Strongly Correlated Bosons
In
One-Dimensional Optical Lattices

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Strongly Correlated Bosons in One-Dimensional Optical Lattices

Master Thesis

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Summary

Recently, the experimental possibility of having a Bose-Einstein condensate in an optical lattice has become available, opening new perspectives in the study of coherence phenomena in the strongly interacting limit. In order to observe strong correlations, the typical interaction energy between two atoms must exceed the single particle (kinetic and/or potential) energies. Since the kinetic energy of the bosons in the lattice decreases exponentially with increasing depth of the lattice potential, one can reach strong coupling in a deep lattice, and this even at low density and small scattering length.

It can be shown that under certain circumstances the dynamics of bosonic atoms with one internal level in an optical lattice generate the Bose-Hubbard model. We have studied this model in the strongly interacting limit with incommensurate filling of the lattice and obtained behavior similar to a discretized Tonks-Girardeau gas.

Strongly interacting bosons in a 1D optical lattice, with two (relevant) internal states, can be made to behave as interacting fermions. In this way, the bosonic system provides us with a method of observing typical 1D fermionic correlation behavior. In particular, we have made a proposal to observe spin-charge separation, a hallmark of 1D Fermi (Luttinger) liquids, in our bosonic system.
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Chapter 1

Introduction

1.1 Motivation

Since the development of quantum mechanics, a vast body of literature has been developed on the quantum-mechanical problem of a gas of particles interacting via a two-body potential. The experimental observation of Bose-Einstein condensation (BEC) in dilute alkali gases [1] has renewed a great interest in this area of research. In a Bose-Einstein condensate, the dilute nature of the gas allows for a rather fundamental description of the interaction effects; the complicated actual interparticle potential is replaced by an effective contact interaction with an interaction strength proportional to the only remaining physical parameter, the s-wave scattering length. The importance of the interaction effects can be estimated by the parameter $\gamma$, which is defined as the ratio between the interaction and kinetic energy per particle.

Up to now, most of the work on BEC has been focused on the regime $\gamma \ll 1$ (for a good introduction, see Ref. [26]). When studying such weakly interacting systems, a mean-field approach reproduces most of the interesting properties such as ground-state properties, interference between two BECs [35], vortices [20] and even matter-wave solitons [22]. The basic notion underlying mean-field theory is that of a macroscopic wavefunction or order parameter, which defines the spatial mode into which a significant fraction of the atoms condense below the critical temperature. This macroscopic wavefunction then obeys a nonlinear Schrödinger equation, the Gross-Pitaevskii equation. The theory is well suited to describing most of the effects of two-body interactions in weakly interacting dilute gases at zero temperature and can be generalized to also explore thermal effects.

Less is known about the strongly correlated regime ($\gamma \gg 1$), although it seems clear that, analogous to the fascinating phenomena encountered in strongly correlated condensed matter systems (ferromagnetism, Cooper pairing and fractional
quantum Hall effect to name a few), interesting physics going beyond a mean-field description should also be observable in cold atomic gases.

An obvious way to go beyond the weak coupling regime is to increase the interaction strength by increasing the s-wave scattering length making use of a Feshbach resonance [10, 29], or to increase the density. Of course, this method is limited by the fact that in this case the associated condensate lifetime strongly decreases due to three-body losses.

Another possibility would be to reduce the dimensionality of the system; recent advances and experiments on ultracold atomic vapors made the 1D regime reachable in a cigar-shaped trap at sufficiently low temperatures and high transverse frequencies [15]. Low dimensions amplify the role of quantum fluctuations and enhance correlations. As a surplus, one-dimensional systems on their own show some remarkable physics not encountered in 2D or 3D (e.g. Luttinger liquid behavior) and on top of that there are a fair number of exactly solvable 1D models, allowing the research of non-perturbative effects.

As an example, the 1D Bose gas with repulsive interparticle interaction, an exactly solvable model [18, 17], becomes more nonideal with decreasing density. This counterintuitive behavior is a typical signature of 1D. It means that in 1D the strongly interacting regime can be reached by lowering the density, so that in principle a Feshbach resonance would not be needed. It can be shown that for strong correlations, the dynamics of the one-dimensional Bose gas reduce to those of a gas of hard-core, or impenetrable point bosons, the “Tonks-Girardeau” gas [30, 5]. The one-to-one mapping of this system to a gas of free fermions, which is only applicable in 1D (see appendix A) ensures a fermionic spectrum and density profile of the Tonks gas. However, the momentum distribution of the homogeneous Tonks gas is fundamentally different from the filled Fermi sea for the corresponding Fermi system; it is known [31] that the momentum distribution for hard-core bosons is sharply peaked in the neighborhood of zero momentum. Although the occupation of this zero momentum state does not scale proportional to the number of particles (so there is no real BEC), the impenetrable bosons will show some coherence effects such as Talbot recurrences following an optical lattice pulse [27] and dark solitonlike behavior in response to a phase-imprinting pulse [6]. It is clear that this mix of fermionic and bosonic behavior in the limit of strong interactions makes this 1D system very interesting to study both theoretically and experimentally.

Recently, the experimental possibility of having a Bose-Einstein condensate in an optical lattice has become available, opening new perspectives in the study of coherence phenomena in both the weak and strongly interacting limit. Since the kinetic energy of the bosons in the lattice decreases exponentially with increasing depth of the lattice potential, one can reach strong coupling in a deep lattice, and this even at low density and small scattering length. Thus in this case it is the
quenching of the kinetic energy, and not the increasing interaction energy, which drives the atoms in the strongly interacting regime.

A remarkable future of these optical lattices is that almost all experimental parameters can be controlled with a high degree of precision which makes trapped gases very clean and flexible systems. The lattice spacing, for example, can be controlled through the wavelength of the interfering laser beams, while the lattice depth is adjustable over a wide range through the intensity of the interfering laser beams. Even the interaction strength can be separately controlled by Feshbach resonances. By a superposition of multiple laser beams it is also possible to generate a variety of different lattice topologies in a perfectly controlled manner. These powerful methods of tuning the relevant parameters are supplemented by versatile techniques to probe the state of the many-boson system, for instance by observing the matter-wave interference pattern after the atoms are released from the lattice.

Making use of this remarkable tunability, the optical lattice systems give access to a lot of fascinating physics concerning strongly correlated systems. Already now, the study of the formation of strongly correlated phases [7] and the observation of the collapse and the revival of the matter-wave field of a BEC have shown some of these diverse applications [8], but a lot of interesting properties remain to be explored. So far, the optical potentials used experimentally have been independent of the internal ground state of the atom. However, it has been suggested that by using spin-dependent lattice potentials one could bring atoms on different lattice sites into contact and thereby realize fundamental quantum gates [3], create large scale entanglement [11] or form a universal quantum simulator [13]. Moreover, cold gases in an optical lattice represent a useful tool to implement solid state systems and to test fundamental theories, often grown and developed in a different area [25].

From the above discussion it becomes clear that these lattice systems form an ideal model system for the investigation of fundamental questions associated with the physics related to fields as diverse as quantum- and atom-optics, quantum information processing and condensed matter physics.

1.2 Contents of the Thesis

In this thesis, the very interesting physics of strongly correlated atomic systems in optical lattices and their versatility is combined with the peculiarity of 1D. The thesis is divided into two main parts.

The lion's share of the work we pursued during the diploma is presented in the first part, where we will consider bosons without internal degrees of freedom
in a 1D lattice. It has already been shown in Ref. [12] that under certain circumstances the dynamics of bosonic atoms on the optical lattice generate the famous Bose-Hubbard model. The Hubbard model depends on two parameters only: the hopping integral, characterizing the kinetic energy of the bosons when they hop between two adjacent lattice sites and a parameter describing the interaction energy when two bosons occupy the same site. In Chapter 2, the realization of the Hubbard model with bosons on a 1D lattice is reviewed and a brief overview of the already known features of this model is given.

Despite the conceptual simplicity of the Bose-Hubbard model, it is considered to exhibit a wealth of interesting phenomena, and a lot of questions concerning the model remain to be answered. In particular, the strongly interacting limit of this model (called the Mott insulator phase) is always taken to have a commensurate filling. But we started to study this Mott phase for fractional filling factors, and we were able to observe typical strongly correlated behavior similar to the Tonks gas. This contradicts the point of view that the particles in an incommensurately filled lattice would form a condensate, which is what people in the community studying lattice gases believe; it is this new physical insight, described in chapter 3, that forms the main result of the thesis.

When considering bosons with internal degrees of freedom, a whole new range of effects becomes available. In the second part of the thesis, we will make use of the proposal that bosons with only two possible internal states in a 1D lattice can be made to behave as interacting fermions [25]. In this way, the bosonic system provides us with a method of observing typical 1D fermionic correlation behavior. The advantage of the approach of using bosons on a lattice to simulate fermions, instead of directly using fermions on a lattice, lies in the fact that fermions are hard to cool down sufficiently in order to trap them on a lattice. A 1D system of bosons with effectively only two internal levels on a lattice however, is already available experimentally [21].

Now, what makes this really interesting is that Fermi-Landau theory which describes interacting fermions in 3D is no longer applicable in a 1D system. Instead, according to Haldane [9], all gapless and interacting 1D fermion systems are so-called Luttinger liquids: they share universal features in their low energy physics corresponding to the exactly solvable Luttinger model [19]. One of the key predictions of this Luttinger model is spin-charge separation. It is a feature of interacting spin-1/2 particles and manifests itself as the complete separation of spin and charge dynamics. Both spin and charge excitations are phononlike, and they have a different propagation velocity. Until now, this fermionic behavior has never been observed clearly in a condensed matter system. However, we will propose a scheme of observing it in a lattice system containing bosons.

In chapter 5, a very short review is given concerning Luttinger liquids, with
emphasis on the differences between Luttinger and Fermi liquids. The explanation for being able to make bosons behave like interacting fermions, based on [25], is a little bit more elaborated.

Chapter 6 presents own work. By using a simple projection technique, we are able to separate spin and charge degrees of freedom in the Hamiltonian describing our lattice system. With this new approach, we can prove rather easily the existence of spin-charge separation, a typical 1D fermionic property, in our bosonic system.

While the separation is then clear from a theoretical point of view, it is much harder to observe it experimentally because, as discussed very shortly in chapter 7, we will see that one would need access to a single well of the lattice, which unfortunately, is not yet feasible.

In reading the thesis, it will become clear that subjects in the second part of the thesis are not treated with the same profoundness as in the first part. The reason for this is that most of my time was spent working on the physics described in the first part. The second part therefore has to be considered as a first step, to give some impression about the tremendous possibilities with strongly correlated bosons on a lattice.
Part I

"Spinless" Bosons in a 1D Lattice
Chapter 2

Bose-Hubbard Model

2.1 Introduction

Cold bosonic atoms can be confined in the periodic potential of an optical lattice generated via the dipole force which atoms experience in a standing, off-resonant field. Following [12], it will be shown that this system can realize the Bose-Hubbard model. Some basic features of this model will then be discussed.

2.2 Realization of the Bose-Hubbard Model with Bosons on a Lattice

The Hamiltonian for a system of bosons in a given internal state in an optical lattice can be written in second quantization as:

\[ H = H_1 + H_2, \]
\[ H_1 = \int d^3x \psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_i(x) \right) \psi(x), \]
\[ H_2 = \frac{1}{2} \iint d^3x d^3y \psi^\dagger(x) \psi^\dagger(y) V_{\text{int}}(x - y) \psi(y) \psi(x), \]

where \( \psi(x) \) is the bosonic field operator for atoms in the fixed internal state. The contribution \( H_1 \) incorporates the kinetic energy of the particles and the optical lattice potential \( V_i(x) \). The second term, \( H_2 \), describes the interaction effects between the particles.

In the simplest case, the lattice potential \( V_i(x) \) generated by three orthogonal standing light fields is given by

\[ V_i(x) = V_{0x} \sin^2(kx) + V_{0y} \sin^2(ky) + V_{0z} \sin^2(kz), \]

where \( k \) is the wavevector of the lasers used. The lattice spacing, denoted by \( a \), is then half of the laser wavelength.
A convenient unit for the strength of the optical lattice potential is the recoil energy \( E_R = \frac{\hbar^2 k^2}{2m} \). The confining potential for an atom on a single lattice site can be approximated by a harmonic potential \( \frac{1}{2m} \sum_{i=1}^{3} \omega_i^2 \) with trapping frequencies \( \hbar \omega_i = 2E_R \sqrt{V_0_i/E_R} \). In a deep optical lattice \( (V_0_i \gg E_R) \), the energies \( \hbar \omega_i \) of local oscillations in each well are much larger than the recoil energy, and each well in the lattice will support many localized bound states, the so-called Wannier states. Such a state is obtained as a linear superposition of Bloch states of the lattice. Since we are interested in the low-energy dynamics of the system (all relevant energies will be smaller than the \( \hbar \omega_i \)), it suffices to consider only the lowest vibrational level at each site. In the language of band structure theory, one says that the atoms are effectively confined to move in the lowest Bloch band of the lattice. It is convenient then to expand the field operators in the Wannier basis, keeping only the lowest vibrational states:

\[
\psi(\mathbf{x}) = \sum_i w(\mathbf{x} - \mathbf{x}_i) a_i, \quad (2.4)
\]

where \( a_i \) annihilates a particle from the lowest energy Wannier state \( w(\mathbf{x} - \mathbf{x}_i) \) centered at site \( i \). The creation and annihilation operators satisfy \([a_i, a_j^\dagger] = \delta_{ij},\) with all other commutators vanishing.

It will also be assumed that the two-body interparticle potential \( V_{\text{int}}(\mathbf{x} - \mathbf{y}) \) can be described within the usual pseudopotential approach; we will replace the actual potential by an effective contact interaction with a strength proportional to the s-wave scattering length \( a_s \) of the real potential:

\[
V_{\text{int}}(\mathbf{x} - \mathbf{y}) = \frac{4\pi a_s \hbar^2}{m} \delta(\mathbf{x} - \mathbf{y}). \quad (2.5)
\]

This approximation will only be valid in the limit \( a_s \ll l_{0j} \), where \( l_{0j} = \sqrt{\hbar/m \omega_j} \) is an estimate for the characteristic size of the lowest vibrational state in the \( x_j \)-direction in a certain well.

Putting the assumptions considered in equations (2.4) and (2.5) in the Hamiltonian (2.1), we obtain:

\[
H_1 = \sum_{i,j} -J_{ij} a_i^\dagger a_j, \quad (2.6)
\]

\[
H_2 = \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} a_i^\dagger a_j^\dagger a_k a_l, \quad (2.7)
\]

where:

\[
-J_{ij} = \int d^3x w^*(\mathbf{x} - \mathbf{x}_i) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_i(\mathbf{x}) \right) w(\mathbf{x} - \mathbf{x}_j), \quad (2.8)
\]
2.2. REALIZATION OF THE BOSE-HUBBARD MODEL

is the hopping matrix element between two sites \( i, j \) and

\[
U_{ijkl} = \frac{4\pi a_s \hbar^2}{m} \int d^3x \ w^*(x - x_i)w^*(x - x_j)w(x - x_k)w(x - x_l), \tag{2.9}
\]
describes the interaction between the particles and also incorporates interaction-mediated hopping. We will only consider repulsive interactions between the particles, so that \( a_s > 0 \).

