Impurity dynamics and nearest-neighbor interactions in one-dimensional lattices

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Abstract
An impurity coupled to a bath is a paradigmatic problem of many-body physics and relevant for various systems. In this work, we study the dynamics due to impurities in one-dimensional lattice systems using the numerical time-evolving block decimation method and analytic calculations. We consider both noninteracting and interacting fermions as the bath, in particular fermions in a singlet superfluid state due to attractive on-site interactions, and baths with a periodic or nearly periodic structure due to nearest-neighbor repulsion. Previous theoretical and experimental research mainly considers homogeneous baths with contact interactions.

We find novel phenomena when the bath is probed with energies above its characteristic energy scale. In publication I, a driven perturbation with velocity above the speed of sound of the interacting fermions retains the ground-state power-law decay of singlet superfluid correlations. In publication III, we study the decoherence of an impurity in terms of the purity of its density matrix. The impurity and the bath fermions have different masses, and we find the fastest decoherence for a light impurity in a heavy bath, whereas the fastest dissipation of energy occurs for equal masses.

In publications II and IV, we consider a bath of fermions with repulsive nearest-neighbor interactions. In a half-filled lattice, the bath is in the Mott insulator state with a particle every two sites. A filling above one half leads to solitons seen as domain walls in the arrangement of the particles. We find that within a resonance region of interactions, the impurity can create an additional soliton-antisoliton pair in the bath. These two excitations have very different dynamics: The antisoliton can form a bound state with the impurity while the soliton excitation propagates. When the ground state of the bath contains solitons, the antisoliton excitation is confined close to its origin. These phenomena are explained by energy conservation, since processes with an energy change larger than the bandwidth are suppressed.

Recent developments in experiments with ultracold gases in optical lattices offer possibilities for testing the theoretical predictions of this work. Long-range interactions in lattice models have been observed in experiments with magnetic atoms and dipolar molecules. Furthermore, single-site addressing techniques allow to create localized impurities and track their motion, and to measure the purity of many-body states.

Keywords Impurity dynamics, domain walls, time-evolving block decimation, extended Hubbard model, decoherence, superfluid correlations

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Tämän työn teoreettiset ennusteet on mahdollista testata kokeissa, joissa ultrakylmiä kasuaja vangitaan optiisiin hiloihin. Kokeissä voidaan toteuttaa hilaistemojia, joissa vierekkäisillä hilapaikoilla olevat hiukkaset vuorovaikuttavat dipoli-dipolivuorovaikutuksella. Lisäksi on mahdollista luoda epäpuhtauksia ja häiriöitä sekä mitata hiukkasten liike yhden hilapaikan tarkkuudella. Myös monen hiukkasin kvanttitilan puhtaus voidaan mitata.

Avainsanat monet kappaleen kvanttysiikka, laajennettu Hubbardin malli, dekoherenssi, supranestekorrelaatiot

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Geneva, March 28, 2017,

Anne-Maria Visuri
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List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.


Author’s Contribution

Publication I: “Moving perturbation in a one-dimensional Fermi gas”

The author did the numerical simulations, participated in the physical interpretation of the results, and was the main writer of the manuscript.

Publication II: “Excitations and impurity dynamics in a fermionic Mott insulator with nearest-neighbor interactions”

The author implemented nearest-neighbor interactions in the numerical algorithm, did the simulations, and participated in the theoretical analysis. The author was the main writer of the manuscript.

Publication III: “Decoherence of an impurity in a one-dimensional fermionic bath with mass imbalance”

The author did the numerical simulations, contributed to the theoretical analysis, and wrote the largest part of the manuscript.

Publication IV: “Impurity and soliton dynamics in a Fermi gas with nearest-neighbor interactions”

The author did the numerical simulations and the analytic calculations and contributed strongly to the physical interpretation. The author was the main writer of the manuscript.
Author’s Contribution
1. Introduction

The field of condensed matter physics describes phases of solid-state materials and fluids where interactions between the particles play an important role. In solids, phenomena such as magnetic ordering and superconductivity arise from the interactions between electrons in a lattice formed by positive ions. The simplest extension to a noninteracting tight-binding model, the Hubbard model [1–3], contains terms for the tunneling of electrons between lattice sites and the interaction of opposite-spin electrons on the same site, and is able to describe these phenomena. Despite its simplicity, an analytic solution of the Hubbard model is only available in one dimension [4, 5], and solving it numerically in higher dimensions is a formidable challenge for current computers.

The Hubbard model was first proposed as an approximate description of electrons in solids but analogous physical systems, which are almost exactly described by the Hubbard model, can be created with ultracold atomic gases in optical lattices [6–8]. In other words, models such as the Hubbard model can be experimentally realized with ultracold atoms. These systems offer new possibilities for simulating strongly-correlated phases of condensed matter, thus operating as quantum simulators [9] – highly controllable quantum systems with tunable parameters which can be used to simulate the dynamics of a complex quantum system. The lattice defects and vibrations in solid materials, which are not taken into account by the Hubbard model, are actually not present in quantum gas experiments. Besides simulating existing physical systems, the tunability of geometries and interactions allows to create many-body states that are not found in nature.

After its introduction, the Hubbard model has been generalized and ex-
tended, for example to bosons and to longer-range interactions. Both the
bosonic and fermionic Hubbard model have been realized in experiments
with ultracold gases, and strongly-correlated phenomena predicted by the
models, such as the superfluid-Mott insulator transition, have been ob-
served [10–17]. Long-range interactions, which are of interest in this
thesis, can be realized with dipolar atoms and molecules [18–27]. Time-
dependent measurements are also possible. In particular, current single-
site imaging techniques allow to track the motion of particles at the reso-
lution of a single lattice site [28–30].

In this thesis, we study dynamical phenomena which occur when fermions
in a lattice are probed with energies above their bandwidth. A finite band-
width imposes an upper bound on energy, and phenomena resulting from
this upper bound in the absence of dissipation, such as repulsively bound
pairs [31] and negative temperatures [32], have been observed in quan-
tum gas experiments. In Publication I of this thesis, we simulate an at-
tractively interacting Fermi gas in a one-dimensional lattice, perturbed
by wave-packet potentials moving with different velocities. Publications
II-IV consider an impurity particle in a bath of fermions with varying
masses and interactions. The motion of impurities of a different spin state
or atom species has also been studied experimentally [33–35].

In the following, we first present the different lattice models studied
in this thesis. These models and their realization with ultracold gases
in optical lattices are discussed in Chapter 2. Chapter 3 introduces the
Tomonaga-Luttinger liquid theory, the low-energy effective theory of gap-
less quantum systems in one dimension. In Chapter 4, we discuss the
impurity and soliton dynamics studied in Publications II and IV. Publica-
tion III studies the decoherence of an impurity as a function of time, and
we present the related concepts and results in Chapter 5. Finally, the nu-
merical time-evolving block decimation method is reviewed in Chapter 6,
and Chapter 7 presents a brief conclusion of the work.
2. Lattice models for fermions

In this chapter, we review the topic of ultracold gases in optical lattices, which is relevant for the experimental realization of the models studied in this thesis. We derive the extended Hubbard Hamiltonian from a general second-quantized many-body Hamiltonian and present a simplified model for the limit of strong nearest-neighbor repulsion. The simplified model is used in Publication IV for studying domain walls in the arrangement of spinless fermions with nearest-neighbor interactions in a one-dimensional lattice.

2.1 Ultracold quantum gases

In quantum mechanics, particles do not have definite trajectories as in classical mechanics but there is an uncertainty to the particles’ coordinates. Mathematically, a particle is described by a wavefunction, connected to a probability distribution in the coordinate space. As hypothesized by de Broglie, particles have also the characteristics of waves, and can for instance interfere. Such quantum effects are observable at small length scales, more specifically, when the distance between the particles is of the same order of magnitude as the wavelength associated with their wave character, called the de Broglie wavelength. The criterion for observing quantum effects in a gas of atoms is that the average distance between the particles is approximately equal to or smaller than the thermal de Broglie wavelength,

\[ n^{-1/3} \leq \lambda_T. \]  

(2.1)
Here, $n$ is the number density of the gas and

$$\lambda_T = \frac{\hbar}{\sqrt{2\pi m k_B T}}, \quad (2.2)$$

where $\hbar$ is the reduced Planck’s constant $\hbar = \frac{h}{2\pi}$, $m$ is the mass of the particles, $k_B$ is the Boltzmann coefficient, and $T$ is the temperature.

Which conditions are required to satisfy this criterion? The particle density of air at room temperature and atmospheric pressure is around $2.5 \cdot 10^{25} \text{ m}^{-3}$, and keeping other parameters fixed, satisfying (2.1) would require a temperature in the range of millikelvins. At such a low temperature, however, air would normally be already in solid form. To maintain the particles in a metastable gaseous phase, much smaller densities are required. For the bosonic atom $^{87}\text{Rb}$, densities are typically $n \approx 10^{-19} \text{ m}^{-3}$, giving an interparticle distance of a few hundred nanometers and a temperature of hundreds of nanokelvins for eq. (2.1) to be valid. Cooling a gas down such remarkably low temperatures requires specialized techniques such as laser cooling and evaporative cooling [36–38].

At room temperature, the possible momenta of gas particles are distributed according to the classical Maxwell-Boltzmann distribution. A gas in the quantum regime, in contrast, follows quantum statistics. The distribution of momenta (or energies) is connected to the intrinsic angular momentum of the particles, called spin. Particles with integer spin follow Bose-Einstein statistics, and are therefore called bosons, while particles with half-integer spin follow Fermi-Dirac statistics and are called fermions. Atoms and molecules are composite particles consisting of elementary fermions, namely, a bosonic atom or molecule consists of an even number of fermions and a composite fermion of an odd number of fermions. For such composites, Bose-Einstein or Fermi-Dirac statistics are in principle approximations [39]. When the size of the composite particle is much smaller than the interparticle distance, the approximation is however very accurate. This is the case in quantum gas experiments. Although the internal structure of the particles is not important for their collective behavior, it can be utilized in experiments for manipulating the atoms, for example for confining them to optical lattices or realizing different (pseudo)spin states.

The Bose-Einstein distribution leads to the prediction of a new phase of matter at a sufficiently low temperature, the Bose-Einstein condensate.
Lattice models for fermions

(BEC). In this phase, a macroscopic number of bosons occupies the lowest-energy state. A BEC of ultracold atoms was first realized in 1995 [40–42]. Furthermore, when bosons are weakly interacting, they can transition to a superfluid state, which has the property of flowing without friction. The superfluid state is analogous to the superconducting state of solid materials, where electric current flows without resistance. Superconductivity and superfluidity of fermionic atoms occur via a different mechanism than bosonic superfluidity since fermions are not able to occupy the same quantum state. In the simplest case, superconductivity and fermionic superfluidity are explained by the Bardeen-Cooper-Schrieffer theory [43], where fermions with an effectively attractive interaction form Cooper pairs which condense.

Whereas the transition from a classical gas to a condensate or a superfluid occurs at a critical temperature due to the suppression of thermal excitations, quantum phase transitions occur at zero temperature as a result of the competition of different energy terms. A well-known example is the superfluid-Mott insulator transition in a lattice system, where the kinetic and interaction energies compete. The critical temperature for the superfluid phase is of the order of the tunneling energy, and a Mott insulator phase can be observed when the temperature is below the energy gap for excitations. The superfluid-Mott insulator transition has been observed in several experiments [10–17]. Many strongly correlated phases, such as the antiferromagnetic phase, require large interactions $U$ compared to the tunneling amplitude $J$. This makes the realization of the antiferromagnetic phase challenging since a temperature close to or smaller than the antiferromagnetic coupling $k_B T \approx \frac{J^2}{|U|}$, around 10-20 nK [7], is required. The experiments are progressing towards lower temperatures, and recently, short-range [44–48] and longer-range [49] antiferromagnetic correlations and string correlations [50] were observed. For a few strongly repulsive atoms, an antiferromagnetic Heisenberg spin chain has also been realized without a lattice [51].

In some cases, the effects of thermal excitations can be accounted for by post-selection techniques [35]. In the simulations done in this work, the temperature is zero. Although ultracold gases are discussed here from the point of view of condensed matter research and the interest is in the many-body perspective of their quantum properties, their application in
the field of quantum information has also been proposed [7, 52–55].

2.2 Optical lattices

Optical lattices created with lasers are the basis for simulating solid-state-like physics with neutral atoms and molecules. The laser frequency is tuned away from transition energies, so that the atoms are not excited but instead feel a potential caused by the electric field. The AC electric field induces an oscillating dipole moment into the atom, and this dipole moment interacts with the electric field. The shift of energy levels due to the interaction is called the Stark effect. Since the oscillation of the electric field is fast, one can consider classically the time-average of the electric field \( E(r) = E_0(r) \hat{e} \), where \( E_0 \) is the amplitude and \( \hat{e} \) the unit vector in the direction of the field. One of the transitions of the atom is usually much closer to the frequency of the laser than others, and therefore the atom can be approximated as a two-level system. This approximation is particularly good for alkali atoms with only one valence electron. The shift of the ground state energy, \( V_L = -d \cdot E \), can be written as [56]

\[
V_L(r) = \frac{|d|^2}{2\hbar(\omega - \omega_0)} I(r),
\]

where \( |g\rangle \) is the ground state and \( |e\rangle \) the excited state of the atom, and \( d = \langle e | d \cdot \hat{e} | g \rangle \) the matrix element of the dipole operator in the direction of the electric field. The laser frequency is denoted by \( \omega \) and the transition frequency between \( |g\rangle \) and \( |e\rangle \) by \( \omega_0 = \frac{E_e - E_g}{\hbar} \). The intensity \( I(r) \) is proportional to the square of the time-average of the electric field, \( I(r) = \frac{1}{2} E^2(r) \). Changing the detuning \( \omega - \omega_0 \) from positive to negative changes the potential from repulsive to attractive, so that the potential minima are either at minima or maxima of the intensity, respectively.

