{\tilde{r}=-r}{=} \int \mathrm{d}^d x \int d\tau \left(\frac{1}{2}|\partial_\tau \phi|^2 + \frac{c^2}{2}|\boldsymbol{\nabla}\phi|^2 - \tilde{\mu}|\phi|^2 + \frac{u}{2}\left(|\phi|^2\right)^2\right) \end{aligned} \tag{4.53}$$

with

$$c^2 = \frac{1}{m\,\partial^2 r/\partial\mu^2} \quad \tilde{\mu} = \frac{\tilde{r}}{\partial^2\tilde{r}/\partial\mu^2} \quad \text{and} \quad u = 2u_0\frac{1}{\partial^2\tilde{r}/\partial\mu^2}$$

$$\Rightarrow S_{\text{eff}}[\bar{\phi},\phi] = \int \mathrm{d}^d x \int d\tau \left(\frac{1}{2}|\partial_\tau \phi|^2 + \frac{c^2}{2}|\boldsymbol{\nabla}\phi|^2 - \tilde{\mu}|\phi|^2 + \frac{u}{2}\left(|\phi|^2\right)^2\right) \tag{4.54}$$

The critical theory of the Mott insulator-superfluid quantum phase transition at the the tips of the Mott-lobes is thus a complex ϕ^4-theory in $d+1$ dimensions. This action has an emergent Lorentz-invariance due to particle-hole symmetry at this specific point. For any point into the Mott-lobes, the gap for particle (hole) excitations is simply the distance in $\mu-$direction, for t fixed, from the upper(lower) phase boundary. The lowest-lying excitation that conserves the total particle number is a particle-hole-exciation. The energy of this excitation is the sum of the particle and hole excitations. This energy is equal to the difference in μ between the top and bottom phase boundary at given t.

$$\text{Gap: } \Delta_g = U\sqrt{w^2 - 4(n+1/2)w + 1} \quad \text{with} \quad w = \frac{zt}{U}$$

The transition at the tip of the Mott-lobes therefore happens without change in the total particle number. It occurs due to the fact that the particles have enough kinetic energy $\sim t$ to overcome the potential energy $\sim U$.

This is a different mechanism than in the first case. The effective actions differ from each other by the order of the time derivative term. One says that they are in different so called **universality classes** where different physical systems act similarly in the vicinity of the critical point.

The first action 4.50 is in the universality class of the vacuum-superfluid transition in a dilute Bose gas and the second one 4.54 is the universality class of the $XY-$ or $O(2)-$model in $d+1$ dimensions.

Additionally, as a conclusion for this section. If one takes the limit where the fields $\bar{\phi}, \phi$ are time and spatially independent, one gets in both cases

$$\begin{aligned} S_{\text{eff}}[\bar{\phi}, \phi] &= \int \mathrm{d}^d x \int d\tau \left(\tilde{\mu} |\phi|^2 + \tilde{u} \left(|\phi|^2 \right)^2 \right) \\ &= V\beta \left(\tilde{\mu} |\phi|^2 + \tilde{u} \left(|\phi|^2 \right)^2 \right) \end{aligned}$$

The term under the integral can be intepreted as a form of energy. Therefore, it can be written as

$$E = \tilde{\mu} |\phi|^2 + \tilde{u} \left(|\phi|^2 \right)^2 . \tag{4.55}$$

This corresponds to the expansion of the free energy in powers of the order parameter ϕ, as it was derived in the relation 3.32.

5 Renormalization Group Analysis

This section follows the discussion of the Renormalization Group in Altland's and Simons's "Condensed Matter Field Theory" [5].

5.1 General Theory

In general, a field theory is given in the form

$$S[\phi] \equiv \sum_{a=1}^{N} g_a \mathcal{O}_a[\phi] \tag{5.1}$$

where ϕ is some (multi-component) field, g_a are coupling constants and $\mathcal{O}_a[\phi]$ a certain set of operators. By "renormalization of the theory" one refers to a scheme to derive a set of **Gell-Mann-low-equations** describing the change of the coupling constants $\{g_a\}$, as fast fluctuations of the theory are successively integrated out. There are different ways to derive the set of **flow equations** from the microscopic theory. All methods share the feature that they proceed in a sequence of three steps. The scheme which will be used is called the **momemntum shell integration**.