Since the Wannier states are very localized, it is sufficient to consider only the hopping terms between neighboring sites in equation (2.8). For the same reason, the most important contribution \( U_{ijkl} \) comes from the on-site interaction (the term \( U_{iii} \)). It is clear that the strength of the on-site interaction will be independent of the site index \( U_{iii} = U \) in equation (2.9)). An estimate for the magnitude of the on-site interaction strength \( U \) can be obtained by approximating each well by a harmonic potential with trapping frequencies \( \hbar \omega_i = 2E_R \sqrt{V_{0i}/E_R} \):

\[
U = \sqrt{\frac{8}{\pi}} k a_s E_R \left( \frac{V_{0x} V_{0y} V_{0z}}{E_R} \right)^{3/4}. \tag{2.10}
\]

The hopping element \( J_{ij} \) will depend on the tunnelling direction because the lattice strength is different in the \( x-, y- \) and \( z- \) directions. In the harmonic approximation, it can be shown that the tunnelling between neighboring sites in a certain direction scales as:

\[
J_{ij(i+1)}^{x,y,z} \sim \left( \frac{V_{0x,y,z}}{E_R} \right)^{3/4} \exp \left( -2 \left( \frac{V_{0x,y,z}}{E_R} \right)^{1/2} \right). \tag{2.11}
\]

In order to obtain a (quasi-) 1D lattice, it is then sufficient to reduce (almost) completely the tunnelling in the \( y- \) and \( z- \) direction by making the coefficients \( V_{0y} \) and \( V_{0z} \) very big. This can be done by increasing the intensity of the relevant lasers. As such, a system of independent parallel chains aligned in the \( x- \) direction results. From now on, we will only consider one of these 1D chains, such that the only coordinate of a lattice site is given by \( x_i \) for site \( i \) on this chain. With all this in mind, the Hamiltonian of our system finally corresponds to the famous Bose-Hubbard Hamiltonian:

\[
H = -J \sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_i n_i(n_i - 1), \tag{2.12}
\]

where \( n_i = a_i^\dagger a_i \) counts the number of bosons on lattice site \( i \). The first term describes the tunnelling of particles between neighboring sites in the chain, the second term describes the interaction between two bosons on the same site. This is made visible in Fig. 2.1.
Before we embark on describing some general facts about the Bose-Hubbard Hamiltonian, let us briefly summarize the assumptions that have lead to a description of our system in terms of this model:

- The model space of the Bose-Hubbard model comprises the lowest energy band only, all excited bands are excluded. Consistency of the model then requires \( \langle n_i - 1 \rangle \ll \hbar \omega_x \) where \( \hbar \omega_x \) is an estimate for the energy separation from the first excited band.

- A pseudopotential approach is assumed to be valid (\( a_s \ll l_{\text{hr}} \)).

- A tight-binding approach is used: only tunneling between neighboring sites and interactions between two particles on the same site are taken into account.

- By selectively decreasing the tunnelling in two orthogonal directions, a (quasi-) 1D chain is obtained.

These assumptions can be readily satisfied in practice.

From now on, it is assumed that we have a finite lattice with \( M \) sites satisfying periodic boundary conditions, i.e. tunnelling between the first and last lattice site is included (if the site index \( M + 1 \) appears in a summation it is implicitly replaced by 1).
2.3 Basic Features of the Bose-Hubbard Model

In order to understand the meaning of the Hamiltonian of the Hubbard model, we discuss the physics encountered in two limiting situations. First, we will have a look at the regime with small interpartiele interactions, where the system behaves as a condensate. Next the strongly interacting limit with commensurate lattice filling is studied, where the system forms a Mott insulator.

2.3.1 Weakly-Interacting System: \( J \gg U \)

First, consider the situation where the on-site interaction \( U \) in the Hamiltonian (2.12) is exactly equal to zero:

\[
H_{U=0} = -J \sum_{i=1}^{M} (a_i^{\dagger}a_{i+1} + a_{i+1}^{\dagger}a_i).
\]  

The Hamiltonian (2.13) can be diagonalized by introducing the operators \( \hat{a}_k \) acting in momentum space:

\[
\hat{a}_k = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} e^{-ikx_i} a_i,
\]  

with \( x_j = ja \) the position of lattice site \( j \) (\( a \) is the lattice spacing). Because of periodic boundary conditions, \( k \) can only take values:

\[
k = \frac{2\pi}{Ma} n, \quad n = 1, \ldots, M - 1.
\]  

The operators \( \hat{a}_k \) satisfy boson commutation relations: \( [\hat{a}_k, \hat{a}_k^{\dagger}] = 0 \) with all other commutators vanishing. In terms of these operators, the Hamiltonian becomes:

\[
H = -2J \sum_{k} \cos(ka) \hat{a}_k^{\dagger} \hat{a}_k.
\]  

So, in the non-interacting limit, the many-body ground state becomes an ideal Bose-Einstein condensate where all \( N \) bosons are in the \( (k = 0) \)-state. This state is therefore called the superfluid state (SF):

\[
|\Psi_{SF} \rangle_{U=0} = (\hat{a}_k^{\dagger})^N |0\rangle = \left( \frac{1}{\sqrt{M}} \sum_{i=1}^{M} a_i^{\dagger} \right)^N |0\rangle,
\]  

where \( |0\rangle \) is the vacuum state corresponding to an empty lattice. The properties of this ground state, which is also called the superfluid state, are well
known: the particles are completely delocalized and, since all particles occupy the same state in momentum space, there is strong phase coherence in the system. Furthermore, elementary excitations consist of promoting one particle from the \((k = 0)\)-state to a state with higher quasi-momentum. In the thermodynamic limit \((M \to \infty, N \to \infty\) and the ratio \(N/M\) kept constant), the quasi-momentum \(k\) from equation (2.15) takes on continuous values so in this limit there is no gap in the excitation spectrum.

If one introduces a small interaction \((U \ll J)\), one can recover a Gross-Pitaevski like description in terms of one macroscopically occupied state. For large enough \(J\) therefore, ordinary BEC behavior is still recovered.

### 2.3.2 Strongly-Interacting System: \(J \ll U\)

In the extreme situation, if one puts the tunnelling term of the Bose-Hubbard model equal to zero, one obtains the Hamiltonian:

\[
H_{J=0} = \frac{U}{2} \sum_{i=1}^{M} n_i (n_i - 1),
\]

with \(U\) positive for repulsive interactions. This Hamiltonian is already diagonal; if one considers the case where the filling factor \(\nu\), which is defined as the ratio between the number of particles and the number of sites \((\nu = N/M)\), is an integer, the ground state will be non-degenerate and will obviously be given by:

\[
|\Psi_{MI}\rangle_{J=0} = \prod_{i=1}^{M} (a_i^\dagger)^{\nu} |0\rangle.
\]

This state is called the Mott-insulator (MI) state.

So, in order to minimize the total interaction energy, the system will choose a configuration with the same number of particles on every site; the particles are localized and perfect correlations in the atom number exist between the lattice sites, but long-range phase coherence is lost. The lowest lying elementary excitations will consist of removing one particle from a certain site, and putting it in another site. The energy of the system will then increase by an amount proportional to \(U\), so there is a energy gap for excitations which remains even in the thermodynamic limit. The ground state for \(\nu = 2\) is depicted in Fig. 2.2, together with one of the first excited states.

If one allows a hopping term with small amplitude \((J \ll U)\), the atoms will remain very localized because the decrease in kinetic energy due to tunnelling is outweighed by the increase of the interaction energy by an amount proportional
2.3. BASIC FEATURES OF THE BOSE-HUBBARD MODEL

Figure 2.2: Schematic representation of the ground state of the Mott insulator phase with integer filling factor $\nu = 2$ in the case of zero tunneling (a), and a first excited state with excitation energy $U$ obtained by moving only one particle (b).

to $U$ (this can also be seen from Fig. 2.2b). Therefore, tunnelling between neighboring sites will likely not occur in the regime $J \ll U$ with integer filling factors, which is therefore called the Mott insulator regime. Of course, this reasoning is only valid if we have an integer filling factor.

For incommensurate filling $\nu = n + m/M$ with $n \in \mathbb{N}$ and $m \in \{1, \ldots, M - 1\}$, there is a number $m$ of particles which can gain kinetic energy by delocalizing over the whole lattice and which do not need to pay the repulsive energy $U$, given that two of those particles will not be simultaneously at the same site (see Fig. 2.3). This situation will be considered in more detail in chapter 3.

Figure 2.3: Strongly interacting regime $J \ll U$ with a fractional filling factor $\nu = 2 + 3/5$. Three particles (dotted) are delocalized on top of a Mott phase with filling factor $\nu = 2$. These particles can tunnel without increasing the interaction energy as long as they do not occupy the same site.

Until now, it is taken for granted in the community studying lattice systems that this delocalized fraction of particles behaves as a condensate (like in the weakly interacting regime) on top of a frozen Mott-insulator phase with integer filling $n$. In chapter 3, we will show that this picture is incorrect; the fraction of particles on top of the Mott-insulator phase will show behavior similar to the
Tonks-Girardeau gas mentioned in the introduction, such that a clear fingerprint of the strong interactions \( J \ll U \) is visible for fractional filling factors in a lattice, and the system does not behave as a condensate at all!

### 2.3.3 The Matter-Wave Interference Pattern

In the previous sections, it was made clear that the ground state of the Bose-Hubbard model with commensurate filling in the weakly interacting limit (superfluid phase) has long-range phase coherence and the particle-hole excitation spectrum is gapless in the thermodynamic limit. By decreasing the parameter \( J/U \), a quantum critical point will be reached at which a gap opens up and long-range phase coherence is lost; one enters the strongly interacting regime (Mott phase). This quantum phase transition from a superfluid to a Mott insulator has recently been verified experimentally \[7\]. In these experiments with cold gases, information on the system is obtained from the matter-wave interference pattern: one prepares the system in a certain state, shuts off the trapping potentials and after some time of flight, an absorption image is taken from the expanding cloud. Because of the experimental relevance of this interference pattern, it is considered here in some more detail.

In order to describe the interference pattern theoretically, one assumes that the interaction between the particles during the expansion is negligible so that the absorption images simply reflect the initial momentum (not quasi-momentum) distribution. By definition, the momentum distribution function \( n_p \) is given by:

\[
    n_p = \int \int dx dy e^{ip(x-y)/\hbar} \rho(x, y),
\]

where \( \rho(x, y) = \langle \psi^\dagger(x)\psi(y) \rangle \), and \( \psi(x) \) is the bosonic field operator. Expanding the field operator in the Wannier basis, one gets:

\[
    \psi(x) = \sum_i w(x-x_i) a_i,
\]

where \( a_i \) annihilates a particle from the lowest energy Wannier state \( w(x-x_i) \) centered at site \( i \). For the momentum distribution, one then obtains:

\[
    n_p = |\tilde{w}(p)|^2 \sum_{m=1}^{M} \sum_{n=1}^{M} e^{ip(x_m-x_n)/\hbar} \langle a_m^\dagger a_n \rangle,(2.22)
\]

with

\[
    \tilde{w}(p) = \int dx \ w(x) e^{ipx/\hbar},
\]
2.3. BASIC FEATURES OF THE BOSE-HUBBARD MODEL

the Fourier transform of the Wannier function $w(x)$.

The momentum distribution is thus completely determined by the correlation function $\langle a_m^\dagger a_n \rangle$. This quantity is easy to calculate for the extreme cases of the non-hopping and non-interacting model considered in the previous section (equations (2.17) and (2.19)). One obtains:

$$\langle \Psi_{SF} | a_m^\dagger a_n | \Psi_{SF} \rangle_{U=0} = \frac{N}{M}, \quad \forall n, m \quad (2.24a)$$

$$\langle \Psi_{MI} | a_m^\dagger a_n | \Psi_{MI} \rangle_{J=0} = \frac{N}{M} \delta_{nm}. \quad (2.24b)$$

From these expressions, it is also clear that there are no long-range correlations in the "ideal" Mott state: the only contribution to $\langle a_m^\dagger a_n \rangle$ comes from terms with $m = n$, whereas for the "ideal" superfluid state (with $U = 0$), one gets the same contribution for all lengths $n - m$ so that the correlation length is infinite. This difference in correlation length is characteristic also in the more general case: in the Mott phase ($J \ll U$) with integer filling factor, the correlations decay exponentially with the distance, whereas they decay only polynomially for the superfluid phase ($J \gg U$).

Let's return to the interference pattern. If one puts the expressions for the correlations, Eq. (2.24), into Eq. (2.22), one obtains the interference pattern for the "ideal" superfluid and Mott states, which is depicted in Fig. 2.4. The interference patterns for both states are strikingly different. For the superfluid state, a series of "Bragg-peaks" show up; this is the expected behavior for the interference pattern in the Mott insulator limit, the interference pattern is a structureless envelope, reflecting the Fourier transform of the Wannier function (which is approximated by a Gaussian). From this, it is clear that the interference pattern allows for a clear distinction of the two phases. It is therefore a perfect instrument in the study of the quantum phase transition from a superfluid to a Mott insulator.
CHAPTER 2. BOSE-HUBBARD MODEL

Figure 2.4: Momentum distribution for the “ideal” Mott insulator state (a) and superfluid state (b) with $N = M = 41$. The momentum is given in units of $\hbar k$, where $k = \pi/a$ with $a$ the lattice spacing. The distribution is normalized to the total number of particles ($\int n_p = N$). This distribution reflects the matter-wave interference pattern of the bosons after release from the optical lattice.
Chapter 3

The Strongly Correlated Limit Revisited

3.1 Introduction

As shown in the previous chapter, the properties of the Bose-Hubbard model are quite well established in both the weakly interacting regime (for all filling factors) and the strongly interacting regime with commensurate filling. With the help of the matter-wave interference pattern, even the quantum phase transition between these two phases has been verified experimentally.

Less is known about the strongly correlated regime \( J \ll U \) with incommensurate filling. We have studied this limit in some more detail, and our results will be discussed in this chapter. As mentioned in section 2.3.2, it is common belief at the moment that for fractional filling factors, a number of particles will exhibit BEC-condensate behavior on top of a Mott insulator phase (see also Fig. 2.3). We have proven this statement wrong.

To make things clearer, here is the Bose-Hubbard Hamiltonian again:

\[
H = -J \sum_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \frac{U}{2} \sum_i n_i (n_i - 1).
\]  

Only repulsive interactions will be considered, so that \( U > 0 \), and we are interested in the limit of strong interactions: \( J \ll U \).

3.2 Filling Factor smaller than 1

We start off with a situation in which the number of particles \( N \) in the lattice is less than the number of available sites \( M \). If the hopping term \( J \) would be zero,
all possible configurations with at most one particle on every site are degenerate ground states of the system. States with higher occupancies on certain sites will carry an energy on the order of \( U \) more than these ground states.

### 3.2.1 An Effective Hamiltonian

For large enough \( U \), the effects of a non-vanishing tunnelling \( J \) can be taken into account by using a simple projection technique. The ground state and the low-energy excitations of the Bose-Hubbard Hamiltonian lie within the subspace of states with no more than one particle on every site because other configurations still have an energy disadvantage on the order of \( U \). Therefore, if one is interested in low-energy properties only, one can limit the complete Hilbert space to states with single occupancy on the sites only. By projecting onto this subspace, one can obtain an effective Hamiltonian acting within the subspace and thereby describing the properties of the ground and low-lying excited states \([4]\) (for a derivation, see appendix B):

\[
H_{\text{eff}} = \mathbb{P}H\mathbb{P} - \frac{1}{U} \mathbb{P}HQH\mathbb{P} + O \left( \frac{J^3}{U^2} \right),
\]

where \( \mathbb{P} \) is a projector on the subspace mentioned above, and \( Q \) projects out of this subspace \((\mathbb{P} + Q = 1)\). The Hamiltonian \( H \) is our Hubbard-Hamiltonian (3.1).