The AC Stark effect is often used in experiments for confining the gas cloud to a harmonic potential created by dipole traps or by the focus of the lattice beams [8]. Such a harmonic potential has an effect on the density distribution of the gas cloud, and is often considered theoretically by a local density approximation where the potential is taken into account as a spatially varying chemical potential. Recently, box traps have also been realized [57–60].

Different types of potentials can be generated by interfering multiple
laser beams, which leads to an interference pattern of intensity. In particular, two counter-propagating beams (or one retroreflected beam) in the $x$ direction produce a standing wave of the form $I_L(x) = I_0 \sin^2(k_L x)$, where $k_L$ is the wave number. The atoms thus experience a periodic potential

$$V_L(x) = V_0 \sin^2(k_L x),$$

where $V_0 = \frac{|d|^2}{2 \hbar (\omega - \omega_0)} I_0$. The wavelength of the standing wave is $\lambda_L = \frac{2\pi}{k_L}$ and the period $\frac{\lambda}{2}$ is the lattice spacing of the optical lattice. Lattice spacings in experiments are typically between 100 nm and 5 $\mu$m [8]. The lattice depth $V_0$ can be tuned by the intensity. It is usually expressed in units of the recoil energy $E_R = \frac{\hbar^2 k_L}{2m}$, where $m$ is the mass of the atoms.

The atoms or molecules in periodic potentials can be thought to simulate electrons in the solid-state ionic crystal.

With two counter-propagating beams in the $x$ direction, the potential is periodic in the $x$ direction and nearly uniform in the $y$ and $z$ directions. Three pairs of counter-propagating beams with orthogonal alignment can be used to create a cubic lattice. Tuning the intensities in different directions allows to create other structures. Arrays of quasi-one-dimensional lattices can be created by making the lattice depth in the transverse directions much larger than in the longitudinal direction. A very deep sinusoidal potential in the transverse direction can be approximated around the minima by a harmonic potential: In cylindrical coordinates, $V_\perp \sin^2(k_L r) \approx V_\perp k_L^2 r^2 = \frac{1}{2} m \omega_\perp^2 r^2$, where $r$ is the distance from the minimum in the radial direction. When the kinetic and interaction energies and the temperature are much below the energy level spacing $\hbar \omega_\perp = 2\sqrt{E_R V_\perp}$, the atoms are confined to the lowest-energy state in the transverse direction and only move along the longitudinal direction. Note that the energy level spacing can be adjusted by the lattice depth. More complex geometries have also been realized [61, 62].

### 2.3 Extended Hubbard model

In this section, we present the derivation of the extended Hubbard model and discuss the experimental control of the parameters.
2.3.1 Continuum Hamiltonian

The (extended) Hubbard model studied in this work can be derived from the second-quantized Hamiltonian

$$H = H_{\text{kin}} + H_{\text{SR}} + H_{\text{LR}},$$

where

$$H_{\text{kin}} = \sum_{\sigma} \int dx \psi_\sigma^\dagger(x) \left[ -\frac{\hbar^2}{2m_\sigma} \nabla^2 + V_L(x) \right] \psi_\sigma(x)$$  \hspace{1em} (2.4)

denotes the kinetic term and the lattice potential,

$$H_{\text{SR}} = g \int dx \psi_\uparrow^\dagger(x) \psi_\uparrow^\dagger(x) \psi_\downarrow(x) \psi_\downarrow(x)$$  \hspace{1em} (2.5)

the short-range (contact) interaction, and

$$H_{\text{LR}} = \frac{1}{2} \sum_{\sigma,\sigma'} \int dx \int dx' V_{\sigma,\sigma'}(x-x') \psi_\sigma^\dagger(x) \psi_{\sigma'}^\dagger(x') \psi_{\sigma'}(x') \psi_\sigma(x)$$  \hspace{1em} (2.6)

the long-range interaction between fermions at positions $x$ and $x'$. We consider a two-component Fermi gas, where the different components are denoted by the spin states $\sigma = \uparrow, \downarrow$. The fermionic field operator $\psi_\sigma(x)$ annihilates a fermion with spin $\sigma$ at position $x$. We discuss here the one-dimensional case, and generalization to higher dimensions is straightforward. The field operators have the anticommutation relations

$$\{\psi_\sigma(x), \psi_{\sigma'}(x')\} = 0,$$

$$\{\psi_\sigma(x), \psi_\sigma^\dagger(x')\} = \delta(x-x')\delta_{\sigma,\sigma'},$$

where $\{A, B\} = AB + BA$. Anticommutation leads to the Pauli exclusion principle, which states that more than one fermion cannot occupy the same quantum state. Therefore, there is no contact interaction between fermions of the same spin.

The interaction $H_{\text{SR}}$ is due to s-wave scattering and is described by a contact potential with the coupling constant $g = \frac{\hbar^2 a_s}{m_r}$, where $a_s$ is the s-wave scattering length and $m_r$ is twice the reduced mass $m_r = \frac{2m_\uparrow m_\downarrow}{m_\uparrow + m_\downarrow}$.

With a magnetic field, the scattering length can be controlled via Feshbach resonances in the two-body scattering [63, 64]. While atoms with short-range van der Waals interactions are used in the majority of quantum gas experiments, in recent years, progress has been made in cooling atoms and molecules with long-range dipole-dipole interactions [65–70]. In particular, long-range terms in lattice models have been realized with polar KRb molecules [21, 23], Rydberg atoms [24, 26], and magnetic atoms [22, 25].
2.3.2 Kinetic term

Let us consider first the kinetic term and the lattice potential. The periodic potential leads to energy bands and gaps. The eigenstates of Hamiltonian (2.4) are the Bloch states \( \phi_k(x) = e^{ikx}u_k(x) \), where \( u_k(x) \) is a periodic function with the period of the lattice spacing \( a \), \( u_k(x + a) = u_k(x) \), and \( k \) is the quasimomentum. In the following, we set \( a = 1 \). When the energy gap between the lowest and next-lowest bands is larger than other energy scales in the system, we can consider only the lowest band.

Instead of the Bloch basis, it is convenient to use the Wannier functions \( w_j(x) = \frac{1}{\sqrt{L}} \sum_k e^{-ikj} \phi_k(x) \) as a basis. These functions are localized around the lattice sites \( j \). The field operators can be written as

\[
\psi_\sigma(x) = \sum_{j=1}^{L} w_j(x)c_{j\sigma},
\]

\[
\psi_\sigma^\dagger(x) = \sum_{j=1}^{L} w^*_j(x)c_{j\sigma}^\dagger,
\]

where \( c_{j\sigma} \) is the fermionic annihilation operator at site \( j \). Substituting eq. (2.7) into eq. (2.4), one arrives at the discrete lattice Hamiltonian

\[
H = -\sum_\sigma\sum_{\langle i,j \rangle} J_\sigma c_{i\sigma}^\dagger c_{j\sigma},
\]

where

\[
J_\sigma = J_{i\sigma} = \int dx u^*_i(x)\left[ \frac{\hbar^2}{2m_\sigma} \nabla^2 + V_L(x) \right] w_j(x)
\]

is the tunneling amplitude and \( \langle i, j \rangle \) denotes neighboring lattice sites. We have left out the term \( J_{ii} \), which for a fixed particle number amounts to a constant shift in energy. For deep lattices, tunneling beyond the neighboring lattice site can be neglected. When the lattice potential is homogeneous and isotropic, \( J \) does not depend on position. In general, position- and spin-dependent tunneling amplitudes are possible. In Publication III, we consider spin-dependent tunneling amplitudes, which according to eq. (2.9) correspond to a mass imbalance between the fermions with different spin. Different lattice potentials can also be used to make the tunneling energy spin-dependent. For a deep lattice, an approximate analytic form can be obtained as \( J \approx \frac{\sqrt{g}}{\sqrt{\pi}} \left( \frac{V_0}{E_R} \right)^{3/4} e^{-\sqrt{4V_0/E_R}} \) [8] and it shows that increasing the lattice depth suppresses tunneling. The lattice depth can thus be used for controlling the relative magnitudes of kinetic and interaction energies.
2.3.3 Single-particle energy spectrum

The dispersion relation of Hamiltonian (2.8) can be obtained by transforming the operators $c_j$ into momentum basis,

$$c_j = \sum_k \phi^j_k c_k,$$

where the Hamiltonian is diagonal. Momentum is equal to $\hbar k$, where $k$ is the wave number, and we set $\hbar = 1$ in the following. For periodic boundary conditions, the basis functions are plane waves $\phi^j_k = \frac{1}{\sqrt{L}} e^{ikj}$, whereas for a box of finite size, corresponding to open boundary conditions, the basis functions are

$$\phi^j_k = \sqrt{\frac{2}{L}} \sin(kj).$$

The dispersion relation is obtained by substituting eq. (2.10) into the Hamiltonian (2.8),

$$H = -J \sum_{j=1}^{L-1} \left( \sum_k \phi^{j+1}_k c_k^\dagger \sum_q \phi^j_q c_q + H. c. \right),$$

where the summation over spin has been omitted. One obtains

$$H = \sum_k \epsilon_k c_k^\dagger c_k,$$

where

$$\epsilon_k = -2J \cos(k)$$

is the single-particle dispersion relation. The dispersion relation is the same in the sine basis as in the plane wave basis, which can be shown as follows. The first term of eq. (2.12) is

$$\sum_{j=1}^{L-1} \sum_k \phi^{j+1}_k c_k^\dagger \sum_q \phi^j_q c_q$$

$$= - \sum_{k,q} \left[ \cos(k)(\delta_{k,-q} - \delta_{k,q}) + 2 \sin(qL) \sin(k(L+1)) \right] c_k^\dagger c_q,$$

where the $\delta_{k,-q}$ terms are zero since the momentum has been chosen to have positive values. The sine terms due to the boundary conditions also vanish since $\sin(qL) = \sin(\frac{\pi}{L} L) = 0$. Adding the Hermitian conjugate, one arrives at eqs. (2.13) and (2.14). The bandwidth is thus $4J$.

The group velocity is defined as $v_g(k) = \left| \frac{\partial \epsilon_k}{\partial k} \right|$, which for eq. (2.14) gives $v_g(k) = 2J |\sin(k)|$. The speed of sound in a noninteracting Fermi gas is
equal to the group velocity at the Fermi momentum $v_g(k_F)$. When the particles interact, the dispersion relation and the speed of sound are modified. In particular, when the one-dimensional system is in a gapless regime, the speed of sound corresponds to the velocity of the collective excitations of a Luttinger liquid, as discussed in Chapter 3.

### 2.3.4 Interaction terms

In the Wannier basis of eq. (2.7), the interaction term in eq. (2.6) can be written as

$$H_{SR} = U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (2.15)$$

where $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ is the particle number operator and

$$U_{ijim} = g \int dx w_i^\dagger(x) w_j^\dagger(x) w_l(x) w_m(x). \quad (2.16)$$

A larger lattice depth makes the Wannier functions more localized, which leads to a larger overlap of functions localized around the same site. For a sufficiently deep lattice, only the on-site term $U = U_{iii}$ is relevant.

Similarly to eq. (2.16), the long-range term $H_{LR}$ becomes

$$H_{LR} = \sum_{\sigma,\sigma'} \sum_j \sum_{\delta \geq 1} V_{\delta,\sigma\sigma'} n_{j\sigma} n_{j+\delta\sigma'}, \quad (2.17)$$

where

$$V_{\delta\sigma\sigma'} = \int dx \int dx' V_{\sigma\sigma'}(x-x') |w_j(x)|^2 |w_{i+\delta}(x')|^2 \quad (2.18)$$

and $\delta$ is the range of the interaction. When only the nearest-neighbor terms with $\delta = 1$ are taken into account, the extended Hubbard model is written as

$$H = -\sum_\sigma \sum_{\langle i,j \rangle} J_\sigma c_{i\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{\sigma,\sigma'} \sum_j V_{\sigma\sigma'} n_{j\sigma} n_{j+1\sigma'}. \quad (2.19)$$

In Publications II and IV, we consider nearest-neighbor interactions among only one of the spin species, so that $V_{\uparrow\uparrow} > 0$ and $V_{\uparrow\downarrow} = V_{\downarrow\downarrow} = 0$. In particular, we consider a large spin imbalance with a varying number of fermions with spin up and only one spin-down impurity. The bath of spin-up fermions with nearest-neighbor interactions can then be mapped to a spin model, as discussed in Sec. 2.4.1.
2.4 Domain walls in the \( V \gg J \) limit

In this section, we consider the spinless extended Hubbard model in the regime of strong nearest-neighbor repulsion, \( V \gg J \). When the lattice is half filled, the number of particles is commensurate with the number of lattice sites and the system is in the Mott insulator state where the particles occupy alternating lattice sites. The transition from a Luttinger liquid to a Mott insulator at half filling is discussed in the context of the sine-Gordon model in Chapter 3. For \( V \gg J \), a phase transition from the Mott insulator to a Luttinger liquid also occurs when the filling deviates from one half. This is called the commensurate-incommensurate phase transition. At incommensurate filling, close to the transition, the excess particles form domain walls in the particle arrangement. Using the terminology of Publication IV, such domain walls can be solitons of two neighboring particles or antisolitons of two neighboring empty sites. We present here a simplified model of the solitons, developed in Publication IV, based on the Jordan-Wigner transformation [71] and the Kramers-Wannier transformation [72, 73]. The fermion system is mapped to the XXZ spin model, and the resulting spin chain is represented in terms of bonds instead of lattice sites. Finally, the bonds where the domain walls are located are mapped back to free fermions. We show that the density distribution obtained from the simplified model agrees well with the numerical solution of the many-body problem.

