Many-particle dynamics of driven-dissipative Bose-Einstein condensates

Master’s thesis
by
Jonathan Stysch

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Main examiner: Priv.-Doz. Dr. Holger Cartarius
Co-examiner: Prof. Dr. Siegfried Dietrich

First Institute of Theoretical Physics
University of Stuttgart
Pfaffenwaldring 57, 70550 Stuttgart
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1 Introduction

1.1 Motivation

Starting in 1995 with the first experimental realizations of Bose-Einstein condensates by Cornell, Wieman, and Ketterle [1, 2], ultracold atoms have provided a fruitful research field for the experimental and theoretical investigation of strongly correlated quantum systems. Initially the emphasis of most works in this field was on analyzing the matter wave properties of systems confined in magnetic traps, which can be described in a mean-field approximation with the Gross-Pitaevskii nonlinear Schrödinger equation. A more recent topic are Bose-Einstein condensates in optical lattices, which provide a versatile tool for the study of condensates in a vast number of different setups with easily controllable system parameters [3]. The Bose-Hubbard model [4] presents a description for the dynamics of ultracold atoms in a deep optical lattice, similarly to the Hubbard model in solid state physics [5], and has been validated experimentally [6]. It can be used for the investigation of many-body non-equilibrium dynamics [7] and transport processes beyond a mean-field description [8]. Moreover, the model provides a framework for the general simulation of lattice models, which might in the future give experimental insight into phenomena such as high-$T_c$ superconductivity, for which to date no rigorous theoretical treatment exists [9].

Particularly interesting in this context are open quantum systems for which an environment provides particle gain and/or loss. On the one hand a balanced gain and loss can give rise to steady states [10] similarly to those found with the Gross-Pitaevskii equation for $PT$-symmetric complex potentials [11]. On the other hand controlled dissipation of particles has been shown to induce correlations in a system [12], which allows for the engineering of pure states required in quantum computation [13]. Dissipation is also conjectured to play an important role for transport phenomena in biological clusters [14]. A well established extension of the Bose-Hubbard model to treat open systems is found with a quantum master equation in Lindblad form [15], which is able to describe localized particle gain and loss as well as phase noise [16]. However, while localized dissipation can reliably be realized with a focused electron beam [17], applying localized particle gain in an optical lattice is far more challenging [18]. It is therefore the central object of this thesis to investigate how a part of a system within the Bose-Hubbard model can act as an environment for the dynamics of a subsystem, instead of using an external Born-Markov environment. To do so, the behavior of two different setups is analyzed independently.
1 Introduction

In the first part of this thesis a closed Hermitian system of six sites on a ring is considered that is divided into two symmetric three-site subsystems acting as an environment for each other. The subsystems are initially separated from each other in the sense that each of them contains a pure Bose-Einstein condensate that shares no phase coherence with the other. The dynamics induced by coupling the subsystems together at \( t = 0 \) is found to be similar to the oscillating behavior in the open system studied in [11]. Moreover, by analyzing the evolution of the purity of the single-particle density matrix, a periodic loss and subsequent restoration of the coherence within the subsystems is observed, which is a characteristic behavior of driven-dissipative open systems [19]. These oscillations of the purity are successfully related to the time evolution of the average contrast in an interference experiment and thereby rendered observable in an experiment.

In the second part of this work a different approach is pursued to simulate an environment. A one-dimensional optical lattice is subject to particle loss at its central site. The system is prepared such that the outer sites of this chain can act as a reservoir for its lossy site. With this setup a quasi-constant filling level of the central site can be sustained over a long time range, analogously to the steady states found in [10] for open many-particle systems with balanced gain and loss. This study is inspired by an experiment [20], in which the central site of an optical lattice was subject to a loss of atoms via an electron beam. In that work a bistable behavior was found with respect to the filling level of the central site. If it is initially filled with the same number of atoms as the adjacent reservoir sites, this ratio is sustained up to a critical loss rate. If it is empty at the beginning of the time evolution, a filling below that of the neighboring sites is stabilized. The combination of several physical processes is made responsible for this bistability. It is investigated in this thesis whether this behavior can be reproduced in a mathematical model containing all of these processes. As will be shown this is not the case. It seems that a further source of incoherence has to be taken into account.