Writing the effective Hamiltonian in terms of the operators that create and annihilate particles in a certain site, one obtains for the lowest order term:

\[
\mathbb{P}H\mathbb{P} = -J \sum_{i=1}^{M} \mathbb{P}(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i)\mathbb{P}.
\]

To first order therefore, particles are able to tunnel only to vacant neighboring sites; tunnelling to an already occupied site is "forbidden" because one leaves the subspace of single occupancies. Also notice that the interaction term in the Hamiltonian (3.1) of course gives a zero contribution to the effective Hamiltonian.

The second order term requires some careful considerations. It can be written as:

\[
-\frac{1}{U} \mathbb{P}HQH\mathbb{P} = -\frac{J^2}{U} \sum_{i,j=1}^{M} \mathbb{P}(a_{i-1}^\dagger a_{i+1}^\dagger a_i Q a_j^\dagger (a_{j-1} + a_{j+1}))\mathbb{P}.
\]

Let us analyze this expression in more detail. The term \( a_j^\dagger (a_{j-1} + a_{j+1})\mathbb{P} \) moves a particle to site \( j \) from a neighboring site. Site \( j \) will then either be singly occupied or doubly occupied; other occupations are not possible because of the operator \( \mathbb{P} \). The operator \( Q \) projects out the possibility of the single occupation at site \( j \); this
3.2. **FILLING FACTOR SMALLER THAN 1**

Operator can therefore be replaced by $a_j^+a_j - 1$ which gives zero if site $j$ is singly occupied, and 1 if it is doubly occupied. Next, the term $(a_{i-1}^+ + a_{i+1}^+ )a_i$ will move a particle from site $i$ to a neighboring site. Now there are two possibilities:

- if $i \neq j$, then after this operation, site $j$ will still be doubly occupied and the projector $\mathbb{P}$ which finally acts gives zero as result.

- if $i = j$, the double occupation of site $j$ is removed, and the final projection could give a nonzero contribution.

So only terms with $i = j$ will give a contribution to the effective Hamiltonian. Replacing the operator $\mathbb{Q}$ like mentioned above, we get for the second order term of the effective Hamiltonian:

$$-rac{1}{U} P H \mathcal{Q} H \mathbb{P} = -\frac{J^2}{U} \sum_{i=1}^{M} \mathbb{P} [a_{i-1}^+ a_i(n_i - 1)a_i^+ a_{i-1} + a_{i+1}^+ a_i(n_i - 1)a_i^+ a_{i+1} + a_{i-1}^+ a_i(n_i - 1)a_i^+ a_{i+1} + a_{i+1}^+ a_i(n_i - 1)a_i^+ a_{i-1}] \mathbb{P}. \quad (3.5)$$

Figure 3.1 shows the two processes taken into account in the second order perturbation theory. The first two terms describe the effect where a particle tunnels, generates a state with double occupation, and subsequently one of the particles tunnels back to the original site so that in the end we are still in the subspace of single occupancies. These terms will give rise to an attractive nearest neighbor interaction of the form $n_{i\pm 1}n_i$ (see Eq. (3.6)). The last two terms in equation (3.5) describe an effective tunnelling of a particle to a next nearest neighbor site, mediated by a neighboring particle.

![Diagram](image)

**Figure 3.1:** Second order processes in the effective Hamiltonian. Hopping back and forth (a) leads to an effective attraction between nearest neighbors. When particles hop forward twice, next nearest neighbor tunnelling results (b).
CHAPTER 3. THE STRONGLY CORRELATED LIMIT REVISITED

After some minor algebra, the effective Hamiltonian up to second order can finally be written as:

\[ H_{\text{eff}} = -J \sum_{i=1}^{M} \mathbb{P}(a_{i+1}^{\dagger}a_{i} + a_{i+1}^{\dagger}a_{i}) \mathbb{P} - \]
\[ 2 \frac{J^2}{U} \sum_{i=1}^{M} \mathbb{P}(n_{i-1}n_{i} + n_{i+1}n_{i} + a_{i+1}^{\dagger}a_{i+1}n_{i} + a_{i}^{\dagger}a_{i-1}n_{i}) \mathbb{P}. \]  (3.6)

3.2.2 \( U \rightarrow \infty \): The Jordan-Wigner Transformation

As a first approximation, one can keep only the first order term and neglect the higher order terms of the effective Hamiltonian (3.6). This treatment gives exact results for the limit \( U \rightarrow \infty \) corresponding to a system of impenetrable bosons for which double occupancies on a site are really forbidden: two particles cannot be created on the same site. This hard-core constraint will be absorbed in the definition of the field operators as follows:

\[ a_{i}^\dagger a_{i} = 0 \quad \forall i. \]  (3.7)

As such, the effect of the projection operator \( \mathbb{P} \) is thus integrated in the commutation relations for the creation and annihilation operators. The Hamiltonian for impenetrable bosons then becomes:

\[ H_{B} = -J \sum_{i=1}^{M} (a_{i+1}^{\dagger}a_{i} + a_{i+1}^{\dagger}a_{i}), \]  (3.8)

with the constraint (3.7).

At first sight, this Hamiltonian might seem trivial to solve; just introduce the operators

\[ \tilde{a}_{k} = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} e^{-i k x_{i}} a_{i}, \]  (3.9)

acting in quasi-momentum space and the Hamiltonian (3.8) then becomes diagonal:

\[ H_{B} = -2J \sum_{k} \cos(ka) \tilde{a}_{k}^{\dagger} \tilde{a}_{k}. \]  (3.10)

Because of the periodic boundary conditions, the quasi-momentum \( k \) can take on only values:

\[ k = \frac{2\pi}{Ma} n, \quad n = 0, \ldots, M - 1. \]  (3.11)
3.2. FILLING FACTOR SMALLER THAN 1

Now, the eigenvalues of the number operator $n_k = \hat{a}_k^\dagger \hat{a}_k$ are completely determined by the commutation relations for the operators $\hat{a}_k^\dagger$ and $\hat{a}_k$; for normal bosonic commutation relations, the occupation of a certain $k$-state can only be a positive integer (or zero), and the ground and excited states can then be easily constructed from the vacuum using the creation operators $\hat{a}_k^\dagger$; the ground state for instance would be $(\hat{a}_{k=0}^\dagger)^N |0\rangle$ with energy $-2JN$.

However, the hard-core constraint (3.7) has a major impact on the commutation rules for the quasi-momentum operators in the case of hard-core bosons; the occupation in quasi-momentum space can take on values more general than natural numbers. As a consequence, it is not immediately clear how to find the ground and excited states for impenetrable bosons directly.

So we have to resort to another method to solve the problem. Analogous to what people have done when studying the 1D gas of impenetrable bosons [5] (without a lattice), we will use a mapping between hard-core bosons and spinless fermions. This mapping is explained in appendix A using the language of first quantization. In second quantization, the mapping between a system of spinless fermions and impenetrable bosons can be described more directly with the so-called Jordan-Wigner transformation between the creation and annihilation operators for impenetrable bosons and fermions (see e.g. [28]). Defining the operators $c_i^\dagger$ as:

$$c_i^\dagger = \prod_{j<i} (1 - 2a_j^\dagger a_j) a_i^\dagger, \tag{3.12}$$

they will obey normal fermionic anti-commutation relations if the bosonic $a$-operators satisfy the impenetrability constraint (3.7); in other words, the operator $c_i^\dagger$ defined above creates an effective fermion on site $i$.

Although the Jordan-Wigner transformation seems quite complicated at first, it has a very easy structure: the operator $(1 - 2a_j^\dagger a_j)$ can only take on the values $-1$ if site $j$ is occupied and 1 if it is unoccupied; other occupations are not allowed because of the constraint (3.7). Now if the number of occupied sites to the left of site $i$ is even, the string operator $\prod_{j<i}(1 - 2a_j^\dagger a_j)$ will have the value 1 and the transformation reads $c_i^\dagger = a_i^\dagger$. If it is odd, the string operator becomes $-1$ and the transformation is $c_i^\dagger = -a_i^\dagger$.

Before we transform the Hamiltonian (3.8), one remark has to be made. We always use periodic boundary conditions, meaning that the operator $a_{M+1}^\dagger$ in the summation is implicitly put equal to $a_1^\dagger$. From the previous discussion however, it should be clear that the corresponding fermion operator becomes:

$$c_{M+1}^\dagger = (-1)^{N-1} a_{M+1}^\dagger = (-1)^{N-1} a_1^\dagger = (-1)^{N-1} c_1^\dagger, \tag{3.13}$$

where $N$ is the number of particles in the lattice. So the Hamiltonian for hard-
core bosons with periodic boundaries will map onto a fermionic one with the same boundaries only if the number of particles in the system is odd! If \( N \) is even, the impenetrable bosons map onto fermions with anti-periodic boundaries. In order to retain periodic boundary conditions after the mapping, it will be assumed from now on that \( N \) is odd. Clearly, for sufficiently large systems, this assumption does not restrict our conclusions. Note that if we had chosen open boundaries, this problem would not have occurred, but it would have complicated further calculations a little bit.

Transforming the bosonic Hamiltonian (3.8) in terms of the fermion operators, one gets:

\[
H_F = -J \sum_{i=1}^{M} (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}).
\]

This is the Hamiltonian for free fermions on a lattice. It can be diagonalized again by introducing the operators in quasi-momentum space, analogous to (3.9):

\[
\tilde{c}_k = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} e^{-ikx_i} c_i,
\]

where the \( k \)-values are again restricted to (3.11). The Hamiltonian is then diagonalized:

\[
H_F = -2J \sum_k \cos(ka) \tilde{c}_k^\dagger \tilde{c}_k.
\]

The difference now is that the fermionic operators in quasi-momentum space satisfy the usual anti-commutation rules: \( \{ \tilde{c}_k, \tilde{c}_k^\dagger \} = \delta_{kk'} \) with all other anti-commutators vanishing. As a direct consequence, the operator \( \tilde{c}_k^\dagger \tilde{c}_k \) has eigenvalues zero and one. Solution of the fermion problem now is trivial: one gets a characteristic Fermi-sea picture where in the ground state, the lowest energy \( k \)-states will be filled up to a certain energy, the Fermi energy. The excitations are particle-hole like, where a particle from the Fermi sea gets promoted to a higher energy state. This is depicted in Fig. 3.2.

Let’s now derive the ground state for the impenetrable bosons in some detail. The system of spinless fermions we map on, has the following ground state:

\[
|\psi_g\rangle_F = \prod_{n=-n_F}^{n_F} \tilde{c}^\dagger_{k_n} |0\rangle, \quad k_n = \frac{2\pi}{Ma} n, \quad n_F = \frac{N-1}{2}.
\]

This corresponds to the visualization in terms of a Fermi-sea (Fig. 3.2). In position space, the states \( c_{x_1}^\dagger c_{x_2}^\dagger \ldots c_{x_N}^\dagger |0\rangle \) with \( x_1 < x_2 < \ldots < x_N \) form a basis, and we can write the ground state as usual:

\[
|\psi_g\rangle_F \sim \sum_{x_1 < x_2 < \ldots < x_N} \left( \det [e^{ik_{x_j} x_i}]_{n=-n_F,\ldots,n_F} \right) c_{x_1}^\dagger c_{x_2}^\dagger \ldots c_{x_N}^\dagger |0\rangle,
\]
3.2. FILLING FACTOR SMALLER THAN 1

Figure 3.2: Visualization of the ground state (a) and first excited state (b) for free fermions in terms of a Fermi sea. The dispersion relation for free fermions on a lattice is given by $\varepsilon_k = -2J \cos(ka)$.

in terms of a Slater determinant $\det[e^{ik_n x_j}]_{n=-n_F, \ldots, +n_F}^{j=1, \ldots, N}$ of the plane waves with lowest momentum. If we do the Jordan Wigner transformation, noting that $c_{x_1}^\dagger c_{x_2} \ldots c_{x_N}^\dagger |0\rangle = a_{x_1}^\dagger a_{x_2} \ldots a_{x_N}^\dagger |0\rangle$ for all $x_1 < x_2 < \ldots < x_N$, we obtain the ground state for impenetrable bosons:

$$|\psi_g\rangle_B \sim \sum_{x_1 < x_2 < \ldots < x_N} \left( \det[e^{ik_n x_j}]_{n=-n_F, \ldots, +n_F}^{j=1, \ldots, N} \right) a_{x_1}^\dagger a_{x_2}^\dagger \ldots a_{x_N}^\dagger |0\rangle. \quad (3.19)$$

Like already said before, according to people working in the field of lattice gases, our system of strong interacting bosons with fractional filling should behave as a condensate (remember the discussion at the end of section 2.3.2. The ground state expression derived above however, proves our statement that this point of view is incorrect; it is clear that the impenetrable bosons do not form a condensate at all because the ground state is generally not expressible as a product state where all particles occupy the same one-particle state! Although the ground states for fermions and bosons look pretty much the same, the ground state for bosons can not be interpreted as a Fermi-sea anymore because of the different commutation relations for the bosonic operators $a_i$. In the next paragraph, we will show that the peculiar (non-condensate) behavior of the system can also be seen in an experiment, by measuring the matter-wave interference pattern.

To conclude, finding the ground and excited states of the Hamiltonian $H_F$ proves to be trivial. Furthermore, the ability to determine the action of operators on any fermion state allows us to perform tractable calculations on the fermion system. It is here that the strength of a mapping between the impenetrable bosons and free fermions lies. However, it should be stressed that this does not mean
that by doing the mapping, the solution of the original problem of impenetrable bosons has become completely trivial. Let me explain this with an example. In section 2.3.3, it was shown that an experimental quantity of interest, the matter-wave interference pattern, is completely determined by the correlation function \( \langle a_i^\dagger a_j \rangle \). If one applies the Jordan-Wigner transformation to this quantity, one obtains:

\[
\langle a_i^\dagger a_j \rangle = \left( \prod_{i<l<j} (1 - 2c_i^\dagger c_l) c_i^\dagger c_j \right) \neq \langle c_i^\dagger c_j \rangle, \quad i < j.
\]

(3.20)

So this quantity is not equal to the corresponding quantity for free fermions. The string-operator makes this quantity quite hard to calculate for impenetrable bosons although the associated fermionic observable \( \langle c_i^\dagger c_j \rangle \) is quite easy to calculate. We will come back to this problem in the next section.

Nevertheless, there are some quantities that are the same for a system of impenetrable bosons and the corresponding system of free fermions. The occupation number operator for instance, is the same for both systems because the mapping will involve the square of the string-operator (which is always equal to 1):

\[
\langle a_i^\dagger a_i \rangle = \left( \prod_{j<i} (1 - 2c_j^\dagger c_i) c_i^\dagger c_i \right) = \langle c_i^\dagger c_i \rangle.
\]

(3.21)

More general, all physical properties expressible in terms of spatial configuration probabilities are the same for these two systems. Furthermore, from comparison of the Hamiltonians (3.10) and (3.16), it is also clear that the two systems will have the same energy spectrum. However, one has to keep in mind that in most cases, the Jordan-Wigner transformation has a strong influence on the calculation of the observables.

### 3.2.3 The Quasi-Momentum Distribution and Interference Pattern

Let us come back to the calculation of the correlation function \( \langle a_i^\dagger a_j \rangle \) for impenetrable bosons. Although it was made clear in the previous paragraph that doing a Jordan-Wigner transformation complicates the things at first sight, it will prove to be a very helpful method in calculating this correlation function.