I. Subdivision of the manifold

One decomposes the integration manifold $\{\phi\}$ into a sector to be integrated out $\{\phi^{>}\}$ and a complementary set $\{\phi^{<}\}$. In the momentum shell integration scheme, the sector to be integrated out is defined to be the shell $\frac{\Lambda}{b} \leq \left|\vec{\mathbf{k}}\right| \leq \Lambda$ with $b > 0$. The **UV-cutoff** Λ is an **intrinsic generic short distance cut off**, e.g. $\Lambda \sim 1/a$ where a is the lattice spacing. The fields $\{\phi^{>}\}$ are in this sector, the large momentum/small length scales modes and the small momentum/ large length scale modes $\{\phi^{<}\}$ are in the sector $|\vec{\mathbf{p}}| \leq \frac{\Lambda}{b}$. Hence, one can decompose ϕ in slow and fast modes in $k-$space as follows

$$\begin{aligned} \phi(x) &= \phi^{>}(x) + \phi^{<}(x) && (5.2)\\ &= \sum_{\Lambda/b<k<\Lambda} \phi^{>}(k) e^{ikx} + \sum_{k<\Lambda/b} \phi^{<}(k) e^{ikx} && (5.3) \end{aligned}$$

II. RG step; Decimation

One integrates out the fast/short distance fluctuations. In general, this step includes approximations which are done in a so called **loop expansion**. The expansion parameter is the number of loops. Here, one has to assume that higher loop numbers become smaller contributions.
The effective action is then of the form

$$S'[\phi^{<}] = \sum_{k<\Lambda/b} \sum_{n} g'_n \mathcal{O}'_n[\phi^{<}] \tag{5.4}$$

where the prime stands for new couplings and operators after the integration.
The integration step therefore changes the coupling constants and possibly generates new terms in the action. It has to be checked if the new generated terms are **relevant** in their scaling behaviour. If they are, one has to include them into the former action with an a priori undetermined coupling constant and repeat the steps until no new terms are generated. Again, one ends up with the action

$$S'[\phi^{<}] = \sum_{k<\Lambda/b} \sum_{n} g'_n \mathcal{O}'_n[\phi^{<}] \tag{5.5}$$

with a new momentum cut-off $\frac{\Lambda}{b}$. It will be necessary to get the action in the initial form, the momenta and frequencies have to be rescaled, which is the third RG step.

III. Rescaling

One has to rescale the frequencies and momenta so that the rescaled field amplitude fluctuates on same scale as the former field

$$k \to bk \quad \text{and} \quad \omega \to b^z \omega \tag{5.6}$$

where z is the **dynamical exponent**. However, ϕ can be rescaled arbitrarily because it is simply an variable of integration. The rescaling

$$\phi \to b^{\Delta_\phi} \phi \tag{5.7}$$

is called **field renormalization**, Δ_ϕ is the scaling dimension of the field. Usually, one chooses Δ_ϕ such that the free non-interacting part of the theory is **scale invariant**, which means it does not change under the RG steps. For instance

$$S = \int \mathrm{d}^d x \int d\tau \left(|\boldsymbol{\nabla}\phi|^2 + |\partial_\tau \phi|^2 \right) \tag{5.8}$$

$$\underset{x'=x/b}{\overset{\phi'=b^{\Delta_\phi}\phi}{\to}} \int \mathrm{d}^d x' \int d\tau' b^{d+z} \left(b^{-2-2\Delta_\phi} \left|\boldsymbol{\nabla}'\phi'\right|^2 + b^{-2(z+\Delta_\phi)} \left|\partial_{\tau'}\phi'\right|^2 \right) \tag{5.9}$$

$$= \int \mathrm{d}^d x' \int d\tau' b^{d+z-2\Delta_\phi} \left(b^{-2} \left|\boldsymbol{\nabla}'\phi'\right|^2 + b^{-2z} \left|\partial_{\tau'}\phi'\right|^2 \right) \tag{5.10}$$

Here one has to choose $z = 1$ so that the space and imaginary time scale in the same manner.

$$S'[\phi'] = \int \mathrm{d}^d x' \int d\tau' b^{d+1-2\Delta_\phi-2} \left(\left|\boldsymbol{\nabla}'\phi'\right|^2 + \left|\partial_{\tau'}\phi'\right|^2 \right) \overset{!}{=} S[\phi] \tag{5.11}$$