1.2 Outline

Chapter 2 provides a review of Bose-Einstein condensation. The purity of the single-particle density matrix is introduced as a measure of the coherence in a quantum system and the Gross-Pitaevskii equation is presented as the mean-field description of the condensate. The chapter is concluded with a discussion of \( PT \)-symmetric complex potentials in the analysis of open systems within the mean-field approach.

In chapter 3 the Bose-Hubbard Hamiltonian is introduced as the many-particle description of a Bose-Einstein condensate in a deep optical lattice. The model is extended in the framework of a quantum master equation that allows for the treatment of interactions with an environment. An approximation of the extended model is found in the Bogoliubov back-reaction method. The full many-body description as well as the approximation are related to the mean-field approach in the final section of the chapter.
The discussion of the six-site Hermitian system divided into two symmetric subsystems is given in chapter 4. A scheme for the construction of the subsystems’ separated many-particle states out of mean-field coefficients is presented and the dynamical behavior induced by the coupling is analyzed. The development of the purity of the subsystems is investigated and linked to the average contrast in an experiment. Finally, the dimensionless units of the theoretical treatment are related to their physical counterparts with a simple ansatz for the trapping potential and the wave functions of the particles.

The one-dimensional optical lattice subject to localized dissipation is treated in chapter 5. Its first two sections provide a discussion of the choice of the initial state and the system parameters as well as the approximation of the Bose-Hubbard model in the regime of high particle numbers. This is followed by an analysis of the dynamics both in the absence of phase noise and in the presence of it, including an investigation of the dominating transport processes in both cases. Chapter 6 concludes the thesis and provides a brief outlook on future topics for investigation.
2 Bose-Einstein condensation

Following Bose’s work on the quantum statistics of photons [21] the concept of Bose-Einstein condensation was introduced in two papers by Einstein in 1924 and 1925 [22, 23]. Einstein showed that in an ideal, non-interacting gas of Bosons below a critical temperature close to absolute zero the majority of particles falls into the lowest accessible quantum state. This fraction of particles occupying the lowest energy level form thereby a macroscopic quantum state referred to as a “Bose-Einstein condensate” (BEC) which can be described with a single wave function. Exhibiting quantum effects on a macroscopic scale, BECs have been related to phenomena like superfluidity and superconductivity. Using the process of laser cooling the first Bose-Einstein condensates where produced in 1995 from diluted gases of rubidium atoms by Cornell and Wieman [1] and sodium atoms by Ketterle [2], for which they received the Nobel price in 2001.

Since then, BECs have been the subject of a vast amount of experimental and theoretical studies, in particular because they can provide a means for the investigation of quantum-mechanical systems in a controllable manner.

2.1 Transition criterion

In his original papers Einstein used a purely quantum statistical argument for a uniform non-interaction Bose gas in the thermodynamic limit to derive the transition temperature $T_c$ below which a finite proportion of the Bosons occupies the lowest energy state. The total count of particles in the exited states $N_{ex}$ is obtained by integrating over the product of the Bose-Einstein distribution function

$$N_k = \frac{1}{e^{(e_k-\mu)/k_BT} - 1}$$  \hspace{1cm} (2.1)

at temperature $T$ with the density of states

$$D(\epsilon) = \frac{V}{4\pi} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\epsilon}.$$  \hspace{1cm} (2.2)

Here $\epsilon_k$ is the energy of the $k^{th}$ state, which is set $\epsilon_1 = 0$ for the ground state and positive for all other states, $\mu \leq 0$ denotes the chemical potential, $k_B$ the Boltzmann constant, $V$ the volume, $\hbar$ the reduced Plank’s constant and $m$ the mass of one atom. The integral

$$N_{ex} = \int_0^\infty \frac{D(\epsilon)}{e^{(e_k-\mu)/k_BT} - 1} d\epsilon$$  \hspace{1cm} (2.3)
yields [24]

$$\frac{N_{\text{ex}}}{V} = \lambda_i^{-3} F_{3/2} \left( e^{\mu/k_B T} \right)$$