Transforming the impenetrable boson operators into fermionic ones, one gets:

\[
\langle a_i^\dagger a_j \rangle = \left( \prod_{i<l<j} (1 - 2c_i^\dagger c_l) c_i^\dagger c_j \right).
\]

(3.22)

The difficulty in calculating the fermionic correlation function lies in the fact that it involves products of more than two operators. With the help of Wick's theo-
3.2. FILLING FACTOR SMALLER THAN 1

rem [34] however, one is able to express the expectation value of a product of multiple operators in terms of products of only two operators. Applying this method, the correlation function above can be written as a determinant of dimension $j - i$ (it is supposed that $i < j$):

$$
\langle a_i^\dagger a_j \rangle = \langle \prod_{i < l < j} (1 - 2c_i^\dagger c_l) c_l^\dagger c_j \rangle \quad (3.23)
$$

$$
= 2^{j-i-1} \begin{vmatrix}
    g_{i,i+1} & g_{i+1,i+1} - 1/2 & g_{i+2,i+1} & \cdots & g_{j-1,i+1} \\
    g_{i+2,i+2} & g_{i+1,i+2} & g_{i+2,i+2} - 1/2 & \cdots & g_{j-1,i+2} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    g_{i,j-1} & g_{i+1,j-1} & g_{i+2,j-1} & \cdots & g_{j-1,j-1} - 1/2 \\
    g_{i,j} & g_{i+1,j} & g_{i+2,j} & \cdots & g_{j-1,j}
\end{vmatrix},
$$

with $g_{l,m} = \langle c_l^\dagger c_m \rangle$. Since our system is translational invariant, the correlation function $\langle a_i^\dagger a_j \rangle$ will only depend on the “distance” $j - i$ between two lattice sites. It suffices therefore to consider only $\langle a_i^\dagger a_{i+\Delta} \rangle$ for arbitrary $i$ and a fixed distance $\Delta$. This gives a better overview over the determinant expression:

$$
C_\Delta = \langle a_i^\dagger a_{i+\Delta} \rangle = 2^{\Delta-1} \begin{vmatrix}
    f_1 & f_0 - 1/2 & f_{-1} & \cdots & f_{-2+\Delta} \\
    f_2 & f_1 & f_0 - 1/2 & \cdots & f_{-3+\Delta} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    f_{\Delta-1} & f_{\Delta-2} & f_{\Delta-3} & \cdots & f_0 - 1/2 \\
    f_\Delta & f_{\Delta-1} & f_{\Delta-2} & \cdots & f_1
\end{vmatrix}, \quad (3.24)
$$

where now $f_l = g_{i,i+l} = \langle c_l^\dagger c_{i+l} \rangle$ with arbitrary $i$.

The non-locality of the Jordan-Wigner transformation becomes clear in this expression; if we want to calculate the correlations for two impenetrable bosons separated by a distance $\Delta$, we have to know the corresponding correlations for fermions separated over all distances $x$ smaller than $\Delta$. Calculating these correlations for fermions is quite easy; going over to quasi-momentum space (equations (3.15) and (3.11)), we can make optimal use of the Fermi-sea picture for the ground state:

$$
f_l = \langle c_l^\dagger c_{i+l} \rangle = \frac{1}{M} \sum_{k,k'} e^{-ikx_i} e^{ik'x_{i+l}} \langle c_k^\dagger \tilde{c}_{k'} \rangle. \quad (3.25)
$$

Since the ground state corresponds to a filled Fermi-sea,

$$
|\psi_g \rangle = \prod_{n=-n_F}^{n_F} \tilde{c}_{kn}^\dagger |0\rangle, \quad k_n = \frac{2\pi}{Ma}, \quad n_F = \frac{N - 1}{2}, \quad (3.26)
$$
the expectation value $\langle c_k^\dagger c_{k'} \rangle$ will be zero if $k \neq k'$, and it will give 1 if $k = k_n$ with $n \in \{-n_F, \ldots, n_F\}$. We therefore obtain:

$$f_i = \frac{1}{M} \sum_{n=-(N-1)/2}^{(N-1)/2} e^{-i\frac{2\pi}{M} n l} = \frac{1}{M} \frac{\sin(\pi v l)}{\sin(\pi l / M)}, \quad v = N / M. \quad (3.27)$$

Putting this expression for $f_i$ into the determinant (3.24), we are able in principle to calculate the correlation function $C_\Delta$ in the ground state for impenetrable bosons. However, despite the very promising form of the determinant (it closely resembles a so-called Toeplitz determinant [2]), we were unable to find a analytical formula until now. But the simplicity of the determinant expression (3.24) and its elements make it well suited for doing numerical calculations on large systems: we can calculate numerically the correlation functions for large systems of over 100 sites very efficiently, in contrast to an exact diagonalization technique where one is limited to at most 20 sites (on a normal PC).

Therefore, we were able to make a curve fit to the numerical calculations on the basis of Eq. (3.24) for $C_\Delta$. For large distances $\Delta$, the numerical results fit perfectly to:

$$C_\Delta = \frac{\pi}{\sqrt{114}} \sqrt{\sin(\pi \nu)} \frac{1}{\Delta^{1/2}}, \quad \nu = N / M. \quad (3.28)$$

This is made visible in Fig. 3.3. The fit makes it clear that the correlations $C_{\Delta}$ decay like $\Delta^{-1/2}$. The simplicity of the expression for the fit also strengthens our belief that it should be possible to find an analytical approximation for the determinant in equation (3.24).

Nevertheless, an analytical result for the correlation function $C_\Delta$ can be obtained with another method: associating an spin-up on site $i$ with having a particle on this site, and a spin-down if there is no particle, our Hamiltonian (3.8) can be mapped onto a spin model, namely the XX-model with a magnetic field:

$$H = \gamma \sum_i (\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) + B \sum_i \sigma^z_i, \quad (3.29)$$

where $\sigma^{x,y,z}$ are the Pauli spin operators. The magnetic field $B$ is used to fix the number of up spins (and as such the filling factor in our original boson problem). This model has been exactly solved [16] by means of a so-called Bethe Ansatz solution [14]. With this solution, one is able to calculate the correlation function $\langle \sigma^z_i \sigma_{i+\Delta} \rangle$, which corresponds to our $\langle a_i^\dagger a_{i+\Delta} \rangle$. The result confirms that $C_\Delta$ has to decay as $\Delta^{-1/2}$ for large distances $\Delta$.

However, our solution by means of the Jordan-Wigner transformation has some clear advantages over the Bethe Ansatz solution. The latter solution is very
Figure 3.3: Numerical fits for the correlation function $C_\Delta$. The curves for $1/C^2_\Delta$ against $\Delta$ for different filling factors (a) are linear and therefore show that $C_\Delta$ decays as $\alpha(\nu) \Delta^{-1/2}$. The square of the coefficient $\alpha$ is plotted as a function of the filling factor $\nu$ in (b) (dots). It corresponds to a sine-function $\pi^2/114 \sin(\pi \nu)$ (solid line).
mathematical; it does not give much physical insight into the problem and it is generally very hard to calculate physical properties with it. Our solution on the contrary gives a very clear picture of the physics behind the model, and it is easier to deal with. Furthermore, the mapping to the solvable XX-model is only possible for our particular Hamiltonian. If one would like to include other terms in the Hamiltonian, for instance a harmonic trapping potential, one cannot, in general, do a mapping to a solvable spin model. However, as long as one adds only one-particle potentials to the Hamiltonian, our Jordan-Wigner scheme will always reduce the many-particle impenetrable boson problem to a one-particle fermionic problem, from which all relevant quantities can be easily calculated.

Now that we are able to calculate the correlation functions between two points separated by a distance $\Delta$, we can turn our attention to another quantity that can give us more information concerning the physics behind our system of impenetrable bosons on a lattice, namely the occupation of the one-particle states in quasi-momentum space:

$$\langle \tilde{a}_k^+ \tilde{a}_k \rangle = \frac{1}{M} \sum_{m,n=1}^{M} e^{-ik(z_m-z_n)} \langle a_m^+ a_n \rangle$$  \hspace{1cm} (3.30a)

$$= \frac{1}{M} \sum_{m=1}^{M} \sum_{\Delta=1-M}^{M-1} e^{-ika\Delta} \langle a_m^+ a_{m+\Delta} \rangle, \hspace{1cm} \Delta = m - n \hspace{1cm} (3.30b)$$

$$= \sum_{\Delta} e^{-ika\Delta} C_{\Delta}. \hspace{1cm} (3.30c)$$

So the quasi-momentum distribution corresponds to the discrete Fourier transform of the correlation function $C_{\Delta}$. Since we know that $C_{\Delta}$ decays as $\Delta^{-1/2}$ for large $\Delta$, the quasi-momentum distribution will decay as $k^{-1/2}$ for small $k$. This $k^{-1/2}$ behavior is universal; for different filling factors, it is just getting renormalized (see the prefactor $\sin(\pi \nu)$ in Eq. (3.28)). For large $k$-values, we were not able to find an expression for the behavior of the distribution. In Fig. 3.4, the distribution is plotted for different values of the filling factor $\nu = N/M$.

According to the ideas that are common in the community that studies the Bose-Hubbard model (see also the end of section 2.3.2), our system of bosons in the strongly interacting regime with filling factors $\nu < 1$ should behave as a BEC. Remember that we started the current section in order to prove this result wrong. And indeed, the calculations we have done so far show that the behavior does not correspond to that of a condensate at all.
3.2. FILLING FACTOR SMALLER THAN 1

Figure 3.4: Ground state quasi-momentum distribution with different filling factors for impenetrable bosons in a 1D optical lattice with 41 sites.

Two arguments that lead to this conclusion are the following:

- the ground state for impenetrable bosons cannot be written as a product state where every particle is in the same one-particle eigenstate.

- the quasi-momentum distribution decays like $k^{-1/2}$ for impenetrable bosons. The distribution is completely different from the one for a superfluid where, in the ideal case, we find a delta peak at $k = 0$.

This behavior was already encountered in the study of a 1D gas of impenetrable bosons (the Tonks-Girardeau gas [5]) in the absence of an optical lattice. Experimentally, it should be possible to observe this typical Tonks gas behavior in the matter-wave interference pattern after releasing the particles from the optical lattice. From comparison of equations (2.22) and (3.30), it is clear that the interference pattern closely resembles the quasi-momentum distribution except for the envelope $|\tilde{w}(p)|^2$. The characteristic behavior mentioned above should therefore be reflected in the interference pattern. This is made visible in Fig. 3.5. We have sharp interference peaks for small filling factors, but with increased filling some intensity appears in between the peaks. Especially for filling factors in the range $0.7 \lesssim \nu \lesssim 0.9$, the absorption image from a real experimental setup should be clearly distinguishable from both the patterns of the superfluid and the Mott phase (see Fig. 2.4 on page 18).
Figure 3.5: Matter-wave interference pattern in function of the filling factor $\nu$ for the ground state of impenetrable bosons in a 1D optical lattice with 41 sites.
3.3. OTHER FRACTIONAL FILLINGS

To conclude, even for filling factors $\nu < 1$ in the strongly correlated limit, a clear fingerprint of the strong interactions remains visible.

3.3 Other Fractional Fillings

Now we turn back to more general filling factors. All fractional filling factors can be written in the form:

$$\nu = n + \frac{m}{M}, \quad n \in \mathbb{N}, \quad m = 0, \ldots, M - 1. \quad (3.31)$$

In the regime of very strong interactions ($J \gg U$), the lowest energy states of the Bose-Hubbard Hamiltonian with a filling given by the above expression will have either a number of $n$ or $n + 1$ particles on the different sites. It is sufficient to only take into account such states when we are interested in the low-energy properties of the system; indeed, states with other occupancies at the sites will have an energy which is of the order of $U$ larger. Analogous to what we have done in the previous section for filling factors smaller than one, we can describe the low-energy properties by projecting the Hamiltonian into the subspace of states with either $n$ or $n + 1$ particles per site. It is clear that in this subspace, since we have a minimum occupancy of $n$ particles at every site, only the particles on top of this minimum occupancy can tunnel. So we have a number $m$ of particles which can hop to neighboring sites on top of a frozen Mott insulator phase with integer filling $n$. This brings us again to Fig. 3.6.

![Figure 3.6: Strongly interacting regime $J \ll U$ with a fractional filling factor $\nu = 2 + 3/5$. Three particles (dotted) are delocalized on top of a Mott phase with filling factor $\nu = 2$. These particles can tunnel without increasing the interaction energy as long as they do not occupy the same site.](image)

Now, the behavior of the particles on top of the Mott phase is very similar to what we had for filling factors smaller than one. In fact, we can map the current problem to the situation we had for $\nu < 1$. This is made clear in Fig. 3.7. From a
CHAPTER 3. THE STRONGLY CORRELATED LIMIT REVISITED

mathematical point of view, we define the frozen Mott phase as the new vacuum state:

$$|\text{vac}\rangle = \frac{1}{(n!)^{M/2}} \prod_{i=1}^{M} (a_i^\dagger)^n |0\rangle,$$  (3.32)

where $|0\rangle$ corresponds to the empty lattice and the new vacuum state is normalized ($\langle \text{vac}|\text{vac}\rangle = 1$). The state $\psi$ with occupancies of $n+1$ at different positions $x_1, x_2, \ldots, x_m$ is then constructed by acting on this vacuum as follows:

$$|\psi\rangle = |x_1, x_2, \ldots, x_m\rangle = \frac{1}{(n+1)^{m/2}} a_{x_1}^\dagger a_{x_2}^\dagger \ldots a_{x_m}^\dagger |\text{vac}\rangle.$$  (3.33)

These normalized states form a basis in the subspace of states with either $n$ or $n+1$ particles on the different sites. The projection to this subspace is accomplished by defining:

$$a_{x_i}^\dagger a_{x_i}^\dagger |\text{vac}\rangle = 0.$$  (3.34)

Now, we will introduce impenetrable boson operators, such that the normalized state $\psi$ can be written by acting with these operators directly on the $|0\rangle$ state:

$$|\psi\rangle = d_{x_1}^\dagger d_{x_2}^\dagger \ldots d_{x_m}^\dagger |0\rangle, \quad d_{x_i}^\dagger d_{x_i}^\dagger = 0.$$  (3.35)

Figure 3.7: System of strongly interacting bosons on a 1D lattice with filling $\nu = n + m/M = 2 + 2/4$, mapped to a system of hard-core bosons on a lattice with filling $m/M = 2/4$.

Of course, special attention has to be paid while doing this mapping because of the normalization. For instance, tunnelling between two sites $i$ en $j$ is described by:

$$a_{x_i}^\dagger a_{x_j} |x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_j, \ldots, x_m\rangle = (n+1) |x_1, x_2, \ldots, x_i, \ldots, x_{j-1}, x_{j+1}, \ldots, x_m\rangle, \quad i \neq j,$$  (3.36)
3.3. OTHER FRACTIONAL FILLINGS

while:

\[ d_d^i d_j |x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_j, \ldots, x_m \rangle = |x_1, x_2, \ldots, x_i, x_{j-1}, x_{j+1}, \ldots, x_m \rangle, \quad i \neq j. \]  

(3.37)

A similar line of reasoning for the terms \( a_i^\dagger a_i \), gives the following equalities:

\[ a_i^\dagger a_j |\psi\rangle = (n + 1) d_d^i d_j |\psi\rangle, \]  

(3.38)

\[ a_i^\dagger a_i |\psi\rangle = (d_d^i d_i + n) |\psi\rangle, \]  

(3.39)

for all states \( \psi \) in the subspace of states with only \( n \) or \( n + 1 \) particles at the different sites. The Bose-Hubbard Hamiltonian, projected to this subspace, can then be written in terms of the impenetrable boson operators as follows:

\[ H = -J(n + 1) \sum_{i=1}^{M} (d_d^i d_{i+1} + d_d^i d_i), \]  

(3.40)

acting on the states (3.35). Apart from the renormalized tunnelling amplitude \( J \), this Hamiltonian is equal to the one for impenetrable bosons, equation (3.8) from the previous section. So the strongly correlated system for fractional filling factors given in equation (3.31) can be mapped to a system of impenetrable bosons with filling factor \( m/M \) smaller than one.