From this demand follows

$$0 = d + 1 - 2\Delta_\phi - 2 \tag{5.12}$$

$$\Delta_\phi = \frac{d+z-2}{2} \overset{z=1}{=} \frac{d+1-2}{2} \tag{5.13}$$

The factor z can be interpreted as an increasing factor for the dimensionality and one gets a effective dimension $d_{\text{eff}} = d + z = d + 1$,[12]. The factor z arises in quantum phase transitions. As result of the RG steps the effective action becomes

$$S[\phi] = \sum_{k<\Lambda} \sum_n g'_n \mathcal{O}_n[\phi] \tag{5.14}$$

Therefore, the effect of the RG is a change of all coupling constants. It is a mapping from the set of old couplings $\vec{\mathbf{g}} = \{g_1, ..., g_n\}$ to a new set of couplings $\vec{\mathbf{g}}' = \{g'_1, ..., g'_n\}$.

$$\vec{\mathbf{g}}' = R(\vec{\mathbf{g}}) \tag{5.15}$$

In general, R is a non-linear function of $\vec{\mathbf{g}}$. It is convinient to set $b = e^l$ and integrate out only a infinitesimal shell ($\Lambda > k\frac{\Lambda}{e^l}, l \to 0^+$). In this process the difference between bare and renormalized coupling is made arbitrarily small and one can be written $\vec{\mathbf{g}}' - \vec{\mathbf{g}} = R(\vec{\mathbf{g}}) - \vec{\mathbf{g}}$ in the form of the Gell-Mann-Low-equations or flow equations.

$$\frac{\mathrm{d}\vec{\mathbf{g}}}{\mathrm{d}l} = \beta(\vec{\mathbf{g}}) \quad \text{where} \quad \beta(\vec{\mathbf{g}}) = \lim_{l\to 0^+} \frac{R(\vec{\mathbf{g}}) - \vec{\mathbf{g}}}{l} \tag{5.16}$$

5.2 Tree-Level scaling

The Renormalization Group (RG) steps will be used on the two effective actions that emerged in the vicinity of the phase boundary,4.54 and 4.50. For the **Tree-Level Scaling**, it will be assumed that the integration over the fast modes $\phi^{>}$ has no effect on the slow modes in the action. The flow equations will be derived in this approximation and analysed. It will be started with the action of the universality class for the dilute Bose gas. Consequently, the flow equations for the action of the XY-model will be written down in analogy to the previous ones. The stated action is

$$S_{\text{eff}}[\bar{\phi},\phi] = \int \mathrm{d}^d x \int d\tau \left[\bar{\phi}\partial_\tau\phi + \frac{1}{2m}|\boldsymbol{\nabla}\phi|^2 + \tilde{\mu}|\phi|^2 + \frac{u}{2}\left(|\phi|^2\right)^2\right]. \tag{5.17}$$

The first RG step is to divide the fields into high and low momentum modes where the frequency/time dependence stays the same. An intrinsic high energy cut-off Λ is inserted

$$\phi(x,t) = \sum_{k<\Lambda/b} \phi(k,t)e^{ikx} + \sum_{\Lambda/b<k<\Lambda} \phi(k,t)e^{ikx}. \tag{5.18}$$

Afterwards the high energy modes $\phi^{>}$ are integrated out and it is assumed that this has no effect on the action.

Hence, the action becomes

$$\begin{aligned} S_{\text{eff}}[\bar{\phi},\phi] &= \int \mathrm{d}^d x \int_0^\beta d\tau \left[\bar{\phi}^{<}\partial_\tau\phi^{<} + \frac{1}{2m}\left|\boldsymbol{\nabla}\phi^{<}\right|^2 + \tilde{\mu}\left|\phi^{<}\right|^2 + \frac{u}{2}\left(\left|\phi^{<}\right|^2\right)^2\right] \\ &\equiv \int \mathrm{d}^d x \int_0^\beta d\tau \left[\bar{\phi}\partial_\tau\phi + \frac{1}{2m}|\boldsymbol{\nabla}\phi|^2 + \tilde{\mu}|\phi|^2 + \frac{u}{2}\left(|\phi|^2\right)^2\right] \end{aligned} \tag{5.19}$$

As the next step, the momenta, frequencies and fields are rescaled in order to get the former UV-cut-off Λ.