(2.4)

with the thermal de Broglie wavelength $\sqrt{2\pi \hbar / \sqrt{mk_B T}}$ and the function $F_{3/2}(x) = \sum_{n=1}^\infty x^n / n^{3/2}$. Since the chemical potential $\mu$ increases with decreasing temperature but cannot become greater than $\epsilon_1 = 0$ there is a critical temperature $T_c$ for $\mu = 0$ below which the occupation density of the exited states $N_{\text{ex}}/V$ is no longer constant,

$$T_c = \frac{2\pi \hbar^2}{k_B m} F_{3/2}(1)^{-2/3} \left( \frac{N}{V} \right)^{2/3}.$$  

(2.5)

Therefore, this temperature marks the point at which the gas transitions into a Bose-Einstein condensate, where the lowest energy state of the system, which is not considered in the integral (2.3), is occupied by a finite fraction of the atoms.

This statistical argument is only valid for an ideal Bose gas, in which the particles do not interact with each other. In an interacting Bose gas the single particle energy levels are no longer defined. In presence of particle interaction a new criterion for condensation can be found using the concept of off-diagonal long range order developed by Penrose, Onsager and Yang [25–27].

All single-particle properties of a system are described by its single-particle density matrix $\hat{\sigma}$ (SPD matrix)

$$\sigma_{jk} = \langle \hat{a}_j^\dagger \hat{a}_k \rangle = \langle j | \hat{\sigma} | k \rangle.$$  

(2.6)

Here $\hat{a}_j^\dagger$ and $\hat{a}_k$ are the creation and annihilation operators creating and annihilating a Boson in the single-particle states $|j\rangle$ and $|k\rangle$, respectively. The SPD matix can be related to the full density operator of the system $\hat{\rho}$ by tracing over all but one of the $N$ indistinguishable particles [28],

$$\sigma_{jk} = N \langle k | \text{tr}_{2\ldots N} \hat{\rho} | j \rangle \equiv N \langle k | \hat{\rho}_1 | j \rangle,$$

(2.7)

with $\hat{\rho}_1$ being called the reduced single-particle density operator.

For an ideal Bose gas the SPD matrix in position space using the bosonic field operators is given by [24]

$$\langle \hat{\psi}^\dagger(y) \hat{\psi}(x) \rangle = \frac{1}{V} \sum_p N_p e^{ip(x-y)/\hbar},$$

(2.8)

where $N_p$ is the number of particles in a state with momentum $p$. Above the transition temperature, where the ground state is not macroscopically occupied, the sum has to vanish in the off-diagonal long range regime $|x-y| \rightarrow \infty$ because of the rapidly oscillating summands. However, below the transition temperature $N_0$ is finite and hence

$$\lim_{|x-y| \rightarrow \infty} \langle \hat{\psi}^\dagger(y) \hat{\psi}(x) \rangle = \frac{N_0}{V}.$$  

(2.9)
2.2 Purity of a Bose-Einstein condensate

This criterion that in a Bose-Einstein condensate some coherence is preserved over arbitrarily long distances can be generalized for interacting Bose gases,

\[
\lim_{|x-y|\to\infty} \langle \hat{\psi}^\dagger(y) \hat{\psi}(x) \rangle \neq 0.
\] (2.10)

In this form, the criterion for Bose-Einstein condensation is not applicable to a finite system. However, Yang was able to show [27] that it is equivalent to the more practical criterion that the SPD matrix \( \hat{\sigma} \) has to have an eigenvalue of order \( N \). For an ideal Bose gas it is easy to see why this has to be true since the SPD matrix is diagonal in the single-particle states with the occupation of each state being the corresponding eigenvalue. Since this final criterion also holds in the presence of particle interaction it will be the one applied in the following. Moreover, it is especially feasible for BECs in deep optical lattices, where the particles are located at the lattice sites and the dimension of SPD matrix is therefore finite.