2.4.1 Mapping to the XXZ model

The extended Hubbard model for spinless fermions

\[
H_0 = -J \sum_{\langle i,j \rangle} c_i^\dagger c_j + V \sum_j \left( n_j - \frac{1}{2} \right) \left( n_{j+1} - \frac{1}{2} \right) \tag{2.20}
\]

can be mapped to the XXZ spin model

\[
H_0 = J_{xy} \left( \frac{1}{2} \sum_{\langle i,j \rangle} S_i^+ S_j^- + \Delta \sum_j S_j^z S_{j+1}^z \right), \tag{2.21}
\]

by the Jordan-Wigner transformation [71]. The interaction term in eq. (2.20) is written slightly differently than in eq. (2.19), which follows from the transformation. For periodic boundary conditions, the difference between \( V \sum_j n_j n_{j+1} \) and \( V \sum_j \left( n_j - \frac{1}{2} \right) \left( n_{j+1} - \frac{1}{2} \right) \) is a constant shift in energy.
Lattice models for fermions

Figure 2.1. Spinless fermions with nearest-neighbor interactions in a one-dimensional lattice can be mapped to an XXZ spin chain. Figure originally published in Publication IV.

Open boundary conditions on the other hand lead to a different potential at the edge sites $j = 1$ and $j = L$. We have studied a system with nearest-neighbor interactions and open boundary conditions in Publications II and IV, and for the parameters used in the publications, the results do not show any noticeable difference between the two interaction terms.

The operators $S^\pm_j = S^x_j \pm iS^y_j$ are the raising and lowering operators of a spin-$\frac{1}{2}$ chain. The spin operators $S^a_j$, where $a = x, y, z$, can be written in terms of the Pauli matrices $\sigma^a_j$ as $S^a_j = \frac{1}{2}\sigma^a_j$. The coupling constant between the spins is denoted by $J_{xy}$ and $\Delta$ is the anisotropy in the $z$ direction. For $\Delta = 1$, this model is known as the Heisenberg model. The parameters in terms of $J$ and $V$ are

$$
J_{xy} = 2J, \\
\Delta = \frac{V}{J_{xy}}.
$$

To go from eq. (2.21) to eq. (2.20), one transforms

$$
S^+_j = c^\dagger_j e^{i\pi \sum_{l=-\infty}^{-1} c^\dagger_l c_l}, \\
S^-_j = n_j - \frac{1}{2},
$$

which gives the kinetic term $S^+_{j+1} S^-_j = c^\dagger_{j+1} e^{i\pi c^\dagger_j c_j} c_j = c^\dagger_{j+1} c_j$ and the interaction term as in eq. (2.20). The mapping between fermions in a lattice and the spin chain is illustrated in Fig. 2.1. The nearest-neighbor exchange interaction has also been realized with ultracold atoms using various techniques [74].

2.4.2 Free-fermion model of the domain walls

A half-filled lattice corresponds to a spin chain with zero magnetization. The Mott insulator state at half filling is thus equivalent to an antiferromagnetic order of the spins. When the magnetization $\sum_j \langle S^z_j \rangle$ is slightly
above or below zero, there are domains with antiferromagnetic order separated by domain walls where two up spins or two down spins, respectively, are next to each other. The spin chain can be represented as a chain of bonds, where the domain walls correspond to filled bonds and the alternating spins to empty bonds. The filled bonds can then be mapped back to fermions in a lattice of size $L - 1$. When the density of domain walls is low, the domain walls can be considered as noninteracting fermions [75], which allows to calculate expectation values analytically. We present here the main points of the transformations and refer to [73] and the Supplemental Material of Publication IV for more details.

We start by writing Hamiltonian (2.21) in terms of the Pauli matrices,

$$H_0 = \frac{J_{xy}}{4} \sum_{j=1}^{L-1} \left( \sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \Delta \sigma^z_j \sigma^z_{j+1} \right).$$  \tag{2.24}$$

The Kramers-Wannier transformation [72, 73] consists in replacing the matrices $\sigma^\alpha$ by bond operators.

$$\tau^z_{j+\frac{1}{2}} = \sigma^z_j \sigma^z_{j+1},$$

$$\tau^y_{j+\frac{1}{2}} = \prod_{i=1}^{j} \sigma^x_i.$$  \tag{2.25}

The indexing of the bonds is illustrated in Fig. 2.2. Changing into the bond indices $l = j - \frac{1}{2}$, the operators $\tau^z_l$ and $\tau^y_l = i (\tau^-_l - \tau^+_l)$ can be transformed into spinless fermion operators using eq. (2.23), where $S^z_l$ is replaced by $\frac{1}{2} \tau^z_l$ and $S^+_l$ by $\tau^+_l$. In terms of the new fermion operators $\tilde{c}_l$, Hamiltonian (2.24) is written as [73]

$$H_0 = \frac{J_{xy}}{2} \sum_{l=2}^{L-2} \left[ (1 - \tilde{c}^\dagger_l \tilde{c}_l) \tilde{c}^\dagger_{l-1} \tilde{c}_{l+1} + \text{H.c.} \right] + \frac{J_{xy}}{2} \sum_{l=1}^{L-1} \tilde{c}^\dagger_l \tilde{c}_l + \frac{J_{xy}}{2} \sum_{l=1}^{L-1} \tilde{c}^\dagger_{l-1} \tilde{c}^\dagger_{l+1} \tilde{c}^-_l + \frac{J_{xy}}{2} \sum_{l=1}^{L-1} \tilde{c}^\dagger_l \tilde{c}_l.$$  \tag{2.26}

The creation of a fermion now corresponds to the creation of a domain wall in the original spin chain, as depicted in Fig. 2.3.

When the density of domain walls is very low, $\langle \tilde{c}^\dagger_l \tilde{c}_l \rangle \approx 0$, and one can approximate $\left(1 - \tilde{c}^\dagger_l \tilde{c}_l \right) \approx 1$. If the nearest-neighbor repulsion is large, the energy cost of creating domain walls is high and one can also expect $\langle \tilde{c}^\dagger_{l-1} \tilde{c}^\dagger_{l+1} \rangle \approx 0$. For a fixed number of domain walls, the last term of
eq. (2.26) gives a constant shift in energy and can be left out. The Hamiltonian (2.26) can therefore be approximated with only the kinetic term,

\[ H_0 \approx \frac{J_{xy}}{2} \sum_{l=2}^{L-2} \left( \hat{c}^\dagger_{l-1} \hat{c}_{l+1} + \text{H.c.} \right), \tag{2.27} \]

in which the new fermions move by next-nearest-neighbor tunneling. The number of fermions \( N \) is equal to the number of domain walls. The \( N \)-fermion ground state of the free Hamiltonian is

\[ |\Psi_{1,2,\ldots,N}\rangle = \sum_{l_1,\ldots,l_N} \varphi_{k_1,\ldots,k_N}^{l_1,\ldots,l_N} |l_1\rangle \otimes |l_2\rangle \otimes \cdots \otimes |l_N\rangle, \tag{2.28} \]

where \( l_\alpha \) denotes the coordinate of fermion \( \alpha \). We denote by \( |l\rangle \) the single-particle states where site \( l \) is occupied and other sites are empty,

\[ |l\rangle = |0, \cdots, 0, l, 0, \cdots, 0\rangle. \tag{2.29} \]

The coefficient \( \varphi_{k_1,\ldots,k_N}^{l_1,\ldots,l_N} \) is given by the Slater determinant

\[ \varphi_{k_1,\ldots,k_N}^{l_1,\ldots,l_N} = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \varphi_{l_1}^{k_1} & \varphi_{l_1}^{k_2} & \cdots & \varphi_{l_1}^{k_N} \\ \varphi_{l_2}^{k_1} & \varphi_{l_2}^{k_2} & \cdots & \varphi_{l_2}^{k_N} \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{l_N}^{k_1} & \cdots & \cdots & \varphi_{l_N}^{k_N} \end{pmatrix}, \tag{2.30} \]

where the single-particle basis states \( \varphi_{l}^{k} \) are given by eq. (2.11).
2.4.3 Domain walls in the density distribution

In the bond representation, the $S^z_j$ operator becomes

$$S^z_j = \frac{1}{2} \sigma^z_j = \frac{1}{2} \prod_{l=1}^{j-1} \left( 2\tilde{c}^\dagger_l \tilde{c}_l - 1 \right).$$  (2.31)

Its expectation value in the ground state of eq. (2.28) is written as

$$\langle \psi_{1,\ldots,N} | S^z_j | \psi_{1,\ldots,N} \rangle = \frac{1}{2} \sum_{l_1,\ldots,l_N} \left| \varphi_{k_1,\ldots,k_N} \right|^2 \prod_{d=1}^{j-1} \left[ 2 \sum_{\alpha=1}^{N} \delta_{d,\alpha} - 1 \right].$$  (2.32)

The density distribution $\langle n_j \rangle = \langle S^z_j \rangle + \frac{1}{2}$ given by eq. (2.32) is shown in the upper panel of Fig. 2.4 together with the numerical solution of the original Hamiltonian (2.20). The numerical solution, shown for both commensurate (half) and incommensurate filling, is obtained by the time-evolving block decimation algorithm, which is discussed in Chapter 6. At half filling, a large nearest-neighbor repulsion $V \gg J$ leads to a density which oscillates between 0 and 1. The ground state is nondegenerate for odd $L$. At incommensurate filling, the phase of the density oscillation changes by $\pi$ at the locations of the domain walls, which means that there are two neighboring maxima or minima in the density distribution.

When the number of spinless fermions in the original system with nearest-neighbor interactions is denoted by $N$, the number of domain walls in the ground state is

$$N_{DW} = \left| 2 \left( \frac{N - L}{2} \right) \mp 1 \right|,$$  (2.33)

where the upper sign corresponds to $N > \frac{L}{2}$ and the lower sign to $N < \frac{L}{2}$. In Publication IV, we have studied the situation where $N > \frac{L}{2}$ and the excess particles form solitons of two neighboring particles. For $N < \frac{L}{2}$, the domain walls would instead be antisolitons of neighboring empty sites. In Fig. 2.4 with $(N - \frac{L}{2}) = 2.5$, there are four domain walls, and we find a good agreement between eq. (2.32) and the numerical result.

For periodic boundary conditions, the solitons would be delocalized, which would lead to a uniform density. In the case of open boundary conditions, as considered here, the solitons are not completely delocalized, and the neighboring maxima or minima in Fig. 2.4 indicate the most probable locations of the solitons. It is known that when the density of solitons is low
and the nearest-neighbor repulsion is large, the solitons behave as free fermions [75]. This is consistent with the results shown in Fig. 2.4, where the analytic result was obtained by approximating the system with the free Hamiltonian of eq. (2.27). Furthermore, one can directly compare the many-body density distribution to the distribution of $N$ free fermions

$$\langle FS | n_j | FS \rangle = \sum_{k = \frac{N\pi}{L+1}}^{k_F} |\varphi_k^j|^2$$

shown in the lower panel of Fig. 2.4. In the sum, $k_F = \frac{N\pi}{L+1}$, and $|FS\rangle = \prod_{k \leq k_F} c_k^\dagger |0\rangle$. The neighboring minima and maxima in the upper panel coincide with the maxima of the free fermion density in the lower panel, which has Friedel oscillations due to the open boundary conditions.
Lattice models for fermions
This chapter presents a low-energy effective theory called the Tomonaga-Luttinger liquid (TLL) theory, which describes a wide variety of interacting fermion and boson systems in one dimension, in equilibrium. The dynamical phenomena studied in Publications I–IV are not in this low-energy region, but the theory helps us to understand the ground states of the attractive Hubbard model and the XXZ spin model studied in this thesis. A brief overview of the relevant points of the TLL theory is given here, based on the several existing reviews [75–79]. We also discuss the density distributions of Sec. 2.4.3 from the point of view of the sine-Gordon model, and present the results of Publication I regarding singlet superfluid correlations.

3.1 Introduction

The discovery of exactly solvable models in one dimension began with Bethe’s ansatz to solve the Heisenberg model in 1931 [80]. Other models were solved with similar methods [4, 81], and a breakthrough in the analytical treatment of fermions in one dimension came with the bosonization technique [82, 83] to solve the Tomonaga-Luttinger model [84, 85]. At the time, these solutions were not thought to have practical importance but were rather mathematical curiosities [79]. Several physical systems have later been found where particles are effectively confined to one dimension and exhibit phenomena which are qualitatively different from the Fermi liquid description of higher-dimensional systems. One of these phenomena is spin-charge separation, where the charge (or density) and spin of a particle separate and move at different velocities. Signs of
spin-charge separation have been observed in effectively one-dimensional compounds [86] and nanowires [87, 88]. Phenomena specific to one dimension have also been observed in ultracold quantum gases confined to one-dimensional tubes [89–97].

In Fermi liquid theory, elementary excitations are nearly-free quasi-particles which consist of a particle or hole dressed by density fluctuations [98]. The effects of repulsive interactions between the quasiparticles can be described by perturbation theory. In one dimension, such a perturbation theory breaks down since the particle-hole susceptibility diverges [75, 76]. This indicates that the ground state of interacting particles is very different from that of noninteracting ones. In an intuitive picture, particles in two and three dimensions can move past each other almost freely, whereas in one dimension, a single particle cannot move without pushing the other particles. Instead of nearly-free quasiparticles, therefore, the elementary excitations in one dimension are collective density fluctuations. A low-energy effective theory, the Luttinger liquid theory, can therefore be built on these free bosonic collective modes [99]. It describes the universal properties of a large class of one-dimensional models. High-energy properties, on the other hand, are model-specific and have to be studied by other means, such as the numerical techniques described in Chapter 6.

3.2 Low-energy excitations

In one dimension, instead of a continuous Fermi surface as in two or three dimensions, there are two Fermi points at $\pm k_F$, as shown in Fig. 3.1. The particle-hole excitations therefore have a different energy spectrum than in two or three dimensions. Particle-hole excitations with energy close to zero, $\epsilon(q) \approx 0$, are only possible for momentum transfer $q \approx 0$ and $q \approx 2k_F$. This results in a gap in the excitation spectrum between $q \approx 0$ and $q \approx 2k_F$ instead of a continuum as in two or three dimensions. Schematic drawings of the excitation spectra are shown in Fig. 3.2. In one dimension, at $q \to 0$, the particle-hole excitations have a linear dispersion relation $\epsilon(q) = vq$ corresponding to sound-like collective excitations. For noninteracting particles, $v$ is the Fermi velocity. Whereas in two or
three dimensions, the continuum of low-energy excitations indicates that a sound mode can decay into quasiparticles, in one dimension, the sound waves are the stable elementary excitations. This has implications for the solution of the problem of interacting fermions in one dimension, as discussed in Sec. 3.4.