$$x' = x/b \quad , \quad \tau' = \tau/b^z \quad \text{and} \quad \phi' = b^{\Delta_\phi}\phi \tag{5.20}$$

Then, one gets

$$\begin{aligned} S_{\text{eff}}[\bar{\phi},\phi] &= \int \mathrm{d}^d x' \int_0^{\beta b^{-z}} d\tau' b^{d+z} \left(b^{-2\Delta_\phi - z}\bar{\phi}'\partial'_\tau\phi' + b^{-2-2\Delta_\phi}\frac{1}{2m}\left|\boldsymbol{\nabla}\phi'\right|^2 + b^{-2\Delta_\phi}\tilde{\mu}\left|\phi'\right|^2 + \frac{u}{2}b^{-4\Delta_\phi}\left(\left|\phi'\right|^2\right)^2\right) \\ &= \int \mathrm{d}^d x' \int_0^{\beta b^{-z}} d\tau' \left(b^{-2\Delta_\phi + d}\bar{\phi}'\partial'_\tau\phi' + b^{d+z-2-2\Delta_\phi}\frac{1}{2m}\left|\boldsymbol{\nabla}\phi'\right|^2 + b^{d+z-2\Delta_\phi}\tilde{\mu}\left|\phi'\right|^2 + \frac{u}{2}b^{d+z-4\Delta_\phi}\left(\left|\phi'\right|^2\right)^2\right) \end{aligned}$$

and if one inserts $\Delta_\phi = \dfrac{d+z-2}{2}$, in analogy to 5.12, this becomes

$$S_{\text{eff}}[\bar{\phi},\phi] = \int \mathrm{d}^d x' \int_0^{\beta b^{-z}} d\tau' \left(b^{2-z}\bar{\phi}'\partial'_\tau\phi' + \frac{1}{2m}\left|\boldsymbol{\nabla}\phi'\right|^2 + b^2\tilde{\mu}\left|\phi'\right|^2 + \frac{u}{2}b^{4-z-d}\left(\left|\phi'\right|^2\right)^2\right) \tag{5.21}$$

It is obvious that the free part of the action is scale invariant for $z = 2$.

The effect of the RG procedure amounts to a change of the coupling constants $\tilde{\mu}$ and u, and also of the inverse temperature β.

$$\tilde{\mu}' = b^2\tilde{\mu} \tag{5.22}$$

$$u' = b^{4-(z+d)}u \tag{5.23}$$

$$\beta' = b^{-z}\beta \Rightarrow T' = b^z T \tag{5.24}$$

From these equation one can writte down the flow equations for the Tree-Level-Scaling where b is chosen to be $b = e^l$

$$\frac{\partial \tilde{\mu}}{\partial l} = 2\tilde{\mu} \tag{5.25}$$

$$\frac{\partial u}{\partial l} = (4 - (z + d))u \tag{5.26}$$

$$\frac{\partial T}{\partial l} = zT \tag{5.27}$$

Where the $\beta-$functions from 5.16 are recognized to be

$$\beta_\mu = 2\mu \quad , \quad \beta_u = [4 - (z + d)]u \quad \text{and} \quad \beta_T = zT \tag{5.28}$$

The zeroes of the $\beta-$functions define the **fixed points** of the flow equations. At these points, the coupling constants do not change and therefore is the action invariant. This defines a new symmetry, the so-called **scale invariance**. The solutions of the flow equations are

$$\tilde{\mu}(l) = e^{2l}\tilde{\mu}(0) \tag{5.29}$$

$$u(l) = e^{(4-(z+d))l}u(0) \tag{5.30}$$

$$T(l) = e^{zl}T(0) \tag{5.31}$$

The prefactors in the exponents are the **scaling dimension of the coupling constants**.

$$\Delta_\mu = 2 \quad , \quad \Delta_u = 4 - (z + d) \quad \text{and} \quad \Delta_T = z \tag{5.32}$$

Their value is significant for the flow of the coupling constants. This result suggest a discrimination between at least three different types of scaling behaviours.

(i) For $\Delta_i > 0 (i = \mu, u, T)$ the flow is directed away from a fixed point. The associated coupling constant is said to be **relevant**.

(ii) In the complementary case, $\Delta_i < 0$, the flow is attracted by the fixed point. Coupling constants with this property are said to be **irrelevant**.

(iii) Finally, coupling constants which are invariant under the flow $\Delta_i = 0$, are termed **marginal**.