2.2 Purity of a Bose-Einstein condensate

A measure for the mixedness of a quantum mechanical state is given by the purity of the density matrix \( \text{tr} \hat{\rho}^2 \), which is equal to one for a pure state and less than one for a superposition of states. A similar approach can be taken to describe the fraction of particles in a condensate sharing the same single-particle state. We define the purity of the reduced single-particle density matrix as

\[
P' = \text{tr} \hat{\sigma}^2 \text{red}, \quad \text{with } \hat{\sigma} \text{red} = \frac{\hat{\sigma}}{\text{tr} \hat{\sigma}},
\] (2.11)

where the trace over the SPD matrix is equal to the total particle number \( N \) for a closed system,

\[
\text{tr} \hat{\sigma} = \sum_j \langle \hat{a}_j^\dagger \hat{a}_j \rangle = N,
\] (2.12)

and equal to the expectation value of the particle number \( \langle N \rangle \) for an open system. Because diagonalizing a matrix leaves the trace invariant, \( P' \) can be conveniently expressed in terms of the eigenvalues of the SPD matrix \( \lambda_j \),

\[
P' = \frac{1}{N^2} \sum_j \lambda_j^2.
\] (2.13)

Since \( \sum_j \lambda_j = N \), it is apparent that this purity has to be maximal if all but one eigenvalue are equal to zero and takes the value \( P' = 1 \) in this case, which describes a system with all particles in the same single-particle state. The lowest possible value of the purity \( P' = 1/D \) depends on the dimension \( D \) of the system and is realized if all
eigenvalues share the same value $\lambda_j = N/D$. To make the purity an even more graphic quantity it is mapped onto the interval $[0, 1]$, 

$$P = \frac{D}{D-1} P' - \frac{1}{D-1}, \quad (2.14)$$

such that $P = 0$ describes the case where none of the particles share the same state and $P = 1$ is still equal to a perfectly pure BEC.

One situation which has not been considered yet is that of a fragmented condensate. If $k \ll D$ of the eigenvalues of $\hat{\sigma}$ are of the order $N$, there are $k$ separate BECs in the system with random relative phases [29]. An example for this would be a system of two spatially separated BECs whose wave functions do not overlap. In this case, even if all particles of their respective condensate share the same single-particle state, the overall purity would still be only $P' = 0.5$. Therefore, when studying a system that is likely to exhibit fragmentation it might be necessary to consider, rather than the purity, the eigenvalues of $\hat{\sigma}$ directly. Alternatively one can consider the purity separately applied to each subspace of the Hilbert space in which one of the fragments exists.

### 2.3 The Gross-Pitaevskii equation

A very successful tool for analysing the dynamics of BECs is the Gross-Pitaevskii equation (GPE) [30, 31]. It is a mean-field approximation assuming all particles of the system to share the same single-particle state $\phi(r)$ forming a Hartree product,

$$\Psi(r_1, r_2 \ldots, r_N) = \prod_{i=1}^{N} \phi(r_i). \quad (2.15)$$

Assuming a perfectly pure condensate, this approach has been shown to be very accurate in the limit $T \to 0$ and $N \to \infty$ [32], but on the other hand it is also not able to describe the collapse of the matter wave field [33] or take into account any many-body effects in the dynamics.

Starting point for this ansatz is a many-particle Hamiltonian in first quantisation treating the particle interactions with an effective contact interaction potential,

$$\hat{H} = \sum_{i=1}^{N} \left[ \frac{\hat{p}_i^2}{2m} + V(\hat{r}_i) \right] + U_0 \sum_{i<j} \delta(\hat{r}_i - \hat{r}_j), \quad (2.16)$$

where $V(\hat{r}_i)$ denotes the external (trap) potential. The effective contact interaction potential

$$V_{\text{eff}}(\hat{r}_i, \hat{r}_j) = U_0 \delta(\hat{r}_i - \hat{r}_j) \quad (2.17)$$

simplifies the inter-particle interaction to be only two-body s-wave scattering with $U_0 = 4\pi\hbar^2a/m$ being the microscopic interaction strength and $a$ the s-wave scattering length.
2.4 $\mathcal{PT}$-symmetric open systems