![Figure 3.1](image1.png)

**Figure 3.1.** a) The dispersion relation of free particles in the continuum, $E(k) = \frac{k^2}{2m}$ (in natural units, $\hbar = 1$). For fermions at zero temperature, momentum states up to the Fermi level are filled. Fermions in one dimension have excitations with energy $\epsilon(q) \approx 0$ only with momentum transfer $q \approx 0$ (b) or $q \approx 2k_F$ (c).

![Figure 3.2](image2.png)

**Figure 3.2.** a) In two and three dimensions, the energy spectrum $\epsilon(q)$ of particle-hole excitations has a continuum between $q = 0$ and $q = 2k_F$ at low energy $\epsilon(q) \approx 0$. b) In one dimension, there is a gap between $q = 0$ and $q = 2k_F$.

In a lattice, the dispersion relation of free particles is $E(k) = -2J \cos(k)$ and the energy is limited by the bandwidth. The dispersion relation and the single-particle excitation spectrum are shown in Fig. 3.3, where the lattice is half-filled and $k_F = \frac{\pi}{2}$. Since the possible excitation energies in the single-band model are limited from above, a perturbation which probes the high-energy region cannot create excitations in the system. This is discussed in Sec. 3.7.
Tomonaga-Luttinger liquid

![Figure 3.3](image)

**Figure 3.3.** a) The dispersion relation of free particles in a lattice $E(k) = -2J \cos(k)$ in the lowest energy band and first Brillouin zone, $k \in [-\pi, \pi]$. b) In the lattice, the excitation spectrum has a finite bandwidth.

### 3.3 Tomonaga-Luttinger model

The Tomonaga-Luttinger (TL) model was initially introduced as an exactly solvable model of interacting massless fermions in one dimension [82, 84, 85]. The Hamiltonian for free fermions is

$$H = \sum_{k=-\infty}^{\infty} \sum_{r=\pm 1} \sum_{s=\uparrow, \downarrow} v_F(rk - k_F)c^\dagger_{r,s}(k)c_{r,s}(k),$$

(3.1)

where the dispersion relation is linear. The interacting case will be discussed in the following sections. The Hamiltonian has been written in terms of left- and right-moving fermions labeled by $r = L, R$ corresponding to $r = \mp 1$,

$$c_{L,s}(k) = \begin{cases} c_s(k), & k < 0 \\ 0, & k > 0 \end{cases}, \quad c_{R,s}(k) = \begin{cases} c_s(k), & k > 0 \\ 0, & k < 0 \end{cases}.$$

To solve the model exactly, one must introduce the Dirac sea of an infinite number of filled negative-energy states [82, 99]. The operators in (3.1) are therefore normally ordered to avoid an infinite total particle number.

Though first considered unrealistic [85], it was proposed by Haldane [99] that this type of a model describes the low-energy properties of a wide class of one-dimensional many-body quantum models, which he named Luttinger liquids. Some of the unifying properties of such Luttinger liquids are a gapless excitation spectrum and correlations which decay as power laws with interaction-dependent exponents. The low-energy regime of the XXZ model and the (extended) Hubbard model studied in this thesis also fall into this category, except for certain parameter regions where the excitation spectrum has a gap. Such situations are the topic of Sec. 3.5.
3.4 Bosonization

Instead of free fermions, as in Fermi liquid theory, the TL model can be solved analytically by making a change of basis into free bosons. This procedure is called bosonization. Bosonization can be applied to any one-dimensional model, which in general can have a nonlinear dispersion relation. One can find by a renormalization group analysis whether the low-energy and long-wavelength properties are described by the exactly solvable TL model. As shown in Figs. 3.2 and 3.3, bosonic collective excitations have a well-defined dispersion relation at $q \rightarrow 0$. These excitations are described by the density fluctuation operator

$$\rho_{r,s}^{\dagger}(q) = \sum_{k} c_{r,s}^{\dagger}(k + q)c_{r,s}(k), \quad (3.2)$$

which creates a collection of particle-hole excitations with the momentum of each particle increased by $q$. The operators (3.2) have bosonic commutation relations, and they can be used as the new basis for the Hamiltonian (3.1). It turns out that the free Hamiltonian is quadratic also in the boson basis and thus it describes free bosons. Furthermore, if the backscattering of fermions with opposite spin is not included, interactions preserve the quadratic form of the TL Hamiltonian.

With a series of transformations, one can construct the continuum Hamiltonian

$$H_0 = \frac{1}{2\pi} \sum_{\nu=\rho,\sigma} \int \left[ \frac{u_{\nu}}{K_{\nu}} (\nabla \phi_{\nu}(x))^2 + u_{\nu}K_{\nu}(\nabla \theta_{\nu}(x))^2 \right] dx, \quad (3.3)$$

which is here written in position space. The Hamiltonian (3.3) is quadratic in the bosonic field operators $\phi_{\nu}(x)$ and $\theta_{\nu}(x)$, which are functions of the density fluctuation operators of eq. (3.2). The indices $\nu = \rho, \sigma$ denote the charge $\phi_{\rho}(x) = \frac{1}{\sqrt{2}} [\phi_{\uparrow}(x) + \phi_{\downarrow}(x)]$ and spin $\phi_{\sigma}(x) = \frac{1}{\sqrt{2}} [\phi_{\uparrow}(x) - \phi_{\downarrow}(x)]$ degrees of freedom which are now decoupled, $H_0 = H_{\rho} + H_{\sigma}$. The fields $\phi_{\nu}(x)$ are physically related to the particle and spin densities, whereas the fields $\theta_{\nu}(x)$ are related to the phase of the fermionic field operator. The parameters $u_{\nu}$ are the propagation velocities of the collective spin and charge excitations, corresponding to the speed of sound. The parameters $K_{\nu}$ are dimensionless and are called the Luttinger liquid parameters. They appear in the exponents of the algebraic correlation functions. In the TL model, the parameters $K_{\nu}$ and $u_{\nu}$ can be expressed in terms of
the coupling constants of different interactions. For other bosonized one-dimensional models, $K$ and $u$ do not necessarily have analytic expressions in terms of the parameters of the model. In such cases, they can be evaluated numerically.

When the Hamiltonian is quadratic, representing the fermionic field operator

$$\psi_{r,s}(x) = \frac{1}{\sqrt{L}} \sum_{k=-\infty}^{\infty} e^{ikx} c_{r,s,k}$$

in terms of the boson fields $\phi_\nu$ and $\theta_\nu$ allows to calculate any correlation functions analytically as Gaussian path integrals [75, 76]. All correlation functions decay as power laws with exponents which depend on $K_\nu$. Due to strong quantum fluctuations, continuous symmetries are not spontaneously broken in one dimension and there is no long-range order corresponding to such symmetry breaking. Instead of a nonzero order parameter, therefore, the phase of the one-dimensional system is determined by the correlation function which has the slowest power-law decay. In a lattice, however, the discrete translational symmetry can be broken and there can be a long-range density order.

### 3.5 Sine-Gordon model

The boson representation of certain models contains other terms in addition to eq. (3.3). This is the case if, for example, the backscattering of fermions with opposite spin, or a lattice potential, is included. Such cases appear in Publications I, II and IV.

#### 3.5.1 Backscattering of fermions with spin

In the case of a nonzero coupling for the opposite-spin backscattering, the Hamiltonian has an additional term which depends on $\phi_\sigma$,

$$H = H_0 + \frac{2g}{(2\pi\alpha)^2} \int \cos(2\sqrt{2}\phi_\sigma(x)) dx.$$ (3.4)

The coupling constant is denoted by $g$ and $\alpha$ is a short-distance cutoff which in a lattice model would be of the order of the lattice spacing. This type of a model is called the sine-Gordon model in analogy to the relativistic Klein-Gordon model.
For the Hubbard model, $g$ is equal to the on-site interaction $U$. The effect of the cosine term depends on the sign of $U$ and can be studied by a renormalization analysis [75, 100]. If the interaction is repulsive, $U > 0$, the term is irrelevant, and the asymptotic low-energy properties are captured by $H_0$. For an attractive interaction $U < 0$, the cosine term is relevant and changes the physics of the spin excitations. The energy of the cosine term is minimized when the field $\phi_\sigma$ is fixed to one of the minima of the cosine. Expanding the cosine term around a minimum and approximating it by the quadratic term gives a mass term $\propto \int \phi_\sigma^2(x)dx$ for this field. This shows that the energy spectrum of spin excitations has a gap, which means that the spin sector is not a Luttinger liquid. The charge excitations remain gapless. The low-energy excitations are thus charge excitations and the low-energy physics is described by $K_\rho$ and $u_\rho$.

The phase of the system is determined by the dominant correlation function. When there is a spin gap, the spin density wave and triplet superfluid correlations related to spin ordering have an exponential decay. The singlet superconducting (SS) and in a charge density wave (CDW) correlations related to charge ordering, on the other hand, decay asymptotically as power laws [75],

$$\langle O_{SS}^\dagger(x)O_{SS}(0) \rangle \propto \left(\frac{\alpha}{x}\right)^{\frac{1}{K_\rho}},$$

$$\langle O_{CDW}^\dagger(x)O_{CDW}(0) \rangle \propto \left(\frac{\alpha}{x}\right)^{K_\rho}.$$  (3.5)

(3.6)

Here, the order parameter for singlet superconducting order is

$$O_{SS}(x) = \psi_{R\uparrow}^\dagger(x)\psi_{L\downarrow}^\dagger(x) + \psi_{L\uparrow}^\dagger(x)\psi_{R\downarrow}^\dagger(x)$$

and the one for charge density wave order is

$$O_{CDW}(x) = \psi_{R\uparrow}^\dagger(x)\psi_{L\uparrow}(x) + \psi_{R\downarrow}^\dagger(x)\psi_{L\downarrow}(x).$$

The system is thus either in the SS or CDW phase, depending on the value of $K_\rho$. It can be seen in eqs. (3.5) and (3.6) that for $K_\rho < 1$, the CDW correlation decays more slowly and is thus the dominant correlation, whereas for $K_\rho > 1$, the SS correlation dominates.

### 3.5.2 Lattice at commensurate and incommensurate filling

In lattice models, a cosine term arises from the umklapp scattering if the wave number of the periodic potential corresponds to a commensurate
filling of the lattice. In umklapp scattering, two particles scatter from one side of the Fermi surface to the other. This is possible in a lattice since momentum is conserved modulo $\frac{2\pi}{a}$, where $a$ is the lattice spacing. For the Hubbard model, umklapp scattering occurs at half filling. The cosine term is responsible for the Luttinger liquid-Mott insulator phase transition in the charge degree of freedom when the on-site interaction changes from attractive to repulsive. For the XXZ spin model of eq. (2.21), a similar phase transition occurs at zero magnetization and $\Delta = 1$. When $0 < \Delta < 1$, the system is in the Luttinger liquid phase with dominant antiferromagnetic correlations, and for $\Delta > 1$, in the gapped Ising antiferromagnet phase, corresponding to a Mott insulator phase of spinless fermions. The transition from a Luttinger liquid to a Mott insulator described by the sine-Gordon model has been observed in an experiment with ultracold bosonic cesium [95].

In Publication II, we study the XXZ model at zero magnetization, which corresponds to spinless fermions with nearest-neighbor interactions at half filling. For the spinless fermions, the cosine term for the umklapp scattering is [75]

$$\tilde{H} = -\frac{J_z}{(2\pi\alpha)^2} \int \cos[4\phi(x)] dx,$$

where the lattice spacing has been set to 1. When $\Delta > 1$, the system is in the commensurate Mott insulator phase, where $\phi(x)$ is fixed to $\phi = \frac{n\pi}{2}$ which minimizes $-\cos(4\phi)$. The local magnetization in terms of the density of spinless fermions is $\langle S^z(x) \rangle = \langle \rho(x) \rangle - \frac{1}{2}$, which at half filling gives [75]

$$\langle S^z_l \rangle = (-1)^l \langle \cos(2\phi) \rangle.$$

This corresponds for spinless fermions to alternating filled and empty sites. The density distribution, which is related to the local magnetization as $\langle S^z_l \rangle$, is shown in Fig. 2.4 for an odd number of sites $L$ and open boundary conditions, in which case the ground state is nondegenerate.

When there is a small deviation from half filling, the field $\phi$ is not fixed to one minimum but changes in steps of $\frac{\pi}{2}$ from one minimum to the next at the locations of the additional or missing particles. These discontinuities in $\phi$ are called phase slips or solitons. In eq. (3.7), it can be seen that when $\phi$ changes by $\frac{\pi}{2}$, the phase of the oscillation in the local magnetization changes by $\pi$. In the incommensurate case in Fig. 2.4, the phase
of the oscillation changes by $\pi$ at places where there are two minima or maxima next to each other, corresponding to the maxima of the soliton distribution. When approaching half filling for a fixed $\Delta > 1$, the parameter $K$ approaches the critical value $K_c = \frac{1}{4}$ at the incommensurate-commensurate phase transition. At this critical value, the solitons can be mapped to free fermions [101, 102].

3.6 Obtaining LL parameters numerically

The parameters $K_\nu$ and $u_\nu$ determine thermodynamic quantities and the asymptotic behavior of correlation functions of the one-dimensional models in the Luttinger liquid universality class. For certain models, these parameters can be obtained analytically by the Bethe ansatz, and in general can be computed numerically. Once the parameters are obtained, the asymptotic forms of the correlation functions are known exactly from the TLL theory. One approach to determine $K_\nu$ and $u_\nu$ numerically is to use the compressibility $\kappa = \frac{K_\pi}{u}$ and the charge stiffness $D = uK$ [103]. They can be expressed as variations of the ground state energy with respect to the particle number or a flux, respectively. Another approach is to use the charge gap and the energy difference between the ground state and the first excited state [104, 105], which depend on $K$ and $u$. The exponents $K_\nu$ can also be determined from fits to the correlation functions, which are calculated numerically. We have used this approach in Publication I [106].