Also, the quasi-momentum distribution will be related to the one we found in the previous section. The quasi-momentum distribution is given by:

\[ \langle \tilde{a}_k^\dagger \tilde{a}_k \rangle = \sum_{\Delta} e^{ik\Delta} \langle a_i^\dagger a_{i+\Delta} \rangle. \]  

(3.41)

Making use of the equalities (3.38), we find after some algebra:

\[ \langle \tilde{a}_k^\dagger \tilde{a}_k \rangle = n(1 - \frac{m}{M}) + (n + 1) \langle \tilde{d}_k^\dagger \tilde{d}_k \rangle, \]  

(3.42)

where \( \langle \tilde{d}_k^\dagger \tilde{d}_k \rangle \) corresponds to the distribution (3.30) for impenetrable bosons from the previous section. We have plotted the quasi-momentum distribution for the ground-state in Fig. 3.8. If we fix the filling \( n \) of the Mott phase, we see that the distribution closely resembles the curves for impenetrable bosons (with filling \( m/M \)). However, the Mott insulator part provides a background signal; even for the smallest \( m/M \), the distribution never becomes zero for \( n \geq 1 \). Instead, one sees that the distribution has an offset of the order of \( n \) (this is easily visible for small \( m/M \)). For a Mott phase with \( n \) particles at every site, it is clear that \( \langle \tilde{a}_k^\dagger \tilde{a}_k \rangle \) is constant at a value \( n \) so the offset for fractional filling factors must be roughly related to this.
Figure 3.8: Quasi-momentum distribution for the ground-state of the Bose-Hubbard model in the strongly correlated limit. For $n = 0$, the result from the previous section is obtained. For higher $n$, the background of particles in the Mott phase results in an offset of the distribution. The behavior as a function of $m/M$ for fixed $n$ is similar to that of impenetrable bosons. The number of sites on the lattice was fixed to 41 in all three plots.
From all this, we can conclude that the Bose-Hubbard system in the strongly interacting limit for incommensurate filling behaves as a Mott insulator with some delocalized particles on top. These delocalized particles will exhibit correlation phenomena which are determined by strong interactions (Tonks gas), in contradiction again with the point of view that the delocalized particles would behave as a condensate and that no signature of strong interactions would be present.

3.4 Including a Harmonic Trap

In an experimental setup, one uses a harmonic trap to confine the particles. This harmonic trap will give rise to an extra term $\hbar \sum \epsilon_i a_i^\dagger a_i$ with $\epsilon_i = (i - M/2)^2$ in the Bose-Hubbard Hamiltonian, thereby destroying the translational invariance in the system. For weak enough traps however, it can be expected that the typical behavior for incommensurate fillings found in the previous sections will still be present.

By applying the Jordan-Wigner transformation, one can map the system to free spinless fermions in the same harmonic trap. For a finite system of $M$ sites, the one-fermion eigenstates can then be found numerically. The many-body ground state is then a Fermi-sea where the eigenstates with lowest energies are filled. Making use of the determinant expression (Eq. 3.24), the correlation function $\langle a_i^\dagger a_j \rangle$ for bosons in the ground state can be calculated, and this completely determines the matter-wave interference pattern. The result for filling factors smaller than one and for a weak harmonic confinement is shown in Fig. 3.9. We can observe again a sharply peaked interference pattern for small fillings, which becomes broader for larger fillings, similar to the results without the trap. However, more detailed (analytical) studies are necessary in order to really understand the influence of the harmonic confinement.
Figure 3.9: Matter-wave interference pattern for harmonically confined impenetrable bosons in a 1D optical lattice. The number of sites is fixed at $M = 40$. The confinement is very weak at $\hbar/J = 0.01$. 
Chapter 4
Conclusion and Outlook

We have seen that bosons in an optical lattice can realize the Bose-Hubbard model. In the limit of weak interaction, ordinary BEC behavior is recovered for both commensurate and incommensurate filling of the lattice. The strongly correlated regime however, poses some problems dependent on the filling factor. For commensurate filling, one obtains the so-called Mott insulator state from which the properties are well established. On the other hand, we have shown that there are some misconceptions concerning incommensurate fillings; until now, it was believed that the system with fractional filling factors behaves as a condensate, even very deep in the regime of strong interactions. However, we were able to obtain some information on the properties of the system by calculating the ground state and its quasi-momentum distribution. From the results, we can conclude that the system exhibits correlation phenomena which are characteristic for strongly interacting bosons and which do not correspond to a condensate at all.

Some work on the strongly correlated regime with incommensurate filling remains to be done. Concerning the ground state properties, it would be nice to have an analytical formula for the determinant description of the two-point correlation functions (Eq. 3.24). Furthermore, analytical approximations for the ground-state of the system and its properties in the case of an additional harmonic confinement should also be looked after.

After establishing the ground-state properties, one could also look for interesting excitations of the system. An example of this could be the following: suppose that we start with a Mott state. The density distribution for this state would be flat (in the absence of a harmonic trap). Now, if we remove particles from a certain site, we will create a dip in the density distribution. When the system evolves in time, this density dip could propagate to other sites without changing its form. In this way, one could create a soliton in the system. Another possibility would be that the dip first disappears and then after some period in time it reappears; as
such, one would be able to observe a periodic focusing.

This shows that there is still some fascinating physics concerning a system of strongly correlated bosons in an optical lattice waiting to be explored.
Part II

"Spin-1/2" Bosons in a 1D Lattice
Preface

As a general remark, it has to be said that the remaining chapters of the thesis will not dig very deep into the subject they treat. Only the section 6.2 in which we ourselves have derived an effective Hamiltonian for a particular limit, and section 5.3 with the formulas behind the idea of making bosons behave like fermions are a little bit more elaborated.

Therefore, the following chapters have to be understood as giving one a first impression of the subject.
Chapter 5
Correlated Fermions in 1D

5.1 Introduction

Correlated fermions in 3D are a well studied problem. Many systems of interacting fermions can be described theoretically by Fermi liquid theory, which is well understood. In 1D however, this description is not valid. Nevertheless, there is a variety of exactly solvable 1D models which have been known for quite some time, and a deeper understanding of their mutual relationships and their relevance for describing the generic low-energy physics of 1D interacting fermions has emerged rather recently. The very fundamental difference between three-dimensional Fermi liquids, and their one-dimensional counterparts, the so-called Luttinger liquids, will be briefly reviewed in the next section (for a more thorough review, see e.g. Ref. [32]). In a later section, it is discussed how one can use bosons to simulate typical properties of interacting fermions. Since fermions are still hard to cool and trap, it is clear that using bosons to simulate interacting fermions, instead of directly using fermions on a lattice, can be a quite advantageous approach.

5.2 Fermi and Luttinger Liquids

In two and three dimensions, many systems of interacting fermions at low temperatures are described by Fermi liquid theory [23], originally developed by Landau. For a non-interacting system at zero temperature, the ground state is determined by the Fermi surface: all one-particle states with energies less than the Fermi energy are occupied, while all states outside the Fermi surface are unoccupied. An elementary excitation consists of annihilating a particle from a state below the Fermi-surface (hole excitation), or creating it in a state with energy higher than the Fermi energy (particle excitation). For a fixed number of particles in the
system, the low-energy excitations therefore consist of particle-hole pairs where some particles from states within the Fermi-surface are promoted to states outside.

When introducing interactions, Fermi liquid theory is based on a picture of quasi-particles evolving continuously out of the particles (holes) of a non-interacting system of fermions by adiabatically switching on the interactions. These quasi-particles are in one-to-one correspondence with the original fermions and therefore obey Fermi statistics, but their dynamical properties are renormalized by interactions. The original one-particle excitations of the free fermions are now accompanied by a cloud of particle-hole pairs, but the picture of ground- and excited states in terms of a Fermi sea of such quasi-particles is still valid.

The free Fermi gas is thus the solvable model on which Landau's Fermi liquid theory is built. It should be noted that this theory only describes the low-energy properties of an interacting two- or three-dimensional system. However, this is sufficient because macroscopic properties of the system are determined only by excitations on energy scales small compared to the Fermi energy.

An important property of Fermi liquids in two or three dimensions is that the one-particle momentum distribution has a finite discontinuity at the Fermi momentum \( k_F \) (see Fig. 5.1a). Also, the various correlation functions show power-law decay at asymptotically long distances and the exponents governing the power-law are universal, meaning that they do not depend on the strength of the interactions.

Figure 5.1: One-particle momentum distribution function. For a system of interacting fermions in more than one dimension, the distribution shows a finite discontinuity at the Fermi momentum \( k_F \) (a). In one dimension, this discontinuity is absent, but there is an inflection point at \( k_F \) (b).

In one dimension, Fermi liquid theory breaks down: a description of the
5.2. FERMI AND LUTTINGER LIQUIDS

The ground state and low-lying excitations in terms of a Fermi-sea picture of quasi-particles is not possible anymore because the quasi-particles are not stable against turning on the interactions. Instead, the elementary excitations are collective charge and spin fluctuations dispersing with different velocities. When adding a single fermion to the system, the fermion will decay into charge and spin excitations which then separate spatially with time. This is the so-called spin-charge separation. If the spin and charge excitations are gapless, and more precisely have dispersions $\omega_\nu \approx v_\nu |q| (\nu = p, \sigma$ for charge and spin) like depicted in Fig. 5.2, the elementary spin and charge excitations are bosonic in nature, in contrast with the fermionic quasi-particles of a Fermi liquid. Most importantly, one can now rewrite any interacting fermion Hamiltonian, provided its charge and spin excitations are gapless, as a harmonic oscillator and find an operator identity allowing to express every fermion operator as a function of these bosons. With this method, called bosonization [33], all physical properties of the system can be calculated. For free fermions, the Hamiltonian describing the excitations out of the ground state can be expressed as a Hamiltonian that is quadratic in the boson-operators:

$$H = \sum_{\nu=p,\sigma} \sum_q v_\nu |q| \left( b^\dagger_{\nu,q} b_{\nu,q} + 1/2 \right), \quad (5.1)$$

where, for a non-interacting system, the charge and spin velocities are both equal to the Fermi velocity, $v_\nu = v_F$.

In the presence of electron-electron interactions, assuming that charge and spin excitations remain gapless, the Hamiltonian is still of the form (5.1), but the

![Figure 5.2: Particle-hole excitations in 1D. The spectrum has no low-frequency excitations with $0 \lesssim |q| \lesssim 2k_F$, unlike in higher dimensions where these states are filled in. For low energies and low momenta, the dispersion becomes linear: $\omega_\nu \approx v_\nu |q|$.](image-url)
interactions will make $v_{\sigma} \neq v_{\rho} \neq v_F$, leading to charge-spin separation. Interactions will also renormalize the physical properties, and by comparing the velocities measuring this renormalization to $v_{\nu}$, the correlation exponents $K_{\nu}$ can be defined. These $K_{\nu}$ only depend on the low-energy properties of the Hamiltonian. By using the bosonization method, the complete physics of a 1D fermionic liquid can then be described in terms of these 4 coupling parameters only.

It is clear that the properties of these gapless 1D systems of interacting fermions will be very different from those of 2D and 3D systems. In particular, the power-law decay of the correlation functions is determined by the coupling constants $K_{\nu}$, which are renormalized with changing interaction strength, so the behavior of these 1D systems is not universal anymore. Also, the momentum distribution does not have a jump anymore at the Fermi-momentum. Rather, there is an inflection point whose form is determined by the same coupling constants (see Fig. 5.1b).

All such properties are generic for 1D systems of interacting fermions, but they were first studied in a model introduced by Luttinger [19]. Therefore, the term 'Luttinger liquid' was coined by Haldane [9] to describe these universal low-energy properties of gapless 1D quantum systems, and to emphasize that a low-energy description can be based on the Luttinger model in much the same way as the Fermi liquid theory in 3D is based on the free Fermi gas.

5.3 Bosons behaving like Interacting fermions

The main title of the second part of this thesis, “spin-1/2 bosons in an optical lattice”, might sound strange at first since bosonic atoms normally have an integer spin. This means that there is an odd number $2F + 1$ of sublevels in each hyperfine level $F$ (e.g., the $F = 1$ level has three sublevels $m_F = -1, 0, 1$). However, by making use of an off-resonant microwave field, some sublevels of a bosonic atom can be shifted up in energy so that, effectively, the atom can occupy only two levels. One of the two available levels will be called the spin-up level, the other one the spin-down level. In the remainder of the thesis, we will consider such bosonic atoms in an optical lattice.

Recently, it has been proposed that these two-level bosons in a one-dimensional optical lattice can be made to behave as interacting fermions [25]. Bosons on a 1D lattice can thus be used to simulate fermionic correlation properties. The basics behind this idea will now be introduced.

In complete analogy to the derivation in section 2.2, making the same assumptions stated there (tight-binding, only lowest band dynamics, effective 1D tunnelling), the Hamiltonian of a system of bosons with two possible internal
5.3. **BOSONS BEHAVING LIKE INTERACTING FERMIONS**

states on an optical lattice can be written as:

\[
H = -J \sum_{i=1}^{M} \sum_{\sigma=\uparrow, \downarrow} (a_{i\sigma}^\dagger a_{i+1\sigma} + a_{i+1\sigma}^\dagger a_{i\sigma}) + \sum_{i=1}^{M} \sum_{\sigma=\uparrow, \downarrow} V_{\sigma} n_{i\sigma}^2 + U \sum_{i=1}^{M} n_{i\uparrow} n_{i\downarrow}, \quad (5.2)
\]

where \( \sigma = \uparrow, \downarrow \) denotes the two relevant internal levels of the bosons, and the operator \( a_{i\sigma}^\dagger \) creates a particle in level \( \sigma \) on site \( i \) of the 1D lattice. These operators satisfy the normal bosonic commutation relations \([a_{i\sigma}^\dagger, a_{j\sigma'}^\dagger] = \delta_{ij} \delta_{\sigma\sigma'}\), with all other commutators vanishing. The operators \( n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma} \) are the corresponding number operators. The interaction strength of two particles on the same site is given by \( U \) if the particles have opposite spin, and by \( V_\sigma \) if they both have the same spin \( \sigma \). We consider again a finite system of \( M \) sites with periodic boundaries, so that the summation index \( M + 1 \) in the above Hamiltonian is implicitly replaced by 1.

The first term in the Hamiltonian describes the tunnelling of particles to adjacent sites, where it is assumed that the tunnelling amplitude \( J \) is independent of the internal level of the hopping particle. We have two interaction terms. The first contribution to the interaction energy comes from having two particles in the same internal level at the same site. The corresponding interaction energy \( V_{\sigma} \) can be spin-dependent. Another contribution comes from having a spin-up and a spin-down boson at the same site (interaction energy \( U \)). Since we will only consider repulsive interactions between the particles, we have \( V_{\sigma}, U > 0 \).

The key point now is that, by making use of the large control one has over the lattice parameters, the interaction energies \( V_{\sigma} \) can be made very large compared to the tunnelling \( J \) and the spin-up spin-down interaction coefficient \( U \). In such a situation, two particles with the same spin are not likely to be found on the same lattice site, because they have to pay a large interaction energy. The ground- and low-energy excited states of the Hamiltonian then lie in a subspace spanned by states for which a site can only be doubly occupied if both particles have opposite spin. As such, the very large interaction between the bosons creates an effective Pauli-exclusion principle due to which only particles with different spin can get paired together. Already here, it becomes clear that bosons can indeed made to behave like fermions.