To gain an equation describing the dynamics of the wave function, the total energy of the system, the expectation value of $\hat{H}$ [24],

$$E = \int dr \left[ \frac{\hbar^2}{2m} |\nabla \psi(r)|^2 + V(r)|\psi(r)|^2 + \frac{1}{2}U_0|\psi(r)|^4 \right], \quad (2.18)$$

has to be considered. Here $\psi(r) = \sqrt{N}\phi(r)$ is the wave function normalized to the total number of particles

$$\int dr |\psi(r)|^2 = N. \quad (2.19)$$

Minimizing the energy (2.18) with respect to $\psi(r)$ under that condition is equivalent to minimizing $E - \mu N$ for a fixed chemical potential $\mu$. This procedure finally yields the time-independent Gross-Pitaevskii equation

$$\left( -\frac{\hbar^2}{2m} \Delta + V(r) + U_0|\psi(r)|^2 \right) \psi(r) = \mu \psi(r), \quad (2.20)$$

which has the form of a nonlinear Schrödinger equation and corresponds to the time-dependent GPE

$$i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m} \Delta + V(r) + U_0|\psi(r, t)|^2 \right) \psi(r, t). \quad (2.21)$$

When analyzing the effect of the nonlinear interaction term it can be very practical to express the equation again in terms the function $\phi(r)$, which is normalized to one,

$$i\hbar \frac{\partial}{\partial t} \phi(r, t) = \left( -\frac{\hbar^2}{2m} \Delta + V(r) + g_0|\phi(r, t)|^2 \right) \phi(r, t). \quad (2.22)$$

This way the strength of the nonlinear interaction is no longer dependent on the particle number via the wave function but instead via the parameter $g_0 = NU_0 = 4\pi N\hbar^2 a/m$, which is called macroscopic interaction strength. By applying external magnetic fields it is possible to tune the scattering length $a$ over several magnitudes through the Feshbach resonances of the type of particle used in the system [34, 35]. This way, the macroscopic interaction strength does not have to posses a determined value for a certain number of atoms in the system but can be controlled.

2.4 $\mathcal{PT}$-symmetric open systems

To ensure that the spectrum of a quantum mechanical system is purely real, the Hamiltonian is usually chosen to be hermitian ($\hat{H} = \hat{H}^\dagger$), which is a sufficient condition but not a necessary one. As shown by Bender and Boettcher in 1998 [36] the weaker condition of being invariant under the $\mathcal{PT}$ transformation can be enough for a Hamiltonian
to possess a purely or partly real spectrum of eigenvalues, where $\mathcal{PT}$ is the combined action of the parity and the time reversal operators. This new class of $\mathcal{PT}$-symmetric Hamiltonians can be very useful in describing open-quantum systems with particle gain and loss, as illustrated in this section.

A linear quantum system is $\mathcal{PT}$-symmetric if the commutator of the Hamiltonian and the combined $\mathcal{PT}$ operator vanishes,

$$[\hat{H}, \mathcal{PT}] = 0. \quad (2.23)$$

The parity and time reversal operators are defined by their effect on the momentum and position operators as well as the imaginary unit:

$$\mathcal{P} \hat{x} \mathcal{P} = -\hat{x}, \quad \mathcal{P} \hat{p} \mathcal{P} = -\hat{p}, \quad (2.24)$$

$$\mathcal{T} i \mathcal{T} = -i, \quad \mathcal{T} \hat{p} \mathcal{T} = -\hat{p}. \quad (2.25)$$

Hence the action of the combined $\mathcal{PT}$ operator is given by

$$\mathcal{PT} \hat{x} \mathcal{PT} = -\hat{x}, \quad \mathcal{PT} \hat{p} \mathcal{PT} = \hat{p}, \quad \mathcal{PT} i \mathcal{PT} = -i. \quad (2.26)$$

It follows directly from (2.26) that a Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad (2.27)$$

is $\mathcal{PT}$-symmetric if the potential fulfills the condition

$$V(\hat{x}) = V^*(-\hat{x}). \quad (2.28)$$

For Hermitian systems no complex potentials are allowed but by considering the time derivative of the probability density $\rho = |\psi(r, t)|^2$ in presence of a complex potential it becomes apparent why they are relevant for effectively describing open systems,

$$\frac{\partial \rho}{\partial t} = \psi^*(r, t)\dot{\psi}(r, t) + \psi(r, t)\dot{\psi}^*(r, t) = \frac{1}{i\hbar} \left( \psi^*(r, t)\hat{H}\psi(r, t) - \psi(r, t)\hat{H}^\dagger\psi^*(r, t) \right)$$

$$= -\frac{i\hbar}{2m} \left( \psi(r, t)\Delta\psi^*(r, t) - \psi^*(r, t)\Delta\psi(r, t) \right) + \frac{1}{i\hbar} (V(r) - V^*(r)) \rho. \quad (2.29)$$