In Publication I, we consider a Fermi gas with attractive interactions in a harmonic trap, described by the Hubbard model with the harmonic potential $V(j) = V_{\text{trap}}(j - j_0)^2$. We calculate $K_\rho$ by fitting eq. (3.5) to the numerically obtained pair correlation, as shown in Fig. 3.4. In terms of the lattice operators, the singlet superconducting (superfluid) order parameter is written as $O_{\text{SS},j}^\dagger = c_{j\uparrow}^\dagger c_{j\downarrow}$ and the correlator as

$$C_{ij} = \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} \rangle. \quad (3.8)$$

For the ground state with the on-site interaction $U = -4J$, we find $K_\rho = 1.22 \pm 0.08 > 1$ indicating that the system is in the singlet superfluid state. The TL model is usually formulated for a translationally invariant system, and to take into account the harmonic trap, a local density approximation has been used [107]. The values of $u_\nu$ and $K_\nu$ depend on
the density, and in the case of an inhomogeneous density they depend on position. We however find that using eq. (3.5) in the case of a harmonic potential with $V_{\text{trap}} = 5 \times 10^{-4} J$ gives a value close to the Bethe ansatz result $K_\rho = 1.28 \pm 0.02$ for a homogeneous system. This value is obtained using the average density at the center of the trap.

![Figure 3.4. The pair correlation of eq. (3.8) with one of the indices fixed to $j = \frac{L}{2}$. The fit $-\frac{1}{\sqrt{2\pi} x} + a$ gives $K_\rho = 1.22 \pm 0.08$, where the errors are given by the 95% confidence bounds. The on-site interaction is $U = -4J$. Figure originally published in Publication I.](image)

3.7 Moving perturbations in the one-dimensional Fermi gas

In Publication I, we study attractively interacting fermions in a harmonic trap, described by the attractive Hubbard model. The fermion cloud is perturbed by a moving potential well or barrier of either Gaussian $V(i, t) = V_0 e^{-(i-vt)^2/2\sigma^2}$ or Lorentzian $V(i, t) = \frac{\gamma}{(i-vt)^2 + \gamma^2}$ shape, where $i$ is the lattice site index, $V_0$ the height and $v$ the velocity of the potential, and $\gamma = \frac{1}{V_0}$.

The initial state is the ground state of the system without the perturbation. We find that the initial density distribution is largely deformed and singlet superfluid correlations broken if the velocity $v$ is smaller than the maximum group velocity $v_{\text{max}}$, whereas for larger velocities there is no considerable change in the density distribution and correlations. The singlet superfluid correlation $|C_{x, \frac{L}{2}}|$ is shown in Fig. 3.4 in the ground state and after perturbing the system with a slow ($v = 0.5J$) and fast ($v = 4J$) potential barrier, as compared to the maximum group velocity $v_{\text{max}} = 1J$.

In order to understand how the moving wave packet perturbations probe the excitation spectrum of the one-dimensional Fermi gas, we have calculated the Fourier transforms of the perturbing potentials in momentum-
frequency space. They are shown in Fig. 3.5 for velocity \( v = 1J \) and an arbitrary potential height. The Fourier transforms are centered around \( \omega = -vk \) and oscillate around this line when the time integral of the Fourier transform is over a finite interval (here, \( t \in [0, 5/J] \)). In the infinite-time limit, the frequency part of the Fourier transform becomes a delta function and the oscillations vanish. Comparing the Fourier transforms to the single-particle excitation spectrum in Fig. 3.3, one can expect that the potentials are most likely to create excitations in the Fermi gas when the velocity is smaller than the slope of the spectrum at \( q = 0 \). On the other hand, for a very large \( v \), there should not be available excitations due to the finite bandwidth. These are the effects that we observe in the simulations.

For noninteracting fermions, the slope of the excitation spectrum at \( q = 0 \) is the Fermi velocity \( v_F \). Because of the interactions and the harmonic trap, the excitation spectrum of the our system is modified from that of Fig. 3.3. When the fermions have an attractive interaction, the low-energy excitations at \( q \to 0 \) are collective charge excitations with the dispersion \( \epsilon(q) = u_\rho k \), where \( u_\rho \) is their velocity. This description does not extend to high-energy excitations, and to our knowledge, the exact excitation spectrum of the attractively interacting fermions in a harmonic trap in one dimension has not been calculated. In the limit \( U \to -\infty \), fermions with opposite spin pair into doublons, which are hard-core bosons and have a spectrum similar to that of Fig. 3.3. One can therefore expect the single-particle description to be valid for large \(|U|\). The single-band approximation does not take into account the possible excitations to higher bands, which could occur for a large \( v \) and \( V_0 \).

The effects of dimensionality and the perturbation strength could be fur-
Tomonaga-Luttinger liquid

ther investigated in order to test the interpretation of the results based on the physical picture of the excitation spectrum and the perturbing potentials in momentum-frequency space. One could for example study the possibility of Andreev bound states or excitations of the amplitude mode [108, 109] which can occur in three dimensions.
4. Dynamics of soliton excitations

An impurity particle interacting with many particles of a different type is a situation encountered in various physical systems, both classical and quantum. Localized impurities are known to lead to diverse phenomena relevant for condensed matter physics [110], and recently, experiments with ultracold gases have made it possible to measure the real-time motion of mobile impurities [35]. Most of the previous research is focused on impurities in homogeneous environments. In this section, we review the main results of Publications II and IV, which consider a mobile impurity or a local quench in a system with a specific arrangement of the particles. As discussed in Sec. 2.4, for strong nearest-neighbor repulsion $V \gg J$, the fermions are in the Mott insulator state at half filling with a particle every two sites. When the filling deviates slightly from one half, domain walls form between Mott-insulator-like domains. The effect of the impurity or local quench in these systems is to create a pair of excitations, a soliton and an antisoliton, which propagate in the lattice. The transport of excitations due to spin flips and quenches in the equivalent XXZ spin model has been studied with various techniques [111–116]. We extend the simplified model of Sec. 2 to describe the time evolution the excitations in the case of a Mott insulator perturbed by a local potential quench. The dynamics of this system is compared to numerical simulations with an impurity particle and a filling above one half. We discuss the phenomena which arise when interactions are larger than the bandwidth of the particles.
4.1 Dynamics with a local potential quench

We study the dynamics of fermions which are initially in the ground state of Hamiltonian $H_0$ of eq. (2.20). The time-evolution due to a local quench in potential is described by

$$H = H_0 + H', \quad (4.1)$$

where $H' = U n_{j_0}$. A potential barrier of height $U$ is thus created at site $j_0$ at the center of the lattice at time $t = 0$. In the simplified domain wall description, we consider the case where the height of the potential barrier is equal to the magnitude of the nearest-neighbor interaction between the fermions, $U = V$. At half filling, the occupation probability of site $j_0$ is close to 1. We assume that for $U = V$, the probability of the fermion at $j_0$ to tunnel to the neighboring site and create a soliton-antisoliton pair is also close to 1, which allows to consider an initial state where the excitations have already been created. The situation is different when the filling deviates from $\frac{1}{2}$, since the site $j_0$ has a finite probability of being empty.

4.1.1 Time evolution of a single domain wall

Similarly as in Sec. 2.4, one can use the bond mapping and the free Hamiltonian (2.27) to calculate time-dependent quantities in the case where solitons and antisolitons can be considered noninteracting. In Publication IV, we consider fermions with nearest-neighbor repulsion in the Mott insulator state, where a local quench in potential creates a soliton-antisoliton pair. We find that the soliton and antisoliton excitation propagate in opposite directions, creating an inversion of the density oscillation, and their motion can be described by the free Hamiltonian (2.27). The system is symmetric on the left and right sides of $j_0$, and we can therefore consider only half of the lattice. The domain wall in the right half can be created either at bond $j_0$ or $j_0 + 1$, as can be seen from Figs. 2.2 and 2.3, and the initial state can be written as a superposition

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|j_0\rangle + |j_0 + 1\rangle) = \frac{1}{\sqrt{2}} \sum_k \left[ \varphi_{j_0k}^* + \varphi_{j_0k+1}^* \right] |k\rangle, \quad (4.2)$$

where $\varphi_{j_0k}$ is given by eq. (2.11). The time-dependent state is

$$|\psi(t)\rangle = e^{-iH_0 t} |\psi(0)\rangle = \frac{1}{\sqrt{2}} \sum_k \left[ \varphi_{j_0k}^* + \varphi_{j_0k+1}^* \right] e^{-i\epsilon_k t} |k\rangle. \quad (4.3)$$
Dynamics of soliton excitations

Figure 4.1. The density distribution in the right half of the lattice given by eq. (4.4) is close to the numerical solution of the many-body problem by TEBD, shown at $t = 0$ (upper) and at $t = 6/J$ (lower). The system is in the Mott insulator state with a nearest-neighbor repulsion $V = 50J$, 31 particles and $L = 61$. In the domain wall model, a domain wall is already created in the initial state.

$$\langle \psi(t) | n_j | \psi(t) \rangle = \frac{1}{4} \sum_l \left[ \sum_k \left( \varphi_{k0}^{*} + \varphi_{k0+1}^{*} \right) \varphi_{k} e^{-i\epsilon_k t} \right]^2$$

where $\epsilon_k$ is given by eq. (2.14). Using eq. (2.31), the particle density is now

$$\langle \psi(t) | n_j | \psi(t) \rangle = \frac{1}{4} \sum_l \left[ \sum_k \left( \varphi_{k0}^{*} + \varphi_{k0+1}^{*} \right) \varphi_{k} e^{-i\epsilon_k t} \right]^2 \times \prod_{d=1}^{j-1} (2\delta_{d,l} - 1) + \frac{1}{2}.$$  (4.4)

The density distribution given by this simplified model is shown in Fig. 4.1 in the initial state and at time $t = 6/J$. The many-body TEBD result is also shown. The motion of the domain wall in the density is quite accurately predicted by the simple model.

4.1.2 Propagation of soliton and antisoliton excitations

When the filling of the lattice is slightly above one half, the excess particles form solitons in the ground state, as discussed in Sec. 2.4. In this case, mapping the excitations to free fermions would be inaccurate since the interaction between the solitons that are present in the ground state and the soliton and antisoliton excitations would have to be taken into account. The numerical solution shows clear differences between the Mott insulator and the incommensurate initial state.

We calculate numerically the distribution of neighboring filled sites $\langle n_j n_{j+1} \rangle$ and the distribution of neighboring empty sites or holes, $\langle n_j^h n_{j+1}^h \rangle = \langle (1 - n_j)(1 - n_{j+1}) \rangle$, corresponding to the distributions of solitons and an-
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Figure 4.2. (a), (b) The soliton distribution \( \langle n_j n_{j+1} \rangle \) as a function of position and time for the (a) commensurate and (b) incommensurate initial states shows clear wavefronts. In panel (b), the solitons which are present in the initial state result in a nonzero distribution at \( t = 0 \). (c), (d) The antisoliton distribution \( \langle n_j^\dagger n_{j+1}^\dagger \rangle \) as a function of position and time for the (c) commensurate and (d) incommensurate initial states. (c) The antisoliton distribution has similar wavefronts as the soliton distributions. (d) In contrast, at incommensurate filling, the antisoliton does not propagate as far but is confined close to its origin. Figure adapted from Publication IV.

tisolitons, respectively. The distributions are shown as functions of time in Fig. 4.2. Note that similar correlations have been measured in experiments with a quantum gas microscope [117]. The soliton and antisoliton distributions for the MI initial state are shown in panels (a) and (c) of Fig. 4.2. The soliton distribution is zero at \( j_0 - 1 \) and \( j_0 \) and develops maxima at \( j_0 - 2 \) and \( j_0 + 1 \) as the fermion at \( j_0 \) tunnels either to the left or to the right. Correspondingly, a maximum of the antisoliton distribution is created at \( j_0 - 1 \) and \( j_0 \). For longer times, both distributions become zero at the center, indicating that the two excitations propagate symmetrically in opposite directions. For incommensurate filling, the soliton excitation does not behave as a free particle but interacts with the other solitons present in the system, which results in a slower propagation in panel (b). The antisoliton excitation on the other hand stays confined to the central region of the lattice. This can be understood for \( V \gg J \) to result from the conservation of energy. The motion of an antisoliton excitation past a soliton would require the two excitations to annihilate. An annihilation has a very small probability since the released energy could not be absorbed
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Figure 4.3. The number of antisolitons \(N_{AS}(t) = \sum_j \langle n^h_j n^h_{j+1}(t) \rangle\) and the number of solitons \(N_S(t) = \sum_j \langle n_j n_{j+1}(t) \rangle\) stay constant after the initial increase. The initial number of solitons \(N_{DW}\) given by eq. (2.33) is subtracted from \(N_S(t)\). The upper lines are for the MI initial state and the lower lines for incommensurate filling. Figure adapted from Publication IV.

In order to further check whether annihilation takes place, we calculate the total number of solitons \(N_S(t) = \sum_j \langle \psi(t) | n^\uparrow_j n^\uparrow_{j+1} | \psi(t) \rangle\) and antisolitons \(N_{AS}(t) = \sum_j \langle \psi(t) | n^h_j n^h_{j+1} | \psi(t) \rangle\). Figure 4.3 shows that \(N_{AS}(t)\) and the increase in the number of solitons \(N_S(t) - N_{DW}\) overlap, which is consistent with the creation of these excitations through the tunneling of a fermion. The numbers are close to zero at \(t = 0\) and increase until \(t \approx 1/J\), which is the time scale of the tunneling. The saturation to a constant value confirms that no annihilation takes place. For incommensurate filling, there is a finite probability of site \(j_0\) being initially empty, in which case excitations are not created. The saturation value for incommensurate filling is approximately the initial occupation probability \(\langle n_{j_0}(0) \rangle\).