Once again, by projecting onto the subspace, a technique which was already successfully implemented in the first part of the thesis (see also appendix B), one can obtain an effective Hamiltonian describing the low-energy physics of the Hamiltonian (5.2). We will again take into account only the first order term of this effective Hamiltonian, a treatment which gives exact results in the limit \( V_{\sigma} \to \infty \) where having two particles with the same spin on the same site is really forbidden. This constraint can be absorbed in the definition of the operators \( a_{i\sigma}^\dagger \):

\[
a_{i\sigma}^\dagger a_{i\sigma}^\dagger = 0. \quad (5.3)
\]
These "impenetrable boson"-operators can be transformed into fermionic ones by using the Jordan-Wigner transformation, which is generalized to particles with spin as follows:

\[ a_{i\sigma}^\dagger = \prod_{j < i, \sigma' = \uparrow, \downarrow} (1 - 2c_{j\sigma}^\dagger c_{j\sigma'}) c_{i\sigma}^\dagger. \] (5.4)

The operators \( c_{i\sigma}^\dagger \) are then spin-1/2 fermionic operators. The bosonic Hamiltonian (5.2), projected to the subspace where no two particles with the same spin can occupy the same site, can now be written as a fermionic Hamiltonian:

\[ H_{FH} = -J \sum_{\sigma = \uparrow, \downarrow} \sum_{i=1}^{M} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + U \sum_{\sigma = \uparrow, \downarrow} \sum_{i=1}^{M} n_{i\sigma} n_{i\bar{\sigma}}, \] (5.5)

where the number operators \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) are fermionic. This Hamiltonian is the famous Fermi-Hubbard Hamiltonian. In different regimes of the parameters \( J \) and \( U \), it will exhibit very rich behavior such as ferro- and ferrimagnetism, antiferromagnetism, superconductivity, and a metal-insulator transition to name a few. Important for us is that, in the regime \( U > 0 \), it is known that the Fermi-Hubbard model describes a Luttinger liquid for filling factors different from 1/2. The filling factor is defined in this chapter as \( \nu = N/2M \), where \( N = N_\uparrow + N_\downarrow \) is the total number of spin-up and spin-down particles.

After this discussion, it should be clear that our original bosons can indeed be made to behave as effective fermions. In short, it is the large interaction energy between two bosons with the same spin which leads to an effective Pauli-exclusion principle for the bosons, and which makes them behave as fermions; they realize the Fermi-Hubbard model.

The 1D Fermi-Hubbard model can be exactly solved by means of a Bethe Ansatz approach [24], meaning that one has access to the energy spectrum as well as the ground-and excited states of the system. One sees from the spectrum that the elementary excitations of the Fermi-Hubbard model are gapless, and therefore the 1D system forms a Luttinger liquid. But, calculating physical properties with this exact solution is a daunting task. However, the spin- and charge-velocities \( v_\sigma \) and \( v_\rho \), and the coupling exponents \( K_\sigma \) and \( K_\rho \) can be found quite easily from the known energy spectrum, so that a complete description of the low-energy properties can also be given in terms of a Hamiltonian (5.1), like showed in the previous section. Then, making use of an identity between fermionic and bosonic field operators, derived in the bosonization theory, the interesting correlation functions can be calculated quite easily.

In the next chapter, we will derive in a more straightforward way the ground- and excited states of the Fermi-Hubbard model in the limit \( U \gg J \). It will be
shown that the charge and spin degrees of freedom in these states are indeed separated: in particular, it will be seen that the eigenstates are product states where the position (charge) part of the state corresponds to a state of free spinless fermions, while the spin-part is an eigenstate of the Heisenberg spin model.
CHAPTER 5. CORRELATED FERMIONS IN 1D
Chapter 6

Luttinger Liquid with Bosons on a 1D Lattice

6.1 Introduction

In the previous chapter, it was seen that a one-dimensional system of interacting fermions could form a Luttinger liquid. One of the hallmarks of such systems is the separation of the spin and charge (= mass) degrees of freedom. This effect has never been observed in a condensed matter system.

It has also been shown that bosons on a 1D lattice can be used to simulate fermionic correlation properties. In particular, they can realize a Fermi-Hubbard model. Stimulated by the extreme flexibility and controllability of the lattice systems we set out to observe spin-charge separation in a system of two-level bosons on a 1D optical lattice.

Luttinger liquids are most often described by a phenomenological method called bosonization [33]. By using a simpler method which we developed ourselves, we were able to show that the ground- and all excited states of our system can be written as a product of a state acting in position space and another one acting in spin space, thereby proving the existence of spin-charge separation in our system.

6.2 Effective Hamiltonian Approach for the Strongly Interacting Limit

We start off with equation (5.5) from the previous chapter, where it was shown that bosons on a 1D lattice can realize the Fermi-Hubbard model. In the limit of strong interactions, \( U \gg J \), the projection technique can be applied again to obtain an
effective Hamiltonian describing the low-energy physics of the Fermi-Hubbard model. Indeed, in this regime, the ground-and low-energy excited states of the Fermi-Hubbard model (Eq. (5.5)) lie in the subspace spanned by states where two fermions with opposite spin cannot be simultaneously at the same site because for such a configuration the system has to pay an energy $U$. Define $\mathcal{P}$ as the projector on this subspace, and $Q$ the projector out of the subspace ($\mathcal{P} + Q = 1$). The low-energy properties of our system can then be described by an effective Hamiltonian, which is given to second order by (see appendix B):

$$H_{\text{eff}} = \mathcal{P}H_{FH}\mathcal{P} - \frac{1}{U}\mathcal{P}H_{FH}QH_{FH}\mathcal{P}.$$  

(6.1)

In terms of the fermionic creation and annihilation operators, the first order term becomes:

$$H_{\text{eff}}^{(1)} = -J \sum_{i=1}^{M} \sum_{\sigma = \uparrow, \downarrow} \mathcal{P}(c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma})\mathcal{P}.$$  

(6.2)

This describes tunnelling of a fermion to an unoccupied neighboring site. The second order term can be written as:

$$H_{\text{eff}}^{(2)} = -\frac{J^2}{U} \sum_{i,j=1}^{M} \mathcal{P}(c_{i-1\sigma}^\dagger c_{i\sigma}^\dagger + c_{i+1\sigma}^\dagger c_{i\sigma}^\dagger)Q^{\dagger}c_{j\sigma'}(c_{j-1\sigma'} + c_{j+1\sigma'})\mathcal{P}.$$  

(6.3)

Let's consider this term step by step: first, a particle tunnels from a neighboring site to site $j$. This site is then either singly occupied, or doubly occupied with two particles with opposite spin. The possibility of single occupation is ruled out by the projector $Q$. This operator could therefore be replaced by $n_{j,-\sigma}$ (remark: if $\sigma = \uparrow$, then $-\sigma = \downarrow$ and the other way round). After that, a particle is moved from site $i$ to a neighboring site. If $i \neq j$, then $j$ will still be doubly occupied afterwards, and the final projection $\mathcal{P}$ will give zero. If $i = j$, the double occupancy at site $j$ can be removed, and a contribution to the effective Hamiltonian will result. So we only have to take into account terms with $i = j$, and we can replace $Q$ by $n_{i,-\sigma}$. The result is:

$$H_{\text{eff}}^{(2)} = -\frac{J^2}{U} \sum_{i=1}^{M} \sum_{\sigma} (c_{i-1\sigma}^\dagger c_{i\sigma}^\dagger n_{i,-\sigma} c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}^\dagger n_{i,-\sigma} c_{i\sigma}^\dagger c_{i-1\sigma})$$  

(6.4a)

$$+ (c_{i-1\sigma}^\dagger c_{i-\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i-1\sigma} + c_{i+1\sigma}^\dagger c_{i-\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i+1\sigma})$$  

(6.4b)

$$+ (c_{i\sigma}^\dagger c_{i\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+\sigma}^\dagger c_{i\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i-\sigma})$$  

(6.4c)

$$+ (c_{i-\sigma}^\dagger c_{i-\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+\sigma}^\dagger c_{i\sigma} n_{i,-\sigma} c_{i\sigma}^\dagger c_{i-\sigma}).$$  

(6.4d)

This term incorporates processes which could be named a cell shift, a spin flip, and a combination of both. They are visualized in Fig. 6.1. The different processes in the figure carry the same label as the corresponding terms in the formula above (6.4a, 6.4b etc.).
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Figure 6.1: Second order processes taken into account by the effective Hamiltonian description of our system: identity (a), spin-flip (b), cell shift with spin-flip (c) and cell shift (d). The different processes (a), (b), ... correspond respectively to the terms (6.4a), (6.4b), ... of Eq. (6.4).
6.2.1 Perturbation Theory

Now, we will introduce some notation which will make the derivation of spin-charge separation in the Fermi-Hubbard model with $U \gg J$ more clear. The subspace considered above, where one can have only single occupancies at every site is spanned by states of the form:

$$|x_1, x_2, \ldots, x_N \rangle \otimes |\sigma_1, \sigma_2, \ldots, \sigma_N \rangle = c_{x_1, \sigma_1}^\dagger c_{x_2, \sigma_2}^\dagger \cdots c_{x_N, \sigma_N}^\dagger |0\rangle,$$

(6.5)

where $N$ is the number of particles. The $x_i$ denote the positions of occupied sites ($x_i = 1, \ldots, M$), and the $\sigma_i$ the spin of the particle at position $x_i$. In order to obtain a unique definition, it is assumed that $x_1 < x_2 < \ldots x_N$. As an example, the state $|269\rangle |\uparrow\uparrow\downarrow\rangle$ has 2 fermions with spin up on sites 2 and 6, and a spin down at site 9. All other sites are unoccupied.

We also define operators $|m\rangle_i \langle n|$ and $|\sigma\rangle_i \langle \sigma'|$ acting separately on respectively the position (=charge) and spin degrees of freedom, as follows:

$$|m\rangle_i \langle n| |x_1, \ldots, x_i = n, \ldots, x_N\rangle = |x_1, \ldots, x_i = m, \ldots, x_N\rangle,$$

(6.6a)

$$|\sigma\rangle_i \langle \sigma'| |\sigma_1, \ldots, \sigma_i = \sigma', \ldots, \sigma_N\rangle = |\sigma_1, \ldots, \sigma_i = \sigma, \ldots, \sigma_N\rangle.$$  

(6.6b)

It is easy to see that all operators acting on states within the considered subspace can be written as products of operators (6.6).

Now, we can write our effective Hamiltonian $H_{\text{eff}}^{(1)} + H_{\text{eff}}^{(2)}$ in terms of these operators.

The first order term, $H_{\text{eff}}^{(1)}$ will only involve operators acting on the position part. Indeed, it will move a particle to a neighboring empty site and it thereby preserves the spin configuration. This is best understood with an example. Consider again the state $|269\rangle |\uparrow\uparrow\downarrow\rangle$. One of the terms in $H_{\text{eff}}^{(1)}$ moves the particle from site 2 to site 3. The resulting state is then $|369\rangle |\uparrow\uparrow\downarrow\rangle$. Notice that the spin configuration did not change.

It is important to note that if we have periodic boundaries, a particle can tunnel from the last site to the first one. Such a process does not conserve the spin configuration. In our example, if we have only 9 sites, then the particle at site 9 can tunnel to the first site. As a consequence: $|269\rangle |\uparrow\uparrow\downarrow\rangle \rightarrow |126\rangle |\downarrow\uparrow\uparrow\rangle$, so that the spin configuration does change in this special case! This boundary effect can be neglected, which will not restrict the conclusions if we consider sufficiently large systems.

The effective Hamiltonian can then be written to first order as:

$$H_{\text{eff}}^{(1)} = \left(-J \sum_{i=1}^{N} \sum_{m=1}^{M} |m+1\rangle_i \langle m| (\sigma_i - |m+1\rangle_{i+1} \langle m+1|) \right) \otimes \Pi_{\Sigma},$$

(6.7)
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where the term \((\Pi_{\rho} - |m+1\rangle_{i+1} \langle m+1|)\) assures that tunnelling takes only place to an empty neighboring site (\(\Pi_{\rho,2}\) is the identity operator, acting in position or spin space). The first order term thus is already spin-charge separated: the position part describes tunnelling of free spinless fermions, whereas the spin part is the identity operator. The eigenstates of \(H_{\text{eff}}^{(1)}\) are trivial to calculate: they are product states \(|\phi\rangle \otimes |\sigma\rangle\) where the \(|\phi\rangle\) are eigenstates of the Hamiltonian for free spinless fermions. These are Slater determinants of plane waves with different momenta:

\[
|\phi\rangle \sim \sum_{x_1 < x_2 < \ldots < x_N} (\det[e^{i k_n x_j \frac{j=1}{N}}]) |x_1, x_2, \ldots, x_N\rangle.
\]

The momenta are restricted to:

\[
k_n = \frac{2\pi}{M} n, \quad n = 0, \ldots, M - 1
\]

because of periodic boundaries. Since this Hamiltonian acts as the identity operator on the spin degrees of freedom, all states \(|\phi\rangle |\sigma\rangle\) with different spin configurations \(|\sigma\rangle = |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle\), but with fixed \(|\phi\rangle\), are degenerate with energy:

\[
E = -2J \sum_n \cos(k_n),
\]

with the \(k_n\) values as in the Slater determinant of \(|\phi\rangle\).

The second order term can also be written in terms of the new operators. After some algebra, one obtains in the end:

\[
H_{\text{eff}}^{(2)} = -\frac{J^2}{U} \sum_{i=1}^{N} \sum_{m=1}^{M} \hat{H}^{(i)}(m) \cdot \hat{H}_{\text{spin}}^{(i)} \quad \text{with}
\]

\[
\hat{H}^{(i)}(m) = 2|m+1\rangle_{i+1} \langle m|_i \langle m+1|_{i+1} + |m+2\rangle_{i+1} \langle m+1|_i \langle m+1|_{i+1} (\Pi - |m+2\rangle_{i+2} \langle m+2|) + |m\rangle_{i+1} |m-1\rangle_i \langle m+1|_{i+1} (\Pi - |m-1\rangle_{i-1} \langle m-1|)
\]

\[
\hat{H}_{\text{spin}}^{(i)} = \sum_{\sigma = 1, -1} \{|\sigma\rangle_{i+1} - |\sigma\rangle_i \langle \sigma|_{i+1} - |\sigma\rangle_{i+1} |\sigma\rangle_i \langle \sigma|_{i+1} \}
\]

It is clear that this part of the effective Hamiltonian is not yet written in a spin-charge separated form, because of the \(i\)-dependence of \(\hat{H}^{(i)}(m)\) and \(\hat{H}_{\text{spin}}^{(i)}\). This will be taken care of now.
Since we are considering the limit $J/U \ll 1$, we can treat $H^{(2)}_{\text{eff}}$ as a perturbation to the first order term $H^{(1)}_{\text{eff}}$. This perturbation will lift the spin degeneracy present when considering $H^{(1)}_{\text{eff}}$ only. From degenerate perturbation theory, one learns that one has to calculate the eigenstates of the perturbation $H^{(2)}_{\text{eff}}$ in every subspace of degenerate eigenstates of the unperturbed Hamiltonian $H^{(1)}_{\text{eff}}$.

### 6.2.2 Non-degenerate eigenstates $|\phi\rangle$

We will first consider the case where all orthogonal spinless fermion eigenstates $|\phi\rangle$ of the unperturbed Hamiltonian $H^{(1)}_{\text{eff}}$ have a different energy. Then, all of the above-mentioned degenerate subspaces are spanned by states of the form:

$$S_\phi = \{|\phi\rangle \otimes |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle : \sigma_i = \uparrow, \downarrow\}, \quad (6.11)$$

for fixed $|\phi\rangle$. So with every $|\phi\rangle$, there corresponds a subspace generated by the different degenerate spin configurations.