The distinction of relevant, irrelevant and marginal coupling constants in turn implies different types of fixed points.

(i) Firstly, there are **stable fixed points**, i.e. fixed points whose coupling constants are alle irrelevant. These points corresponds what can be called stable phases of matter. When you release a system in parameter space surrounding any of these attractors, it will scale towards the fixed point and eventually sit there.

(ii) Complementary to stable fixed points there are **unstable fixed points**. Here, all coupling constants are relevant. These fixed point can not be reached and, even if you approach it closely , the system will eventually flow away from it.

(iii) A fixed point which has both relevant and irrelevant coupling constants is associated with **phase transition,** see in [5] the chapter about Renormalization Group. The fixed point in the considered case is at

$$\tilde{\mu}^* = 0 \quad , \quad T^* = 0 \quad \text{and} \quad u^* = 0 \tag{5.33}$$

which is called **Gaussian fixed point**. The scaling dimension of $\tilde{\mu}$ and T are positive, therefore they are relevant couplings. Whether u is a relevant or irrelevant coupling depends on the number

of dimensions d.

$$\Delta_u = 4 - (z+d) \underset{z=2}{=} 2 - d \equiv \varepsilon = \begin{cases} > 0 & \text{for} \quad d < 2 \\ = 0 & \text{for} \quad d = 2 \\ < 0 & \text{for} \quad d > 2 \end{cases} \tag{5.34}$$

From this one can see that the interaction u becomes irrelevant for $d > 2$. The dimension $d_c = 2$ is therefore called **upper critical dimension**.
Hence, for $d > 2$ the couplings $\tilde{\mu}$ and T are relevant for the fixed point $\tilde{\mu}^*$, $T^* = 0$ and $u^* = 0$ in which u is irrelevant. This indicates a phase transition at these values for the couplins or rather a quantum phase transition because of $T = 0$.

The action at this fixed point is

$$S_{\text{eff}}^{BG}[\bar{\phi}, \phi]0 \int \mathrm{d}^d x \int_0^\infty d\tau \left(\bar{\phi}\partial_\tau \phi + \frac{1}{2m} |\boldsymbol{\nabla}\phi|^2 + \frac{u}{2} \left(|\phi|^2 \right)^2 \right) \tag{5.35}$$

as in 4.51.

For the XY-model, the only difference to the theory before is the order of the term with the time derivative.

$$S_{\text{eff}}^{XY}[\bar{\phi}, \phi] = \int \mathrm{d}^d x \int_0^\beta d\tau \left(\frac{1}{2} |\partial_\tau \phi|^2 + \frac{c^2}{2} |\boldsymbol{\nabla}\phi|^2 - \tilde{\mu}|\phi|^2 + \frac{u}{4!} \left(|\phi|^2 \right)^2 \right) \tag{5.36}$$

The RG steps after the rescaling lead to the action

$$S_{\text{eff}}^{XY}[\bar{\phi}', \phi'] = \int \mathrm{d}^d x' \int_0^{\beta b^{-z}} d\tau' \left(b^{2-2z} \frac{1}{2} \left| \partial_{\tau'} \phi' \right|^2 + \frac{c^2}{2} \left| \boldsymbol{\nabla}' \phi' \right|^2 - b^2 \tilde{\mu} \left| \phi' \right|^2 + b^{4-(d+z)} \frac{u}{4!} \left(\left| \phi' \right|^2 \right)^2 \right) \tag{5.37}$$

where it was again inserted that $\Delta_\phi = \dfrac{d+z-2}{2}$. The only difference in the scaling behaviour to the action for the dilute Bose gas is the value of the dynamical exponent z. Which has to be chosen properly such that the free part is scale invariant. The dynamical exponent z has to be set one so that this demand is satisfied. The flow equations are

$$\tilde{\mu}' = b^2 \tilde{\mu} \tag{5.38}$$

$$T' = bT \tag{5.39}$$

$$u' = b^{3-d} u \tag{5.40}$$

or if one sets $b = e^l$ and let l seek to 0^+

$$\frac{\partial \tilde{\mu}}{\partial l} = 2\tilde{\mu} \tag{5.41}$$

$$\frac{\partial T}{\partial l} = T \tag{5.42}$$

$$\frac{\partial u}{\partial l} = (3-d)u \equiv \varepsilon u \tag{5.43}$$

The upper critical dimension for this critical theory where the interaction constant u becomes irrelevant is $d_c = 3$.