4.2 Dynamics with an impurity particle

We compare the local potential quench to a more complicated situation where instead of a potential barrier, an impurity particle is created at \(j_0\). In the following, we denote the impurity particle by \(\downarrow\) and the majority component fermions, which can be thought of as an environment or bath, by \(\uparrow\). The term \(H_0\) of eq. (4.1) is then written as

\[
H_0 = -J \sum_{\langle i,j \rangle} c^\dagger_i c^\uparrow_j + V \sum_j \left( n^\uparrow_j - \frac{1}{2} \right) \left( n_{j+1}^\uparrow - \frac{1}{2} \right) \tag{4.5}
\]
Figure 4.4. A schematic drawing of the time evolution after creating an impurity in a Mott insulator bath. Here, the bath fermion with spin up hops to the left but the symmetric case is equally likely. 1) The impurity can either stay at $j_0$, in which case the soliton and antisoliton propagate in opposite directions, or 2) it can oscillate between the empty sites forming the antisoliton, creating a “bound state” of the impurity and the antisoliton. Figure adapted from Publication II.

and the term $H'$ is replaced by

$$H' = -J \sum_{\langle i,j \rangle} \hat{c}^\dagger_i \hat{c}^\dagger_j + U \sum_j \left( n_{j\uparrow} - \frac{1}{2} \right) n_{j\downarrow}.$$

(4.6)

The motional degree of freedom of the impurity results in differences in the dynamics compared to the static potential barrier. In particular, the motion of the antisoliton excitation is affected by the impurity since these two can form a bound state. Extending the simplified domain wall description to a situation with an impurity particle remains a topic of future work.

4.2.1 Bound state

Besides creating a soliton and an antisoliton excitation, the impurity can tunnel to the neighboring site. The time evolution is shown schematically in Fig. 4.4 and is a superposition of different configurations, where either the two excitations propagate to opposite directions or only the soliton propagates and the antisoliton stays fixed. The superposition leads to a smaller amplitude of the density oscillation between the two domain walls than for the potential barrier, as shown in Fig. 4.5. The impurity can move past a bath fermion only in a second-order process with an effective tunneling amplitude $\frac{J^2}{U}$ [118], which for $U \gg J$ results in the very slow
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Figure 4.5. The density distribution of the bath fermions and the impurity for (a) the Mott insulator initial state and (b) incommensurate filling. The density of the bath fermions is shown at $t = 0$ and the density of the impurity and bath fermions at (a) $t = 6/J$ and (b) $t = 8/J$. In the case of the impurity particle, the superposition of different evolutions leads to a smaller amplitude of the density oscillation in the final state. Figure adapted from Publication IV.

motion of the impurity.

Unlike in Fig. 4.2(c) and (d), where the antisoliton propagates away from the center, a maximum of the antisoliton distribution remains at the center in Figs. 4.6(c) and (d). The maximum indicates a bound state of the impurity and the antisoliton. The interference pattern in Figs. 4.6(c) and (d) indicates that the antisoliton can be in several momentum states since part of the momentum in the direction of the antisoliton can be absorbed by the impurity. These differences are also seen in the line profiles of Fig. 4.7 at a fixed time $t = 6/J$. Panels (e) and (f) show that the same characteristics of the antisoliton distribution are observable for weaker and experimentally more relevant interactions $U = V = 10J$. While strong interactions can lead to the population of higher bands [119], in recent experiments, band gaps of an order of magnitude larger than the bandwidth were used to ensure the validity of the single-band approximation [22, 25].

4.2.2 Resonance in the interactions

We find that the probability of creating a soliton and an antisoliton excitation depends on the difference between the interactions $U$ and $V$. In Publication II, we study an impurity particle in a bath which is in the Mott insulator state, and vary the on-site interaction $U$ around a fixed value of
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Figure 4.6. (a), (b) The soliton \(\langle n_j n_{j+1}\rangle\) and (c), (d) the antisoliton \(\langle n_j^h n_{j+1}^h\rangle\) distributions as in Fig. 4.2 after an impurity particle is created at the center of the lattice at \(t = 0\). Whereas the soliton distributions are almost identical for the static barrier and the impurity, the antisoliton distribution has a maximum at the center in the case of the impurity, indicating the impurity and antisoliton can form a bound state. Figure adapted from Publication IV.

\[ V \]

The total number of doublons \(N_{\uparrow\downarrow} = \sum_j \langle n_j^\uparrow n_j^\downarrow \rangle\) indicates whether the soliton and antisoliton excitations are created. Initially, \(N_{\uparrow\downarrow} = 1\) when the impurity is created at a site occupied by a bath fermion, as shown in Fig. 4.8. When \(U \gg J\) and \(U\) and \(V\) are far apart, the probability of excitations is very small since the process where the bath fermion moves to the neighboring site would not conserve energy. In this case, the bath fermions stay fixed and the impurity tunnels on the occupied sites in a second-order process, as discussed in Publication II. The average number of doublons is conserved, as shown in Fig. 4.8(a) for \(V = 100J\) and \(|V - U| = 10J\). When \(|V - U| \lesssim 3J\), the number of doublons decays to a value close to zero. Similarly, the number of solitons \(N_S\) increases to a value close to 1 when \(U\) is sufficiently close to \(V\). We suppose that this "resonance region" is related to the ranges of kinetic energies of the particles involved, since in order to conserve energy, the difference in \(U\) and \(V\) should be provided or absorbed by transitions in kinetic energy.
Figure 4.7. Soliton $\langle n_j \uparrow n_{j+1} \uparrow \rangle$ and antisoliton $\langle n_j \uparrow n_{j+1} \uparrow \rangle$ distributions for the static barrier and the impurity at time $t = 6/J$. In panels (a)-(d), $U = V = 50J$, and in panels (e) and (f), $U = V = 10J$. (b) The difference in the soliton distribution with respect to the initial state $\langle \Psi(t) | n_j \uparrow n_{j+1} \uparrow | \Psi(t) \rangle - \langle \Psi(0) | n_j \uparrow n_{j+1} \uparrow | \Psi(0) \rangle$ is similar for the two perturbations and shows that the excitations propagate slower in the incommensurately filled lattice. (c) The distribution of antisolitons has wavefronts and a minimum at the center in the case of the static barrier and a maximum in the case of the impurity. (d) For incommensurate filling, the antisoliton distribution is confined to the central region and the maximum in the impurity case is more pronounced. (e), (f) The same characteristics are observed for a weaker nearest-neighbor repulsion $V = 10J$. Figure adapted from Publication IV.
Figure 4.8. (a) The number of doubly occupied sites $\langle N_{\uparrow \downarrow}(t) \rangle$ calculated by TEBD with $V = 100J$ and varying $U$. When $U$ is sufficiently close to $V$, $\langle N_{\uparrow \downarrow}(t) \rangle$ decays as a function of time. (b) The number of solitons $N_S = \sum_j \langle n_j \uparrow n_j \uparrow + 1 \rangle$ as a function of time shows the same resonance behavior when $V = 50J$ and $U$ is varied. The evolution is very similar for the static potential barrier (solid lines) and the impurity (dashed lines). Figure adapted from Publications II and IV.
5. Decoherence in a many-body system

The process through which a quantum system becomes classical due to coupling to an environment is called decoherence. In the study of such open quantum systems, typically treated by master equations, the environment is a large thermal reservoir, and decoherence is connected to thermalization. In Publication III, we study decoherence during the unitary time evolution of a closed and finite system at zero temperature. The system of interest is an impurity particle, which interacts and becomes entangled with an environment of free fermions. Such controlled environments have been realized in experiments where an impurity atom or ion interacts with an ultracold gas of atoms of a different type [120–124].

In this Chapter, we present the related concepts of entanglement and decoherence via the Schmidt decomposition and the purity of reduced density matrices. We also present the central results related to decoherence in Publication III.

5.1 Schmidt decomposition

The Schmidt decomposition is a certain representation of a pure state in a finite-dimensional bipartite Hilbert space, and can be used for characterizing the entanglement between the two subsystems that partition the pure state. In a general form, a pure bipartite state can be written as

\[ |\Psi\rangle = \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} c_{i,j} |i\rangle_A \otimes |j\rangle_B , \]

where \(|i\rangle_A\) and \(|j\rangle_B\) are the orthonormal basis states of the subspaces A and B. When coefficients \(c_{i,j}\) are formed into a matrix \(c\), the matrix can be
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decomposed with the singular value decomposition (SVD)

\[ c = U \Lambda V^\dagger. \]  

(5.1)

The matrices \( U \in \mathbb{C}^{N_A \times \min(N_A, N_B)} \) and \( V \in \mathbb{C}^{N_B \times \min(N_A, N_B)} \) are unitary. The matrix \( \Lambda \) of size \( \min(N_A, N_B) \times \min(N_A, N_B) \) is diagonal and contains the singular values \( \lambda_\alpha \in \mathbb{R}_{\geq 0} \) on the diagonal. Using the SVD, eq. (5.1) can be written as

\[ |\Psi\rangle = \sum_{i,j} \sum_{\alpha=1}^{\chi} U_{i,\alpha} \lambda_\alpha V_{\alpha,j}^* |i\rangle_A |j\rangle_B \]  

(5.2)

\[ = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B, \]  

(5.3)

where the tensor product sign has been omitted. The new basis states are \( |\alpha\rangle_A = \sum_i U_{i,\alpha} |i\rangle_A \) and \( |\alpha\rangle_B = \sum_j V_{\alpha,j}^* |j\rangle_B \), and the number of nonzero singular values is denoted by \( \chi \leq \min(N_A, N_B) \). Equation (5.3) is called the Schmidt decomposition. The singular values, also called Schmidt coefficients, satisfy

\[ \sum_{\alpha=1}^{\chi} \lambda_\alpha^2 = 1. \]

The Schmidt number or Schmidt rank \( \chi \) is a measure of entanglement: The subsystems are entangled only if \( \chi > 1 \), whereas \( \chi = 1 \) corresponds to a product state \( |\Psi\rangle = |\alpha\rangle_A \otimes |\alpha\rangle_B \) with no entanglement. We can illustrate this by applying the Schmidt decomposition to two possible states of two qubits and identifying whether they are entangled. For the state \( |\Psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B) \), the matrix \( c \) in \( |\Psi\rangle = \sum_{i,j=0}^{1} c_{i,j} |i\rangle_A |j\rangle_B \) is

\[ c = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \]

In the SVD of eq. (5.1),

\[ U = V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Lambda = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \]

and the Schmidt number \( \chi = 2 \) shows that the state is entangled. For another example state \( |\Psi\rangle = \frac{1}{2} (|0\rangle_A |0\rangle_B + |0\rangle_A |1\rangle_B + |1\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B) \), one finds \( \lambda_1 = 1 \) and \( \lambda_2 = 0 \). In this case, \( \chi = 1 \), and \( |\Psi\rangle \) is the product state

\[ |\Psi\rangle = \lambda_1 |\alpha = 1\rangle_A |\alpha = 1\rangle_B = \frac{1}{2} (|0\rangle_A + |1\rangle_A) (|0\rangle_B + |1\rangle_B). \]

Since the dimension of \( \Lambda \) is \( \min(N_A, N_B) \), one could expect that in general, \( \chi \) grows approximately linearly with the number of states of the subsystems, which grows exponentially with the system size. It has been
shown however that in many cases, $\chi$ grows slower. These results are known as area laws [125]. For gapped one-dimensional systems in particular, the entanglement saturates to a constant with increasing system size [126]. For many gapless systems, entanglement also grows very slowly [127–130]. This observation is at the basis of algorithms which simulate large one-dimensional lattice systems by using a truncated representation of the state. Such algorithms, in particular the TEBD algorithm used in this work, are discussed in Chapter 6.

### 5.2 Purity of the density matrix

The description of a system coupled to an environment requires the distinction between a coherent superposition and a statistical mixture. A state in a coherent superposition of eigenstates is called a pure state and is described by a wavefunction $|\Psi\rangle$. Coherence means that there is a definite phase relation between the states in the superposition, which in measurements is seen as interference patterns. A coupling to an environment causes the system to evolve into a statistical mixture of certain states and destroys the superpositions of these states [131]. A statistical mixture of pure states is called a mixed state and cannot be described by a wave function. A general quantum state is described by a density matrix $\rho$, and for a pure state, $\rho = |\Psi\rangle \langle \Psi|$.

One measure of the quantum coherence of the state is the purity of the density matrix $\text{Tr}(\rho^2)$, which has values between 1 for a pure state and $\frac{1}{N}$ for a totally mixed state, where $N$ is the dimension of the density matrix. A similar measure is the von Neumann entropy $S(\rho) = -\text{Tr}(\rho \ln \rho)$. The purity of a subsystem can be accessed via its reduced density matrix. For a pure bipartite state as in eq. (5.3), the reduced density matrix of subsystem A is

$$\rho_A = \text{Tr}_B(\rho) = \sum_{\beta=1}^X \langle \beta |_B (|\Psi\rangle \langle \Psi|) |\beta \rangle_B = \sum_{\alpha=1}^X \lambda_{\alpha}^2 |\alpha \rangle_A \langle \alpha |_A,$$

and similarly, $\rho_B = \text{Tr}_A(\rho) = \sum_{\alpha=1}^X \lambda_{\alpha}^2 |\alpha \rangle_B \langle \alpha |_B$. The reduced density matrices of the subsystems have the same purity,

$$\text{Tr}(\rho_A^2) = \text{Tr}(\rho_B^2) = \sum_{\alpha=1}^X \lambda_{\alpha}^4.$$  

(5.4)
Decoherence in a many-body system

In a product state, $\chi = \lambda_1 = 1$ and $\text{Tr}(\rho_{A,B}^2) = 1$, whereas entanglement leads to $\lambda_\alpha < 1$ and a lower purity of the reduced density matrices even though the combined system continues to be in a pure state.

The Schmidt bases $|\alpha\rangle_A$ and $|\alpha\rangle_B$ are in fact the eigenbases of the reduced density matrices. In the eigenbasis, the density matrix is diagonal, whereas in some other basis it can have off-diagonal elements. The diagonal elements of the density matrix give the populations of the corresponding states, whereas off-diagonal elements are called coherences and indicate that the system is in a superposition. In Publication III, we study the density matrix of an impurity particle in the position basis. For a system in a pure state, the off-diagonal elements are largest in this basis, whereas for a mixed state, the density matrix is close to diagonal.