Using the definition of the probability current density $\mathbf{j} = i\hbar(\psi \nabla \psi^* - \psi^* \nabla \psi)/2m$ this yields the continuity equation for complex potentials

$$\frac{\partial}{\partial t} \rho(r, t) + \nabla \mathbf{j}(r, t) = \frac{2}{\hbar} \text{Im} V(r) \rho. \quad (2.30)$$

In contrast to the standard continuity equation for Hermitian quantum mechanics, where $\text{Im} V(r) = 0$, this equation allows for sources and sinks of the probability density generated by the imaginary part of the potential. It is therefore possible to use complex
potentials to describe the coupling to an environment for which particle exchange is permitted.

However, the spectrum of a Hamiltonian obeying relation (2.23) is only then purely real if the eigenstates of $H$ can be constructed from eigenstates of the $\mathcal{PT}$ operator (i.e. the eigenstates are $\mathcal{PT}$ symmetric) \[37\]. This case is referred to as unbroken $\mathcal{PT}$ symmetry, while in the opposite case, where some or all eigenvalues are complex, one speaks of broken $\mathcal{PT}$ symmetry. Complex eigenvalues occur always in pairs of complex conjugates and their respective eigenfunctions can be mapped onto each other using the $\mathcal{PT}$ operator. Although there is no general criterion for which Hamiltonians the spectrum is real, real eigenvalues are usually found if the imaginary part of the potential is small relative to its real part.

For a nonlinear equation as the GPE (2.20) the commutator relation (2.23) cannot be applied as a criterion for $\mathcal{PT}$ symmetry anymore. A general nonlinear Schrödinger equation has the form

$$
\hat{H}_{\text{lin}}\psi + \hat{f}(\psi)\psi = \mu\psi,
$$

(2.31)

where $\hat{H}_{\text{lin}} = \hat{p}^2/2m + V(\hat{x})$ is the linear part of the Hamiltonian and $\hat{f}(\psi)$ a general nonlinear function that is invariant under a change of the global phase

$$
\hat{f}(e^{i\alpha}\psi) = \hat{f}(\psi), \quad \alpha \in \mathbb{R}.
$$

(2.32)

For systems of the form (2.31) the requirement for $\mathcal{PT}$ symmetry reads

$$
\mathcal{PT}\left[\left(\hat{H}_{\text{lin}} + \hat{f}(\psi)\right)\psi\right] = \left(\hat{H}_{\text{lin}} + \hat{f}(\mathcal{PT}\psi)\right)\mathcal{PT}\psi.
$$

(2.33)

If $\hat{H}_{\text{lin}}$ obeys the commutator relation (2.23) this requirement reduces to a condition for the non-linearity,

$$
\mathcal{PT}\hat{f}(\psi) = \hat{f}(\mathcal{PT}\psi)\mathcal{PT}.
$$

(2.34)

In position space this condition holds if the real part of the nonlinearity $f(\psi(\mathbf{r}))$ is symmetric and the imaginary part is antisymmetric, which is possible for the nonlinearity based on the contact interaction $f(\psi(\mathbf{r})) = U_0|\psi(\mathbf{r})|^2$ in the GPE (2.20).