5.3 Wilson-Fisher fixed point

As mentioned in the beginning of the section, analytical RG computations requirea pertubative treatment of the interaction term. For $d < d_c$ these grow under RG transformations, i.e. interactions

are relevant in the RG sense below d_c. For the $|\boldsymbol{\nabla}\phi|^4$-theories 4.54 and 4.51 the critical fixed point with non-linearity $u = 0$, the Gaussian fixed point is unstable with respect to finite u. An unstable fixed point is one where all coupling constants are relevant. Therefore the critical fixed point for $d < d_c$ will be characterized by a finite value of u, the so-called **Wilson-Fisher fixed point**. The relevance of the interaction implies that bare pertubation theory is divergent at criticalicity, see [5]. This problem can be overcome using the so-called $\varepsilon-$**expansion**. A theory of the $|\phi|^4-$type can be analysed in an expansion around the upper critical dimension, i.e. in $\varepsilon = d_c - d$. This approach is based on the observation that the fixed point value of renormalized coupling, u, is small near $d = d_c$, and a double expansion in u and ε allows for controlled calculations. In the XY-model, the RG equations, describing the flow of the dimensionless non-linear coupling, u, upon changing b reads

$$\frac{\partial u}{\partial l} = \varepsilon u - \frac{5}{3}u^2 \tag{5.44}$$

with a fixed point at $u^* = \frac{3}{5}\varepsilon$ where $\varepsilon = d_c - d$.

For the dilute Bose gas one gets with a redefined interaction coupling $u \to \frac{\Lambda^{2-d}}{2mS_d}u$ and where $S_d = \frac{2}{\Gamma(d/2)(4\pi)^{d/2}}$ is the usual phase space factor

$$\frac{\partial u}{\partial l} = \varepsilon u - \frac{u^2}{2} \tag{5.45}$$

With the stable fixed point at

$$u^* = 2\varepsilon \tag{5.46}$$

Physically, the finite value of u at criticality implies strong self-interactions of the order parameter of the bosons for $d < d_c$.

Observables at and near criticality require different treatments, depending on whether $d > d_c$ or $d < d_c$. Above the upper-critical dimension, bare perturbation is usually sufficient. Below d_c, one can employ a renormalized perturbation expansion, perturbation theory is formulated in terms of renormalized quantities, and in the final expressions the couplings are replaced by their fixed point values, and the results are interpreted as arising from an ε expansion of the expected power-law behaviour, i.e. power laws are obtained by re-exponentiating the perturbation series. The renormalized perturbation expansion can thus be understood as a certain resummation technique of bare perturbation theory.

6 Conclusion and Outlook

It was seen that the quantum phase transition right at the tips of the Mott-lobes which leaves the average integer filling of the lattice sites unchanged, happens due to the fact that the bosons have enough energy to overcome the repulsive interaction potential. This bosons can be interpreted as free particles which immediately condense and generate the superfluid phase. The effective theory describing this transition has a emergent lorentz invariance in $(d+1)-$dimensional space. It is in the same universality class as the XY-model. This symmetry is due to the equality of the excitation gaps of quasiparticles and quasiholes out of the Mott-insulating phase.
Anywhere else on the phase boundary the transition is accompined with a change of the average particle number per lattice site. The excess particles or holes over the average integer filling act like a free dilute Bose gas. These free constituents then condense and lead to the superfluid phase. The effective filed theory describing this transition is in the universality class of a dilute Bose gas.
The perspective of the Renormalization Group, let one suggest that the quantum critical point is at $T = 0$ and where the mass term in the actions of the theories vanishes. The interaction term scales differently dependent on the dimension d. There are different fixed points to which the theories scale.
As an outlook, the derived fixed points which describes the quantum phase transition are not unique universal quantities. They depend on the method used to derive them.
Universal quantities which can be measured in experiment are the so-called **critical exponents**. These can be determined from the fixed point values and state how thermodynamic quantities scale in the vicinity of the phase boundary,[5].

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Selbstständigkeitserklärung

Hiermit erkläre ich, die vorliegende Arbeit selbständig verfasst zu haben und keine anderen als die in der Arbeit angegebenen Quellen und Hilfsmittel benutzt zu haben.

Petar Čubela München, 14.02.2019