5.3 Decoherence of an impurity particle coupled to a bath

In Publication III, we study a closed system of an impurity and a bath of free fermions in a one-dimensional lattice. The impurity and bath are initially decoupled, $|\Psi(t = 0)\rangle = |\Psi_{\uparrow,\text{GS}}\rangle \otimes |\Psi_{\downarrow}\rangle$, and thus in pure states, $\text{Tr}(\rho_{\downarrow}^2(t = 0)) = \text{Tr}(\rho_{\uparrow}^2(t = 0)) = 1$. The bath, denoted by $\uparrow$, is initially in the ground state and the impurity, denoted by $\downarrow$, is localized at the center of the lattice. The time evolution is described by the Hamiltonian

$$H = -\sum_{j=1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} J_{\sigma} (c_{j\sigma}^\dagger c_{j+1\sigma} + \text{H.c.}) + U \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow}. \quad (5.5)$$

We study the decoherence of the impurity particle in terms of $\text{Tr}(\rho_{\downarrow}^2(t))$ due to the on-site interaction $U > 0$ with the bath. The impurity and bath fermions have different masses, which is reflected by the different tunneling energies $J_{\sigma}$. The tunneling energy is inversely proportional to the mass, so that for example $J_{\uparrow} < J_{\downarrow}$ means that the bath atoms are heavier than the impurity. In experiments with ultracold atoms in optical lattices, besides using atoms with different masses, the tunneling energies can be adjusted by the lattice potential [132, 133]. Quantum gas microscope techniques also allow to measure directly the purity of many-body states [134, 135].

We find the fastest decoherence when the bath particles are infinitely more massive than the impurity, $J_{\uparrow} / J_{\downarrow} \to 0$. The tunneling energy of the
impurity is used to set the scale for the time, $\frac{1}{J}$, and for the interaction $U$. The reduced density matrix of the impurity is shown in Fig. 5.1 at a fixed time $t = 6 \frac{1}{J}$ for two mass imbalances. One can see that a heavy impurity in a light bath with $J_\uparrow = 10 J_\downarrow$ (a) stays coherent with $\text{Tr}(\rho_\downarrow^2(t)) \approx 0.99$, whereas a light impurity in a heavy bath with $J_\uparrow = 0.1 J_\downarrow$ (b) loses its coherence faster. A high purity is connected to ballistic propagation, as seen in Fig. 5.2. The density distribution of an impurity in a light bath ($J_\uparrow = 10 J_\downarrow$) overlaps with the analytic solution for a single particle, which is always in a pure state. In a heavy bath ($J_\uparrow = 0.1 J_\downarrow$), the propagation is diffusive and characterized by a maximum of the density distribution at the initial position.

One can understand the fast decoherence in the heavy bath by considering the limiting case of an infinitely heavy bath, a large interaction $U$, and a very low filling of the bath, in which case possible bound states can be neglected. The entanglement of the impurity with the bath can be thought of as a measurement of the state of the impurity. Alternatively, the impurity can be thought to "measure" the state of the bath at the sites that it reaches. The part of the reduced density matrix of the bath corresponding to these sites becomes diagonal in the position basis, leading to the decay of purity. The purity of the reduced density matrix of the impurity decays equally (see eq. (5.4)). This simplified model is detailed.
Figure 5.2. The density distribution $\langle n_{i\downarrow}\rangle$ of the impurity particle interacting with a light ($J_{\uparrow} = 10J_{\downarrow}$) and a heavy ($J_{\uparrow} = 0.1J_{\downarrow}$) bath at time $t = 6\frac{J_{\downarrow}}{J_{\uparrow}}$. In the light-bath case, the density distribution overlaps with that of a single particle calculated analytically and has strong wave fronts and a minimum at the center, which are characteristic for ballistic (coherent) transport. In the case of the heavy bath, there is a maximum at the center, which characterizes diffusive transport. Figure originally published in Publication III.

in the Supplementary Material of Publication III. Note that even though the bath particles are immobile in the limit $\frac{J_{\uparrow}}{J_{\downarrow}} \to 0$, and the impurity experiences them as potential barriers, the situation is different from a particle in a fixed random potential which would be a one-body problem with no decoherence.

Decoherence is often connected to the dissipation of energy. In Publication III, we find that unlike decoherence, the dissipation of energy is fastest when the masses of the impurity and bath particles are equal. We study the linear density response of the noninteracting bath and find that the maximum dissipation at equal masses is connected to a peak in the integrated dynamic structure factor. We will leave out further discussion of linear response theory here and refer the reader for example to [136].
6. The time-evolving block decimation algorithm

The description of quantum many-body phenomena often leads to the formulation of problems which are not exactly solvable. An effective approach for three-dimensional systems are approximate mean field theories, but in some cases, such as low-dimensional systems, such approximations are inaccurate. Due to the low entanglement, however, quantum many-body models in one-dimensional lattices are often solvable numerically with high accuracy. A central advance in this field was the density matrix renormalization group (DMRG) algorithm [137–139] introduced by S. White in 1992. While the algorithm was originally designed to find the ground state of finite one-dimensional lattice models at zero temperature, similar algorithms have been devised to treat time-dependent problems [140–143], infinite lattices [144–146], higher-dimensional lattices [147], and finite-temperature and dissipative systems [148–150] also in higher dimensions [151], among other extensions and generalizations [130, 152, 153]. What these methods have in common is the representation of the many-body state as a product of matrices – a matrix product state (MPS) – which allows to truncate the state in the optimal way and to make computations feasible.

In this Chapter, we present briefly the time-evolving block decimation algorithm used in this work. The code has been developed earlier in the Quantum Dynamics research group at Aalto University and is based on the formulation by Vidal. More details on several points can be found in [140–142, 154–156]. Many open-source implementations of MPS-based algorithms also exist [157–159].
The time-evolving block decimation algorithm

6.1 The matrix product state

The size of the Hilbert space, which is the number of possible states, of a quantum many-body system grows exponentially with the size of the system. For a lattice of size $L$ with $S$ local states, there are $S^L$ possible states if the total particle number is not constrained. In the case of spinless fermions, for instance, $S = 2$ since a lattice site can be either empty or occupied. The exact diagonalization of the Hamiltonian which describes the many-body system is only possible up to $L \approx 10$. The size of the Hilbert space can however be significantly reduced by keeping only the most relevant states and discarding the rest, which allows to simulate systems larger by one or two orders of magnitude.

The matrix product representation is formed by expressing the Hilbert space of the one-dimensional lattice system as a tensor product of the local Hilbert spaces at each lattice site. A pure state on a one-dimensional lattice of size $L$ can be written as

$$|\Psi\rangle = \sum_{\sigma_1=1}^{S} \sum_{\sigma_2=1}^{S} \cdots \sum_{\sigma_L=1}^{S} c_{\sigma_1,\sigma_2,\ldots,\sigma_L} |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \cdots \otimes |\sigma_L\rangle \quad (6.1)$$

where $|\sigma_j\rangle$ are the local basis states denoted by the numbers $\sigma_j = 1, \ldots, S$. For the Hubbard model, the local basis can be constructed of the spin states $|\emptyset\rangle, |\uparrow\rangle, |\downarrow\rangle$, and $|\uparrow\downarrow\rangle$, and the size of the local Hilbert space is $S = 4$.

The idea of MPS representations is to write the coefficients $c_{\sigma_1,\sigma_2,\ldots,\sigma_L}$ as a tensor product,

$$c_{\sigma_1,\sigma_2,\ldots,\sigma_L} = A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_L} = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{L-1}} A_{\alpha_1}^{\sigma_1} A_{\alpha_2}^{\sigma_2} \cdots A_{\alpha_{L-1}}^{\sigma_L}, \quad (6.2)$$

where the tensors $A^\sigma$ are reshaped into matrices in the course of the algorithm. In the usual formulation for open boundary conditions, the tensors at the edges $j = 1, L$ have a different structure than the others: $A^\sigma_1$ is a row vector and $A^\sigma_L$ a column vector in order to produce a scalar. The different varieties of MPS-based algorithms employ slightly different notations for the tensor product. In the proceeding Sections, we will use the notation of [140–142].
The SVD is repeated on the coefficients $c_{\sigma_1\sigma_2\cdots\sigma_L}$, or equivalently applying the Schmidt decomposition (5.3) repeatedly on the state $|\Psi\rangle$. To apply the SVD, the coefficient $c_{\sigma_1\sigma_2\cdots\sigma_L}$ can be shaped into a matrix $c_{\sigma_1,(\sigma_2\cdots\sigma_L)}$ of dimension $S \times S^{L-1}$. The SVD is then

$$c_{\sigma_1,(\sigma_2\cdots\sigma_L)} = \sum_{\alpha_1=1}^{r_1} U_{\sigma_1,\alpha_1} \lambda_{\alpha_1} V_{\alpha_1,(\sigma_2\cdots\sigma_L)^\dagger}. \quad (6.3)$$

In the DMRG notation [130], $U_{\sigma_1,\alpha_1}$ is identified with $A_{\alpha_1}^{\sigma_1}$ of eq. (6.2). The Schmidt number for the first decomposition is $r_1 \leq S$ and it grows towards the center of the lattice as the dimensions of the decomposed matrix change. In Vidal’s description [140–142], $U_{\sigma_1,\alpha_1}$ of eq. (6.3) is denoted by $\Gamma_{\alpha_1}^{\sigma_1}$, and the sum over $\alpha_1$ is expanded to a fixed number $\chi$, so that $\lambda_{\alpha_1} = 0$ for $\alpha_1 > r_1$.

$$c_{\sigma_1\sigma_2\cdots\sigma_L} = \sum_{\alpha_1=1}^{\chi} \Gamma_{\alpha_1}^{\sigma_1} \lambda_{\alpha_1} V_{\alpha_1,(\sigma_2\cdots\sigma_L)^\dagger}. \quad (6.4)$$

The SVD is repeated on $V_{\alpha_1,(\sigma_2\cdots\sigma_L)^\dagger}$ shaped as $V_{(\alpha_1\sigma_2),(\sigma_3\cdots\sigma_L)^\dagger}$.

$$V_{(\alpha_1\sigma_2),(\sigma_3\cdots\sigma_L)^\dagger} = \sum_{\alpha_2=1}^{\chi} U_{(\alpha_1\sigma_2),\alpha_2} \lambda_{\alpha_2} V_{\alpha_2,(\sigma_3\cdots\sigma_L)^\dagger}. \quad (6.5)$$

where $U_{(\alpha_1\sigma_2),\alpha_2}$ is identified with $\Gamma_{\alpha_1\alpha_2}^{\sigma_2}$ and

$$c_{\sigma_1\sigma_2\cdots\sigma_L} = \sum_{\alpha_1=1}^{\chi} \sum_{\alpha_2=1}^{\chi} \Gamma_{\alpha_1}^{\sigma_1} \lambda_{\alpha_1} \Gamma_{\alpha_1\alpha_2}^{\sigma_2} \lambda_{\alpha_2} V_{(\alpha_2\sigma_3),(\sigma_4\cdots\sigma_L)^\dagger}. \quad (6.6)$$

By repeating this procedure, one arrives at

$$c_{\sigma_1\sigma_2\cdots\sigma_L} = \sum_{\alpha_1=1}^{\chi} \sum_{\alpha_2=1}^{\chi} \cdots \sum_{\alpha_{L-1}=1}^{\chi} \Gamma_{\alpha_1}^{\sigma_1} \lambda_{\alpha_1} \Gamma_{\alpha_1\alpha_2}^{\sigma_2} \lambda_{\alpha_2} \cdots \lambda_{\alpha_{L-1}} \Gamma_{\alpha_{L-1}}^{\sigma_{L-1}} \Gamma_{\alpha_{L-1}}^{\sigma_{L}} \cdots \lambda_{\alpha_L} \Gamma_{\alpha_L}^{\sigma_L} |\sigma_1\sigma_2\cdots\sigma_L\rangle. \quad (6.7)$$

One can think of the vector or diagonal matrix $\lambda^{[j]}$ with elements $\lambda_{\alpha_j}$ as associated to bond $j$ and the tensor $\Gamma^{[j]}$ to the link between bonds $j$ and $j+1$. The time-evolving block decimation algorithm
The number of coefficients $c_{\sigma_1,\sigma_2,\cdots,\sigma_L}$ in the representation of eq. (6.1) is $S^L$, and in eq. (6.7), the number of parameters required to write the state is $(L - 2)\chi^2 S + 2\chi S + (L - 1)\chi$. For eq. (6.7) to be exact, $\chi \approx S^{\frac{L}{2}}$, and the number of parameters is of the order $S^L$ as in the original representation. A significantly smaller $\chi$ is however sufficient to describe the state with high accuracy. This truncation is done by selecting the most relevant states in the superposition, with largest Schmidt coefficients $\lambda_\alpha$, and normalizing the state accordingly. Numerical analysis has shown that the coefficients $\lambda_\alpha$ decay exponentially with increasing $\alpha$ [141]. At quantum phase transitions, entanglement has been shown to grow logarithmically with $L$ [127], and therefore a larger $\chi$ is required to represent the state accurately than in non-critical parameter regimes where the entanglement saturates. In this work, we have used $L$ between approximately 60 and 100 and $\chi \approx 100$.