Referring to the solutions of the nonlinear equation (2.31) as eigenvalues and eigenstates for simplicity, a similar statement as for the linear case can be made regarding the spectrum. An eigenvalue is real if and only if the corresponding eigenstate is $\mathcal{PT}$ symmetric and for every eigenstate $\psi$ with complex eigenvalue $\mu$ the state $\mathcal{PT}\psi$ is also a solution with the complex conjugated eigenvalue $\mu^\ast$. The only difference to the linear case is that the superposition principle does not hold anymore in the nonlinear case and therefore it is not possible to choose $\mathcal{PT}$ symmetric eigenstates for degenerate eigenvalues.
A simple but rich example for both a condensate described by a dimensionless version of the GPE (2.22) and an open system is given with the one-dimensional $\mathcal{PT}$-symmetric double well potential \[ V(x) = \omega_x x^2 + v_0 e^{-\sigma x^2} + i\gamma x e^{-\rho x^2}, \tag{2.35} \]
which is displayed in figure 2.1. The strength of the harmonic part of the potential is characterized by $\omega_x$, while the height and width of the potential barrier are determined by $v_0$ and $\sigma$, respectively. The strength of the imaginary part is given by $\gamma$ and the parameter $\rho$ is chosen as
\[ \rho = \frac{\sigma}{2\ln(v_0\sigma/\omega_x^2)} \tag{2.36} \]
so that the extrema of the imaginary part coincide with the minima of the real part. Here, the left well is subject to particle loss and the right well subject to particle gain since the imaginary part of the potential is negative for $x < 0$ and positive for $x > 0$. As discussed in [38] there exist at least two real eigenvalues $\mu$ of the GPE if the strength of the imaginary potential $\gamma$ is below a critical value, which is for the choice of parameters in figure 2.1 around $\gamma_c \approx 0.04$ and depending on the strength of the nonlinearity $g$. The corresponding eigenstates are $\mathcal{PT}$-symmetric and referred to as quasi-stationary states since they possess a phase gradient resulting in a constant current through the system but posses all other properties of a stationary state of a Hermitian quantum system.

Figure 2.1: $\mathcal{PT}$-symmetric double well potential for $\omega_x = 0.5$, $v_0 = 4$, $\sigma = 0.5$ and $\gamma = 0.02$
Hence, there is a steady transport of probability density from the right well to the left well while the expectation values of all observables like the number of particles in each well stay constant.
3 The Bose-Hubbard model

Although the Gross-Pitaevskii equation (2.21) presented in the previous chapter is a powerful tool to investigate the structure of a BEC in a trap and the dynamics of its collective modes, it does not consider any many-body effects explicitly because it is a mean-field approximation. Since all particles share the same wave function in this description, the purity of the condensate (2.11) is always assumed to be $P = 1$. Furthermore, using a mean field equation it is not possible to describe a system with two or more initially separated, incoherent BECs as the one under investigation in chapter 4. On the other hand, however, because of the very complex nature of many-body quantum mechanics, no system without simplifications can be computationally accessible in practice.

One feasible way to study BECs as many-particle systems that has gathered a lot of interest during the last two decades [4, 10, 39, 40] is the Bose-Hubbard model, which describes a BEC in a deep optical lattice potential. In this model the dimensionality of the system is rendered finite by assuming the particles to be localized at the lattice sites, and hence discretizing position space.

The first section of this chapter briefly introduces the concept of optical potentials, after which the Bose-Hubbard (BH) Hamiltonian is motivated. These descriptions are loosely based on a review article by Jaksch [41], who was the first to apply the BH model to BECs. In the sections following, a master equation is presented as a mathematical framework to describe open systems within the Bose-Hubbard model, and finally the BBGKY hierarchy and the Bogoliubov back-reaction method are considered to give a computationally cheap approximation of the model.

3.1 Optical lattices

Optical lattices are harmonic potentials created by counter-propagating laser beams via the AC Stark effect. The underlying principle can be made clear by considering the simple model of a two-level atom with ground state $|g\rangle$ and exited state $|e\rangle$ separated by $\hbar \omega_0$ and illuminated by the electromagnetic field $E(x, t) = E(x)e^{i\omega t}$. The dipole interaction Hamiltonian is given by $\hat{H}_{\text{dip}} = -\hat{\mu}E(x, t) + \text{h.c.}$, where the dipole operator takes the form $\hat{\mu} = \mu_{eg} |e\rangle \langle g| + \text{h.c.}$ with $\mu_{eg} = \langle e|\hat{\mu}|g\rangle$. For a relatively small laser detuning $\delta = \omega - \omega_0$ with $|\delta| \ll \omega_0$, the interaction Hamiltonian can be expressed as