Doing perturbation theory now corresponds to calculating the matrix elements $\langle \vec{\sigma} | \langle \phi | H^{(2)}_{\text{eff}} | \phi \rangle | \sigma' \rangle$ in such a subspace and diagonalize the resulting matrix.

The matrix elements are given by:

$$\langle \vec{\sigma} | \langle \phi | H^{(2)}_{\text{eff}} | \phi \rangle | \sigma' \rangle = -\frac{J^2}{U} \sum_{i=1}^{N} \sum_{m=1}^{M} \langle \phi | \hat{H}^{(i)}(m) | \phi \rangle \cdot \langle \vec{\sigma} | \hat{H}^{(i)}_{\text{spin}} | \sigma' \rangle. \quad (6.12)$$

Now, it can be proven (see appendix C) that $\sum_{m=1}^{M} \langle \phi | \hat{H}^{(i)}(m) | \phi \rangle = \gamma(\phi)$ is independent of $i$, so that the Hamiltonian can be seen to act as

$$H^{(2)}_{\text{eff}} = -\frac{J^2}{U} \gamma(\phi) H_{\text{spin}}, \quad (6.13)$$

in every subspace $S_\phi$. In this expression, $H_{\text{spin}}$ is given by:

$$H_{\text{spin}} = \sum_{i=1}^{N} \sum_{\sigma = \uparrow, \downarrow} \hat{H}^{(i)}_{\text{spin}}, \quad \text{and} \quad (6.14)$$

$$\gamma(\phi) = \sum_{m=1}^{M} \langle \phi | \hat{H}^{(i)}(m) | \phi \rangle. \quad (6.15)$$

Let's consider this spin-Hamiltonian in some more detail:

$$H_{\text{spin}} = \sum_{i=1}^{N} \sum_{\sigma = \uparrow, \downarrow} \{|\sigma\rangle_i \langle \sigma |_{i+1} - |\sigma\rangle_i \langle -\sigma |_{i+1} - |\sigma\rangle_i \langle \sigma |_{i+1} - |\sigma\rangle_i \langle -\sigma |_{i+1} \rangle. \quad (6.16)$$
The first term will change a \(| \downarrow \uparrow \rangle\) configuration in \(| \uparrow \downarrow \rangle\). It is therefore similar to a term \(S_m^+ S_{m+1}^-\) in terms of Pauli operators. The second term just gives a contribution if there are two neighboring opposite spins, while it gives zero in other cases. This term is therefore related to \(S_m^z S_{m+1}^z - 1/4\). Indeed, by carefully mapping our operators to Pauli operators, it can be seen that the spin Hamiltonian corresponds to the Heisenberg model:

\[
H_{\text{spin}} = 2 \sum_{m=1}^{M} (\vec{S}_m \cdot \vec{S}_{m+1} - 1/4), \quad \vec{S}_i = (S^x_i, S^y_i, S^z_i). \tag{6.17}
\]

After this lengthy derivation, let me summarize the results we have found. In the limit \(U \gg J\), the Fermi-Hubbard Hamiltonian can be written in a spin-charge separated form:

\[
H_{\text{FH}} = H^{(1)}_{\text{eff}} + H^{(2)}_{\text{eff}} = H_\rho + H_\Sigma, \tag{6.18}
\]

\[
H_\rho = -J \sum_i c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i, \tag{6.19}
\]

\[
H_\Sigma = -\frac{2J^2}{U} \gamma(\phi) \sum_{m=1}^{M} (\vec{S}_m \cdot \vec{S}_{m+1} - 1/4). \tag{6.20}
\]

The Hamiltonian \(H_{\text{charge}}\) corresponds to a Hamiltonian for free spinless fermions, while \(H_\Sigma\) corresponds to the Heisenberg model. The eigenstates of the Hamiltonian then are product states \(|\phi\rangle \otimes |\bar{\sigma}\rangle\), where the position part \(|\phi\rangle\) corresponds to an eigenstate of \(H_{\text{charge}}\), and the spin state \(|\bar{\sigma}\rangle\) is an eigenvector of the Heisenberg chain with coupling dependent on \(\phi\). The energy spectrum of these states is then also very simple; the energy of a product state corresponds to the energy of the spinless fermion state plus the energy of the spin eigenstate (which depends on \(\phi\)).

### 6.2.3 Degenerate eigenstates \(|\phi\rangle\)

Now consider the situation where some eigenstates of \(H^{(1)}_{\text{eff}}\) have the same energy. To keep things clear, we will consider the situation where only two orthogonal eigenstates \(|\phi\rangle\) and \(|\phi'\rangle\) have the same energy.

Now, we have to calculate the matrix elements of \(H^{(2)}_{\text{eff}}\) between states lying in the subspace:

\[
S_{\phi,\phi'} = \{|\psi\rangle \otimes |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle : \psi = \phi, \phi' \text{ and } \sigma_i = \uparrow, \downarrow\}. \tag{6.21}
\]
The matrix elements are given by:

$$
\langle \sigma | \left( \psi | H_{ef}^{(2)} | \psi' \right) | \sigma' \rangle = -\frac{J^2}{U} \sum_{i=1}^{N} \sum_{m=1}^{M} \langle \psi | H^{(1)}(m) | \psi' \rangle \cdot \langle \sigma | \tilde{H}_{\text{spin}}^{(1)} | \sigma' \rangle, \quad \psi, \psi' \in \{ \phi, \phi' \}. 
$$

(6.22)

It can be proven, in a completely similar way to what has been done in appendix C, that the terms \( \sum_{m=1}^{M} \langle \psi | \tilde{H}^{(1)}(m) | \psi' \rangle \) are independent of \( i \), so that in this case, the Hamiltonian \( H_{ef}^{(2)} \) acts in the subspace \( S_{\phi,\phi'} \) like:

$$
H_{ef}^{(2)} = -\frac{J^2}{U} \Gamma_{\phi,\phi'} \otimes H_{\text{spin}}. 
$$

(6.23)

where \( H_{\text{spin}} \) corresponds to the Heisenberg chain \( 2 \sum_{i=1}^{M} (\tilde{S}_m \tilde{S}_{m+1} - 1/4) \). The matrix \( \Gamma_{\phi,\phi'} \) is given by:

$$
\Gamma_{\phi,\phi'} = \begin{pmatrix}
\gamma(\phi, \phi) & \gamma(\phi, \phi') \\
\gamma(\phi', \phi) & \gamma(\phi', \phi')
\end{pmatrix}, 
$$

(6.24)

$$
\gamma(\psi, \psi') = \sum_{m=1}^{M} \langle \psi | \tilde{H}^{(1)}(m) | \psi' \rangle, \quad \psi, \psi' \in \{ \phi, \phi' \}. 
$$

(6.25)

The key point is that the charge and spin degrees of freedom are again separated, as can be seen from Eq. (6.23), and the eigenstates of the complete Hamiltonian are thus product states. The spin-part still corresponds to an eigenstate of the Heisenberg chain, and the charge eigenstate will be a linear combination of the states \( |\phi\rangle \) and \( |\phi'\rangle \). The correct linear combination is found as an eigenstate of the matrix \( \Gamma_{\phi,\phi'} \). The corresponding energies are again sums of the energies of the spin- and charge state.

Generalization of this line of reasoning to cases where more than two eigenstates of \( H_{ef}^{(1)} \) are degenerate is now trivial: the only difference will be that the dimension of the matrix \( \Gamma \) increases.

### 6.2.4 Spin-charge separation for the bosons

Although it is clear that the ground and excited states of the Fermi-Hubbard model are product states, remember that we used the Jordan-Wigner transformation to map our original bosonic system to a fermionic one (see section 5.3). In the first part of the thesis, it was shown that this transformation can modify the behavior of certain observables measured on the fermionic system compared to a measurement of the same observable on the bosonic system. Therefore, it remains still to
be shown that the product form of the eigenstates is conserved if we do the inverse Jordan-Wigner transformation.

This is quite simple to see. An eigenstate of the Fermi-Hubbard model is a product state, so that we can write:

\[ |\phi\rangle_F \otimes |\chi\rangle_F = \sum_{x_1 < x_2 < \ldots < x_N} \phi(x_1, x_2, \ldots, x_N) |x_1, x_2, \ldots, x_N\rangle \otimes \sum_{\sigma_1, \ldots, \sigma_N} \chi(\sigma_1, \ldots, \sigma_N) |\sigma_1, \ldots, \sigma_N\rangle \]

\[ = \sum_{x_1 < \ldots < x_N} \sum_\sigma \phi(x_1, \ldots, x_N) \chi(\sigma_1, \ldots, \sigma_N) c_{x_1, \sigma_1}^\dagger c_{x_2, \sigma_2}^\dagger \ldots c_{x_N, \sigma_N}^\dagger |0\rangle. \] 

Now, since \( x_1 < x_2 < \ldots < x_N \), the inverse Jordan-Wigner transformation just makes:

\[ c_{x_1, \sigma_1}^\dagger c_{x_2, \sigma_2}^\dagger \ldots c_{x_N, \sigma_N}^\dagger |0\rangle = a_{x_1, \sigma_1}^\dagger a_{x_2, \sigma_2}^\dagger \ldots a_{x_N, \sigma_N}^\dagger |0\rangle. \] 

This means that the wavefunctions of the bosonic Hamiltonian are still products:

\[ |\phi\rangle_B \otimes |\chi\rangle_B = \sum_{x_1 < x_2 < \ldots < x_N} \sum_\sigma \phi(x_1, \ldots, x_N) \chi(\sigma_1, \ldots, \sigma_N) a_{x_1, \sigma_1}^\dagger \ldots a_{x_N, \sigma_N}^\dagger |0\rangle. \] 

This completes the derivation of spin-charge separation in our system. The derivation was quite technical, but straightforward.

### 6.3 Conclusions

We proposed to observe spin-charge separation, one of the hallmarks of Luttinger liquid theory, with a system of strongly interacting bosons on a 1D optical lattice. Following [25], it was shown first that this system can realize the fermionic Hubbard model. By using a quite simple perturbation approach, the ground- and low lying excited states were shown to be product states: the position state corresponded to a free spinless fermion eigenstate, whereas the spin state was an eigenstate of the Heisenberg model. From a theoretical point of view, the spin-charge separation is thereby proven.

In the next chapter, a discussion will follow concerning the question of how the spin-charge separation could be observed in a realistic experimental setup based on our system of bosons in an optical lattice.
Chapter 7

Experimental Observation of Spin-Charge Separation

It is quite easy to observe experimentally the product form of the eigenstates in Eq. (6.27) derived in the previous chapter. Making use of the dipole force of a high-intensity laser, one could move a few particles from the sites on which the laser is pointed to other sites. By tuning the resonance frequency of the laser, one can choose to create a spin-excitation by removing only the spin-up or spin-down particles, or create a charge excitation by removing both spin components. However, it should be remarked that the product form of the eigenstates only is not a characteristic feature of 1D systems; it can also be a property of certain 3D systems. The spin-charge separation characteristic for Luttinger liquids only becomes apparent if we can create a single hole or particle excitation by removing resp. adding only one particle. Luttinger liquid theory tells us that these one-particle excitations will also decay into charge and spin degrees of freedom, in contrast with the 3D situation where a description of these excitations in terms of stable quasi-particles is imminent.

To show the separation of the spin and charge degrees of freedom of a one-particle excitation, one could in principle do an experiment as described below.

If we have a translationally invariant system, the charge- and spin distributions in the ground state, given respectively by \( \langle n_{ii} \rangle + \langle n_{i+1} \rangle \) and \( \langle n_{ii} \rangle - \langle n_{i+1} \rangle \) as a function of the site number \( i \), are flat over the entire lattice. After moving a single particle from a certain site out of the system, we will create a dip in the charge and spin distributions. From the Luttinger liquid theory described in section 5.2, we know that if we add or remove a particle from the system, the particle (or hole) will decay into charge and spin excitations which separate spatially in time. The idea now is that as a result, the dip in the charge distribution will start moving with a different velocity than the dip in the spin distribution. The dips will not change
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their form because of the linear dispersion of the charge and spin excitations.

There are two problems with this scheme. First of all, one should be able to measure the spin- and charge distribution. This is not a very strong constraint: by making spin-dependent absorption images of the particles after releasing them from the lattice, it should be possible to obtain information on the charge and spin-distributions. By varying the time interval between removing a single particle and releasing the remaining particles from the trap, and by collecting the absorption images after these different experiments, it should be possible to obtain a picture of the time evolution of the spin- and charge distributions and see the separation of the spin- and charge degrees of freedom.

But still, it has to be shown what precise signature of the spin-charge separation can be observed in the absorption images, in particular what the exact relation is between the spin- and charge distributions and the spin-dependent absorption images.

A much more fundamental difficulty arises from the fact that we should be able to add or remove a single particle only in order to create the one-particle excitation. The lattice parameter is equal to $\lambda/2$, while a fundamental limit for the size of the waist $w_0$ of a collimated laser can be obtained from the formula $\theta = Pi/(\lambda w_0)$, where $\theta$ is half the divergence angle. Because of course $\theta < Pi/2$, we get that the smallest waist diameter of a collimated laserbeam is $w_0 < 2\lambda$.

Therefore, one is not able to collimate a laser to a single lattice site in order to remove a single particle. Even if this was possible with some tricky other method, like using a laser with a large wavelength to produce the lattice while creating the excitation with a small wavelength laser, one would not create a single hole in the system because the particle that is removed from its site will not leave the system: instead, it will jump to a neighboring site. With a laser, one can only create particle-hole excitations, and not a single hole-excitation. Therefore, it is possible to let a few particles on a number of neighboring sites jump to other sites, but really removing only one particle from the whole system remains a technological challenge, and this makes the observation of spin-charge separation in our system not yet feasible.

Conclusions

A possible experimental observation of the separation of the energy spectrum and eigenstates of our system was shown to be possible. However, to prove the characteristic 1D Luttinger liquid spin-charge separation, one will always have to create a single particle- or hole excitation to see the spin- and charge degrees of freedom of such an excitation separate. This poses a serious constraint because it means that access to a single lattice site is always necessary in order to create the
one-particle excitation, whatever proposal one makes for an experimental setup. Unfortunately, this single site access is not yet feasible so that the experimental verification of the Luttinger liquid spin-charge separation in our system thus has to be delayed.
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Part III

Appendices
Appendix A

Mapping of 1D Impenetrable Bosons to Spinless Fermions

The symmetry postulate of quantum mechanics tells us that the many-body wavefunction for a system of identical particles should be anti-symmetric (for fermions) or symmetric (for bosons) under permutations of the single-particle dynamical variables. It can be shown [5] that the eigenstates of a one-dimensional Hamiltonian describing a system of bosons with infinite repulsive delta function interaction can be obtained from a fermionic state which is a solution of the same Hamiltonian without the hard-core interactions. This will be considered here in a little bit more detail.