### 6.3 Operating with single-site operators

For Hamiltonians with up to nearest-neighbor terms, calculating the ground-state and time-evolved wave functions and observables involves operations on single lattice sites and pairs of neighboring sites. Such operations can be done conveniently within the matrix product formalism. Operating on the state with a single-site operator only requires updating the $\Gamma$ tensor at the site which is operated on. An operator $O_j$ acting on site $j$ can be written $O_j = \sum_{s_j,s'_j=1}^S O_{s_j}^{s'_j} |s_j\rangle \langle s'_j|$. In order to operate on site $j$, one divides the state (6.7) into subsystems

$$|\Psi\rangle = \sum_{\alpha_{j-1},\alpha_j} |\varphi_{\alpha_{j-1}}^{[1\cdots j-1]}\rangle \lambda_{\alpha_{j-1}} \sum_{\sigma_j} \Gamma^{\sigma_j}_{\alpha_{j-1}\alpha_j} |\sigma_j\rangle \lambda_{\alpha_j} |\varphi_{\alpha_j}^{[j+1\cdots L]}\rangle,$$

where

$$|\varphi_{\alpha_{j-1}}^{[1\cdots j-1]}\rangle = \sum_{\alpha_1,\cdots,\alpha_{j-2}} \sum_{\sigma_1,\cdots,\sigma_{j-1}} \Gamma^{\sigma_1}_{\alpha_1} \lambda_{\alpha_1} \cdots \lambda_{\alpha_{j-2}} \Gamma^{\sigma_{j-1}}_{\alpha_{j-2}\alpha_{j-1}} |\sigma_1\cdots\sigma_{j-1}\rangle$$

and

$$|\varphi_{\alpha_j}^{[j+1\cdots L]}\rangle = \sum_{\alpha_{j+1},\cdots,\alpha_{L-1}} \sum_{\sigma_{j+1},\cdots,\sigma_L} \Gamma^{\sigma_{j+1}}_{\alpha_{j+1}\alpha_{j+1}} \lambda_{\alpha_{j+1}} \cdots \lambda_{\alpha_{L-1}} \Gamma^{\sigma_L}_{\alpha_{L-1}} |\sigma_{j+1}\cdots\sigma_L\rangle.$$
One can see that operating on site \(j\) with \(O_j\) results in updating \(\Gamma_{\alpha_{j-1}\alpha_j}\) as
\[
\tilde{\Gamma}_{\alpha_{j-1}\alpha_j} = \sum_{s_j} O_{s_j}^\sigma \Gamma_{\alpha_{j-1}\alpha_j}^\sigma.
\] (6.9)

For fermion systems, one has to account for the anticommutation relations, which can produce an additional minus sign depending on \(O_j\) and \(s_j\).

### 6.4 Nearest-neighbor operations

Operating with a two-site operator on neighboring sites \(j\) and \(j+1\) results in updating \(\Gamma_{\alpha_{j-1}\alpha_j}, \lambda_{\alpha_j},\) and \(\Gamma_{\alpha_j\alpha_{j+1}}\). A nearest-neighbor operator can be written as
\[
O_{j,j+1} = \sum_{s_j,s_{j+1}}^{s_j,s_{j+1}} \langle s_j s_{j+1} | r_j r_{j+1} \rangle.
\] (6.10)

Similarly as for the single-site operations, the state can be decomposed into the relevant two sites and the remaining parts:
\[
|\Psi\rangle = \sum_{\alpha_{j-1}\alpha_j,\alpha_{j+1}} \lambda_{\alpha_{j-1}} \sum_{\sigma_j}^{\Gamma_{\alpha_{j-1}\alpha_j}} |\sigma_j\rangle \times \lambda_{\alpha_j} \sum_{\sigma_{j+1}}^{\Gamma_{\alpha_{j}\alpha_{j+1}}} |\sigma_{j+1}\rangle \lambda_{\alpha_{j+1}} |\varphi^{[j+2:]_{L}}\rangle.
\] (6.11)

Operating on \(|\Psi\rangle\),
\[
O_{j,j+1} |\Psi\rangle = \sum_{\alpha_{j-1}\alpha_{j+1}} \lambda_{\alpha_{j-1}} \sum_{\sigma_j,\sigma_{j+1}} \theta_{\alpha_{j-1}\alpha_j,\sigma_{j+1}} |\sigma_j\rangle |\sigma_{j+1}\rangle \lambda_{\alpha_{j+1}} |\varphi^{[j+2:]_{L}}\rangle,
\] (6.12)

where
\[
\theta_{\alpha_{j-1}\alpha_j,\sigma_{j+1}} = \sum_{s_j,s_{j+1}}^{s_j,s_{j+1}} O_{s_j,s_{j+1}}^\sigma \Gamma_{\alpha_{j-1}\alpha_j}^\sigma \Gamma_{\alpha_j\alpha_{j+1}}^{\sigma_{j+1}} \lambda_{\alpha_j} \lambda_{\alpha_{j+1}}.
\] (6.13)

One has to now return the state into the form of the original decomposition (6.11). This is done by performing an SVD on the \(\theta\) tensor written as an \(S_{\chi} \times S_{\chi}\) matrix:
\[
\theta_{(\sigma_j\alpha_{j-1},(\sigma_{j+1}\alpha_{j+1})} = \sum_{\beta=1}^{S_{\chi}} U_{(\sigma_j\alpha_{j-1}),\beta} \lambda_{\beta} V_{(\sigma_{j+1}\alpha_{j+1}),\beta}^\dagger
\] (6.14)
\[
\approx \sum_{\beta=1}^{\chi} U_{(\sigma_j\alpha_{j-1}),\beta} \lambda_{\beta} V_{(\sigma_{j+1}\alpha_{j+1}),\beta}^\dagger.
\] (6.15)

On the second line, the dimension \(\beta\) of the matrices is truncated from \(S_{\chi}\) to \(\chi\) in order to retain the original Schmidt number. One can now identify
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the matrices $U$ and $V^\dagger$ with the new tensors $\tilde{\Gamma}^j$ and $\tilde{\Gamma}^{j+1}$, respectively,

$$\theta_{\alpha_{j-1}\alpha_j}^{\sigma_j\sigma_{j+1}} \approx \sum_{\beta=1}^{\chi} \tilde{\Gamma}^{\sigma_j}_{\alpha_{j-1}\beta} \lambda_{\beta}^{\sigma_{j+1}} \tilde{\Gamma}^{\sigma_{j+1}}_{\alpha_j+1} \beta$$  \hspace{1cm} (6.16)

Accuracy and efficiency can be improved by choosing position- and time-dependent Schmidt numbers based on a maximum tolerance on the truncation error $\epsilon_j = \sum_{\alpha>\chi} \lambda_{\alpha_j}^2$ [130]. The errors of the algorithm used in this work are discussed in Sec. 6.7. The Hamiltonians considered here contain only single-site and nearest-neighbor operators but longer-range terms have also been implemented [157, 160–162].

6.5 Time evolution

The state (6.7) can be evolved in time by applying the unitary time-evolution operator $U = e^{-iHt}$. This procedure is often called real-time evolution to distinguish it from imaginary-time evolution, which can be used for simulating finite temperatures and calculating the ground state. In this work, we consider Hamiltonians of the form $H = \sum_j H_{j,j+1}$. The operator $e^{-iHt}$ operates on the whole system, and has to be decomposed into two-site operators in order to update the state according to Sec. 6.4. This can be done with the help of the Suzuki-Trotter (ST) decomposition $e^{x(A+B)} = e^{xA}e^{xB} + O(x^2)$, where $A$ and $B$ are non-commuting operators and $x$ is a small parameter [163, 164]. The operators $H_{j,j+1}$ with $j$ odd do not generally commute with the operators with $j$ even. It is therefore convenient to divide the Hamiltonian to odd and even parts, $H = H_{\text{odd}} + H_{\text{even}}$, where $H_{\text{odd}} = \sum_{j \text{ odd}} H_{j,j+1}$ and $H_{\text{even}} = \sum_{j \text{ even}} H_{j,j+1}$. Using the ST decomposition,

$$e^{-i\delta t(H_{\text{odd}}+H_{\text{even}})} = e^{-iH_{\text{odd}}\delta t}e^{-iH_{\text{even}}\delta t} + O(\delta t^3),$$  \hspace{1cm} (6.17)

where $\delta t$ is a small time step. Since all the terms in $H_{\text{odd}}$ commute, and respectively for $H_{\text{even}}$, one can divide the time-evolution operator into a product of two-site operators,

$$e^{-iH_{\text{odd}}\delta t}e^{-iH_{\text{even}}\delta t} = \prod_{j \text{ odd}} e^{-iH_{j,j+1}\delta t} \prod_{j \text{ even}} e^{-iH_{j,j+1}}.$$

Evolving the state from 0 to $t$ now requires $\frac{t}{\delta t}$ repeated operations, which in practice are performed in consecutive sweeps across the lattice [154].
The error accumulated due to the approximation (6.17) scales with $\frac{t}{\delta t} \cdot \delta t^2 = t\delta t$. Equation (6.17) employs the first-order ST decomposition, and higher-order decompositions produce smaller errors. The second-order decomposition with an error scaling as $t\delta t^2$ has been used in this work for the real-time evolution. Any state stored in the MPS form can be used as an initial state, for example a product state or a previously calculated ground state.

6.6 Finding the ground state

While many algorithms utilize the Suzuki-Trotter decomposition for the real-time evolution, different approaches are used for the ground state search. In the original formulation of DMRG, block Hamiltonians are diagonalized for shifting bipartitions of the lattice [137, 138]. Most of the current MPS implementations minimize the energy locally. The ground state of the total system is found by repeating local operations in sweeps across the lattice. Another method, suggested in [141] and applied in this work, is to operate with an imaginary-time evolution operator on the local states to reach the ground state.

The procedure of the imaginary-time evolution is similar to the real-time evolution described in Sec. 6.5. The ground state $|\Psi_{GS}\rangle$ is obtained by operating on the state with $e^{-i(-it)H} = e^{-tH}$:

$$
|\Psi_{GS}\rangle = \lim_{t \to \infty} e^{-tH} |\Psi_0\rangle = \lim_{t \to \infty} \sum_{n=1}^{\infty} e^{-tE_n} a_n |\varphi_n\rangle,
$$

where $|\Psi_0\rangle$ is the initial state and $\parallel \cdots \parallel$ denotes the norm. The initial state can be written as a sum of the eigenstates $|\varphi_n\rangle$ of the Hamiltonian, and $E_n > 0$ are the eigenenergies. The term with lowest energy $E_1$ decays slowest and therefore $|\varphi_1\rangle = |\Psi_{GS}\rangle$ is the only term which remains at $t \to \infty$, assuming that $|\Psi_0\rangle$ and $|\Psi_{GS}\rangle$ are not orthogonal.

As an indicator for convergence, one can monitor the sum of discarded Schmidt coefficients $\sum_{\alpha > \chi} \lambda_\alpha^2$ or the change in the Schmidt coefficients or $\Gamma$ tensors. The convergence of observables can also be used as a criterion. Numerical noise can potentially lead the imaginary-time evolution to convergence to a state with a different particle number than the one of $|\Psi_0\rangle$ if such a state has a lower energy. This can be prevented by imposing the conservation of the particle number [155]. Utilizing different types of
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symmetries also improves the efficiency of the algorithms [130, 165–168].

6.7 Errors in the time evolution

The approximations used in the real-time evolution result in two types of errors. The first error source is the Suzuki-Trotter decomposition (eq. (6.17)), and the second one is the truncation after two-site operations, as in eq. (6.15). The ST error can be decreased by using a smaller time step $\delta t$ or a higher-order ST decomposition. With a smaller time step, the number of operations required to reach a certain simulation time increases. This means that more truncations are made, which leads to an increasing truncation error.

Figure 6.1 illustrates the behavior of these different error sources, similarly as in [169]. The time-dependent wave function $|\Psi(t)\rangle$ can be solved analytically for the XX model with the initial state $|\Psi(t = 0)\rangle = |\uparrow \uparrow \cdots \uparrow \downarrow \cdots \downarrow \rangle$ [170]. As an error estimate, one can use the deviation in the local magnetization between the TEBD solution and the exact solution. The maximum deviation

$$\Delta_{\text{max}}(t) = \max_l |\langle S_{l,\text{TEBD}}(t)\rangle - \langle S_{l,\text{exact}}(t)\rangle|$$

is shown as a function of time in Fig. 6.1. A smaller time step $\delta t$ leads to a smaller $\Delta_{\text{max}}(t)$ in the beginning of the time evolution. For each $(\delta t, \chi)$ pair, there is a "runaway time" after which $\Delta_{\text{max}}(t)$ starts deviating from the initial behavior as the number of states kept in the truncation is not sufficiently large anymore. For $\delta t = 0.001\frac{1}{J}$ and $\chi = 20$ for example, this occurs around $t = 4\frac{1}{J}$. In Publications I–IV, we have used different values of $\chi$ to check that the observables do not depend on $\chi$. 

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Figure 6.1. The maximum deviation in local magnetization $\Delta_{\text{max}}(t)$ between the TEBD solution and the exact solution for different values of $\delta t$ and $\chi$. 
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7. Conclusions

In this work, we have studied the dynamics of fermions in one-dimensional lattices, perturbed by local potentials or impurity particles, using the numerical time-evolving block decimation method and analytic arguments. For fermions with an attractive on-site interaction, we have showed that fast wave-packet potentials with a velocity above the maximum group velocity do not create excitations and preserve the initial correlations, whereas slow potentials deform the fermion cloud and destroy correlations. We have also studied decoherence in a mass-imbalanced system with an impurity particle in a bath of free fermions. The decoherence of the quantum state of the impurity is fastest when the bath is infinitely massive compared to the impurity, whereas the dissipation of energy is fastest for equal masses.

For fermions with a nearest-neighbor repulsion, a strong repulsion compared to the kinetic energy leads to interesting dynamical phenomena. In particular, we have found a resonance region in the interactions between the bath fermions and between an impurity and the bath, within which a soliton and an antisoliton excitation are created in the bath. The soliton and antisoliton have different dynamics since the impurity can form a bound state with the antisoliton. In addition, the presence of solitons in the initial state restricts the motion of the antisoliton. We have developed a simplified analytic model of the soliton excitations in the limit of a strong repulsion and a low soliton density, where solitons can be mapped to free fermions. This model provides a starting point for understanding soliton excitations in lattice systems. Ultracold gases in optical lattices offer possibilities to test these predictions experimentally. Nearest-neighbor interactions in lattice models have recently been demonstrated.
Conclusions

with dipolar atoms and molecules, and the motion of impurity particles has been tracked with single-site resolution using a spin-resolved quantum gas microscope. The recent observations of short-range antiferromagnetic correlations suggest a possibility to observe the dynamics of basic excitations of the antiferromagnetic state.
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