Consider a system of \( N \) bosons in a one-dimensional box of length \( L \) with open boundary conditions (hard walls at \( x = 0 \) and \( x = L \)). The Hamiltonian of this system can be given generally by:

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + V(x_1, x_2, \ldots, x_N, t). \tag{A.1}
\]

We will suppose that the bosons do not have any internal degrees of freedom, so that the position coordinates \( x_j \) describe all the degrees of freedom of the Bose gas. Furthermore, every realistic potential \( V \) will be symmetric under exchange of the coordinates. Now, the two-particle interaction potential is assumed to contain a hard-core. Instead of treating this interaction as an infinite contribution to \( V \), it will be taken care of by the following constraint on the wavefunction \( \Psi \):

\[
\Psi(x_1, x_2, \ldots, x_N, t) = 0 \quad \text{if} \quad x_i = x_j, \quad 1 \leq i < j \leq N. \tag{A.2}
\]

The potential \( V \) in equation (A.1) will then contain all other (finite) interactions and external potentials.
APPENDIX A. MAPPING OF BOSONS TO FERMIONS IN 1D

Assume that $\Psi_F$ is a fermionic solution to the time-dependent many-body Schrödinger equation

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}, \quad (A.3)$$

with the Hamiltonian from equation (A.1). As a result of the Pauli exclusion principle, $\Psi_F$ will automatically satisfy the condition (A.2). Next, one introduces an anti-symmetric function as follows:

$$A(x_1, x_2, \ldots, x_N) = \prod_{i<j} \text{sgn}(x_i - x_j), \quad (A.4)$$

where $\text{sgn}(x)$ is the algebraic sign of the coordinate difference $x = x_i - x_j$. Since both $A$ and the fermionic wavefunction $\Psi_F$ are anti-symmetric under permutation of the position coordinates, the product

$$\Psi_B = A(x_1, x_2, \ldots, x_N)\Psi_F(x_1, x_2, \ldots, x_N, t) \quad (A.5)$$

will be symmetric. Moreover, it is easy to see that $\Psi_B$ is a solution of the Schrödinger equation (A.3), and it satisfies the open boundary conditions and the hard-core constraint (A.2) because $\Psi_F$ does. So we have constructed a bosonic wavefunction for impenetrable bosons starting from a wavefunction for spinless fermions. This completes the mapping.

A few remarks are in place:

• It is clear that, since $A^2 = 1$, observables related to the density will be equal for the system of impenetrable bosons and the corresponding system for spinless fermions because they depend on the square of the wavefunction. Most observables measurable on a certain bosonic state however, will have different values than the ones measured on the corresponding fermionic state.

• The advantage of the mapping becomes very clear when the potential $V$ in equation (A.1) can be written as a sum of external potentials which act on a single particle (remember that this is possible because the hard-core interactions are not part of $V$ since they were included as a constraint on the many body wavefunction (A.2)):

$$V(x_1, \ldots, x_N, t) = \sum_i V(x_i, t). \quad (A.6)$$
Since now \( H = \sum_i H'(x_i, t) \), solving the time-dependent many-body Schrödinger equation (A.3) (TDMBSE) with the Hamiltonian (A.1) reduces to finding solutions to the one-body Schrödinger equation:

\[
H'(x, t)\psi(x, t) = \frac{i\hbar}{\partial t}\frac{\partial \psi(x, t)}{\partial t},
\]

with a constraint (A.2) on the many-body wavefunction. If one has found the one-body solutions, the many-body states for fermions will be Slater determinants of the one-body solutions which satisfy the condition (A.2) automatically. By making use of the mapping, one can then construct the solutions to the TDMBSE for impenetrable bosons. This, in general will be much easier than solving the Schrödinger equation (A.3) with the constraint (A.2) for bosons directly.

- If the potential \( V \) is independent of the time \( t \), solving the TDMBSE is reduced to finding many-body eigenstates of the Hamiltonian (A.1). If \( \psi_F \) is a fermionic eigenstate, then \( \psi_B = A\psi_F \) will be a bosonic eigenstate with the same energy. So the system of impenetrable bosons and the corresponding system of spinless fermions will have the same spectrum.

- In the preceding discussion, open boundary conditions were assumed. The situation becomes a little bit more complicated for periodic boundary conditions. First of all, the factor \( A \) has to be defined "modulo \( L \)"

\[
A(x_1, \ldots, x_i + L, \ldots, x_N) = A(x_1, \ldots, x_i, \ldots, x_N) \quad \forall i \in [1, N].
\]

(A.8)

Suppose now that one starts with periodic boundary conditions for the fermi-wavefunction: \( \Psi_F(x_1, \ldots, x_{N-1}, L) = \Psi_F(0, x_1, \ldots, x_{N-1}) \). To make things clearer, it is assumed in the following that

\[
0 < x_1 < x_2 < \ldots < x_N < L
\]

(A.9)

so that \( A(x_1, \ldots, x_{N-1}, L) = (-1)^{N-1} \) and \( A(0, x_1, \ldots, x_{N-1}) = 1 \). Now, the wavefunction for hard-core bosons can be constructed following equation (A.5):

\[
\Psi_B(x_1, \ldots, x_{N-1}, L) = A(x_1, \ldots, x_{N-1}, L)\Psi_F(x_1, \ldots, x_{N-1}, L)
\]

\[
= (-1)^{N-1}\Psi_F(0, x_1, \ldots, x_{N-1})
\]

\[
= (-1)^{N-1}\Psi_B(0, x_1, \ldots, x_{N-1}).
\]

(A.10)
So depending on the number of particles $N$ in the system, one ends up with periodic (for $N$ odd) or anti-periodic (for $N$ even) boundary conditions for the wavefunction for impenetrable bosons. If we want the solution for an even number of hard-core bosons with periodic boundary conditions, it can be seen by the line of reasoning mentioned above (Eq. (A.10)) that we need anti-periodic boundaries for the fermions we map on. Or otherwise stated, the system of $N$ impenetrable bosons with periodic boundary conditions can be mapped to the corresponding system of spinless fermions with periodic boundaries if $N$ is odd, and with anti-periodic boundaries if $N$ is even.
Appendix B

Description of a Perturbation with an Effective Hamiltonian

For many systems, the eigenstates of the Hamiltonian $H$ cannot be exactly determined. In such a case, a perturbative method can give some information about the system. In this appendix, the case of a Hamiltonian $H$ having energy levels $E_{\alpha}$ grouped into manifolds $\varepsilon_\alpha, \varepsilon_\beta, \ldots$ which are well separated in energy from each other is considered. The Bose Hubbard model in the strongly interacting limit with incommensurate filling clearly satisfies this criterion (Fig. B.1). It will be shown that in this case the low-energy dynamics of the system can be correctly described by an effective Hamiltonian acting only in the lowest manifold.

The operator $\mathbb{P}$ is defined as the projector over the lowest manifold. The operator $\mathbb{Q}$ projects out of this manifold, so $\mathbb{P} + \mathbb{Q} = 1$. For projection operators we also have $\mathbb{P}^2 = \mathbb{P}$, and $\mathbb{Q}^2 = \mathbb{Q}$. The exact eigenstates and energies of the Hamiltonian under consideration have to be calculated from the time-independent Schrödinger equation:

$$H\psi = E\psi. \quad (B.1)$$

Letting the projection operator $\mathbb{P}$ act on both sides of this equation, and including the identity operator $\mathbb{P} + \mathbb{Q}$ between $H$ and $\psi$ gives:

$$\mathbb{P}H(\mathbb{P} + \mathbb{Q})\psi = E\mathbb{P}\psi. \quad (B.2)$$

By projecting with the operator $\mathbb{Q}$, we get analogously:

$$\mathbb{Q}H(\mathbb{P} + \mathbb{Q})\psi = E\mathbb{Q}\psi. \quad (B.3)$$

This last equation can be written as:

$$\mathbb{Q}\psi = (-1)(\mathbb{Q}H\mathbb{Q} - E)^{-1}\mathbb{Q}H\mathbb{P}\psi. \quad (B.4)$$
Figure B.1: For the Bose-Hubbard model with incommensurate filling and without the tunnelling term $J = 0$, the energy spectrum consists of degenerate levels separated by energies of the order of $U$. Including a small tunnelling term as a perturbation, the degeneracy will be lifted, but the energy levels are still clustered into manifolds which are well separated in energy.
Putting equation (B.4) into (B.2), one gets:

\[(PHP - PHQ(QHQ - E)^{-1} QHP)P\psi = EPP\psi.\]  \hfill (B.5)

By making a power expansion of \((QHQ - E)^{-1}\), one obtains an effective Schrödinger equation for \(P\psi\); to first order for instance, one can put \((QHQ - E)^{-1}\) equal to \(1/U\), where \(U\) is the energy splitting between the two lowest manifolds (see Fig. B.1). One then obtains:

\[\left(\frac{1}{U}PHQHP + O\left(\frac{1}{U^2}\right)\right)P\psi = H_{\text{eff}}P\psi = EPP\psi.\]  \hfill (B.6)

This indeed is an effective Schrödinger equation for the wavefunction \(\psi\) projected onto the lowest manifold. If one would sum all orders, this equation would exactly describe the low-energy dynamics of the system; the first term describes the physics within the lowest manifold while the terms of order \(1/U\) and higher describe the coupling with the higher manifolds.

So we have found an effective Hamiltonian which:

- is Hermitian,
- has only nonzero matrix elements between two states in the lowest manifold
- and has the same eigenvalues and eigenstates as the Hamiltonian \(H\) in the lowest manifold.

This completes the derivation.
Appendix C

Proof of equation (6.13)

In order to prove Eq. (6.13), we show that the terms $\langle \phi | \hat{H}^{(i)}(m) | \phi \rangle$ in Eq. (6.12) are independent of $i$.

The state $|\phi\rangle$ was written as a Slater determinant:

$$|\phi\rangle \sim \sum_{x_1 < x_2 < \ldots < x_N} \det \begin{pmatrix} e^{ik^{(1)}_1 x_1} & e^{ik^{(2)}_1 x_1} & \cdots & e^{ik^{(N)}_1 x_1} \\ e^{ik^{(1)}_2 x_2} & e^{ik^{(2)}_2 x_2} & \cdots & e^{ik^{(N)}_2 x_2} \\ \vdots & \vdots & \ddots & \vdots \\ e^{ik^{(1)}_N x_N} & e^{ik^{(2)}_N x_N} & \cdots & e^{ik^{(N)}_N x_N} \end{pmatrix} |x_1, x_2, \ldots, x_N\rangle,$$

(C.1)

where the $k^{(i)}$ have the form:

$$k^{(i)} \in \left\{ \frac{2\pi}{M} n : n \in \{0, \ldots, M-1\} \right\}.$$

(C.2)

$M$ was the number of available sites, and $N$ the number of particles in the system.

The operator $\hat{H}^{(i)}(m)$ was defined as:

$$\hat{H}^{(i)}(m) = 2|m+1\rangle_{i+1} \langle m|_i (m+1\rangle_i (m+1\rangle_{i+1} (H - |m+2\rangle_{i+2} \langle m+2|)$$

$$+ |m\rangle_{i+1} \langle m-1|_i (m+1\rangle_i (m+1\rangle_{i+1} (H - |m-1\rangle_{i+1} \langle m-1|).$$

(C.3)

We will only show the independence of $i$ for the first term of this operator. The other ones can be calculated by using the same techniques derived below.

Making use of the expression of $|\phi\rangle$ in terms of a Slater determinant (Eq. (C.1)), we find, for any given $i$:

$$\langle \phi | |m+1\rangle_{i+1} \langle m_i (m+1\rangle_{i+1} | \phi \rangle = \sum_{x_1 < \ldots < x_{i-1} < x_{i+2} < \ldots < x_N} \text{mod}(\det A)^2,$$

(C.4)
APPENDIX C. PROOF OF EQUATION (6.13)

where mod is the modulus function. The determinant \( \text{det}(A) \) is given by:

\[
\text{det}(A) = \begin{vmatrix}
\ e^{i k^{(1)} x_1} & e^{i k^{(2)} x_1} & \ldots & e^{i k^{(N)} x_1} \\
\vdots & \vdots & \ddots & \vdots \\
\ e^{i k^{(1)} x_{i-1}} & e^{i k^{(2)} x_{i-1}} & \ldots & e^{i k^{(N)} x_{i-1}} \\
\ e^{i k^{(1)} m} & e^{i k^{(2)} m} & \ldots & e^{i k^{(N)} m} \\
\ e^{i k^{(1)} x_{i+2}} & e^{i k^{(2)} x_{i+2}} & \ldots & e^{i k^{(N)} x_{i+2}} \\
\vdots & \vdots & \ddots & \vdots \\
\ e^{i k^{(1)} x_N} & e^{i k^{(2)} x_N} & \ldots & e^{i k^{(N)} x_N} \\
\end{vmatrix}. \tag{C.5}
\]

Now, we can multiply column \( j \) with \( e^{-i k^{(j)} m} \). Doing this for all columns, we obtain:

\[
\text{det}(A) = \alpha \begin{vmatrix}
\ e^{i k^{(1)} (x_1 - m)} & e^{i k^{(2)} (x_1 - m)} & \ldots & e^{i k^{(N)} (x_1 - m)} \\
\vdots & \vdots & \ddots & \vdots \\
\ e^{i k^{(1)} (x_{i-1} - m)} & e^{i k^{(2)} (x_{i-1} - m)} & \ldots & e^{i k^{(N)} (x_{i-1} - m)} \\
\ 1 & 1 & \ldots & 1 \\
\ e^{i k^{(1)} (x_{i+2} - m)} & e^{i k^{(2)} (x_{i+2} - m)} & \ldots & e^{i k^{(N)} (x_{i+2} - m)} \\
\vdots & \vdots & \ddots & \vdots \\
\ e^{i k^{(1)} (x_N - m)} & e^{i k^{(2)} (x_N - m)} & \ldots & e^{i k^{(N)} (x_N - m)} \\
\end{vmatrix}. \tag{C.6}
\]

The prefactor \( \alpha \) is equal to \( e^{i (k^{(1)} + k^{(2)} + \ldots + k^{(N)}) m} \). Since we have to consider the modulus of the determinant, we can forget about this prefactor.

Now, we introduce the distances \( y_i \) as follows (see also Fig. C.1):

\[
\begin{align*}
y_1 & = x_{i+2} - m, \\
y_2 & = x_{i+3} - m, \\
\vdots & \\
y_{N-i-1} & = x_N - m, \\
y_{N-i} & = M + (x_1 - m), \\
y_{N-i+1} & = M + (x_2 - m), \\
\vdots & \\
y_{N-2} & = M + (x_{i-1} - m).
\end{align*}
\]

Since we sum over \( x_1 < x_2 < \ldots < x_N \), these distances are all positive. Chang-
Figure C.1: Change of variables from $x_i$ to $y_j$.

ing the summation variables $x_i$ to the corresponding $y_j$, noticing that $e^{i k_j M} = 1$ because of periodic boundaries (Eq. C.2), we obtain finally:

$$
\langle \phi | m+1 \rangle_{i+1} | m \rangle_i \langle m | m+1 \rangle_{i+1} | \phi \rangle = 
\sum_{y_1 < y_2 < \ldots < y_{N-2}} \text{mod} \left( \begin{array}{cccc}
1 & e^{i k_1 y_{N-2}} & \ldots & e^{i k_N y_{N-2}} \\
e^{i k_1 y_{N-3}} & 1 & \ldots & e^{i k_N y_{N-3}} \\
e^{i k_1 y_{N-4}} & e^{i k_2 y_{N-4}} & \ldots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
e^{i k_1 y_{N-2}} & e^{i k_2 y_{N-2}} & \ldots & e^{i k_N y_{N-2}} 
\end{array} \right)^2 .
$$

(C.7)

Now, this result is indeed independent of the value of $i$ we have chosen in the beginning. If we take another value $i$, the only difference is that the order of the rows in the determinant is changed. But, by rearranging the rows, we can bring the determinant always in the form above. The value of the determinant will not change by doing these elementary row-operations, except maybe for a minus sign that we pick up. However, this minus sign is not important because only the square of the determinant appears in the expression above. This completes the proof.
Bibliography


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