$$\hat{H}_{\text{dip}} = -\frac{\hbar \Omega(x)}{2} |e\rangle \langle g| + \text{h.c.} \quad (3.1)$$
in the rotating wave approximation with the Rabi frequency $\Omega(x)$ being defined through $\hbar \Omega(x) = 2E(x) \mu_{ge}$. If the detuning is large relative to the Rabi frequency $|\delta| \gg \Omega(x)$, the lattice potential acting on the atom can be obtained by applying second-order perturbation theory, which yields

$$V_{\text{lat}}(x) = \frac{\hbar |\Omega(x)|^2}{4|\delta|}.$$ (3.2)

In this far detuned regime absorption processes are negligibly rare and the field of the laser beams acts merely as a conservative potential on the atom. Moreover, the potential is proportional to the quotient of the light intensity $I(x)$ and the detuning, $V_{\text{lat}}(x) \propto I(x)/|\delta|$, and hence its strength can be controlled easily. For blue detuned lasers ($\delta > 0$) the lattice potential is repulsive and its minima coincide with the minima of the intensity, whereas for red detuned lasers ($\delta < 0$) the potential is attractive.

For two counter-propagating laser beams of wavelength $\lambda$ with $E_{\pm}(x,t) = E_0 e^{i(\omega \pm k x)}$ the lattice potential (3.2) can be expressed as

$$V_{\text{lat}}(x) = V_0 \sin^2(kx)$$ (3.3)

with the magnitude of the wave vector $k$ being $k = 2\pi/\lambda$. Therefore the periodicity of the potential (the lattice constant) is in this case $a = \lambda/2$. The lattice can easily be expanded to two or three dimensions by adding one pair or two pairs of lasers orthogonally to the first one.

Due to the periodicity of the lattice potential, the bosonic wave functions of the atoms can be expressed in terms of Bloch functions $\phi^{(n)}_q(x)$, where $q$ is the quasi momentum for the one-dimensional case and $n$ denotes the band index. Already if the lattice depth $V_0$ is just a few times higher than the recoil energy $E_R = k^2/2m$, the separation between the lowest bands is much larger than their extend. In this case the particles in those bands can be described with the orthonormal Wannier functions localized at site $j$

$$w_n(x - x_j) = \Theta^{-1/2} \sum_q e^{-iqx} \phi^{(n)}_q(x)$$ (3.4)

with $\Theta$ being a normalization constant. These functions are a good basis to describe particles in a deep lattice since they allow for a mean position $x_j$ to be awarded to each particle and make it easy to treat interactions of particles localized at the same site.

### 3.2 The Bose-Hubbard Hamiltonian

Based on the Hubbard model for fermions in solid state physics the Bose-Hubbard model was introduced by Gersch and Knollman in 1963 [42]. It was first proposed to study ultracold atoms in an optical lattice by Jaksch et al. in 1998 [4] and has been validated as an viable description in an experiment [6].
3.2 The Bose-Hubbard Hamiltonian

Starting point for the derivation of the BH Hamiltonian is the full many-body Hamiltonian for a system with contact interaction (2.17),

\[ \hat{H} = \int d^3x \hat{\psi}^\dagger(x) \left( \frac{\mathbf{p}^2}{2m} + V_{\text{lat}}(x) + V_T(x) \right) \hat{\psi}(x) + \frac{U_0}{2} \int d^3x \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x) \].

(3.5)

Here \( \hat{\psi}(x) \) is the Bosonic field operator, \( V_{\text{lat}}(x) \) the lattice potential (3.3) and \( V_T(x) \) a slowly varying external trapping potential. By assuming that for very low temperatures all particles are in the lowest Bloch band of the optical lattice, \( \hat{\psi}(x) \) can be expanded in terms of the Wannier functions (3.4),

\[ \hat{\psi}(x) = \sum_i \hat{a}_i w_0(x - x_i) \]

(3.6)

with \( \hat{a}_i \) being the annihilation operator at site \( i \). This ansatz yields the Hamiltonian

\[ \hat{H} = -\sum_{i,j} J_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \]

(3.7)

with \( J_{ij} = -\int d^3x w_0^*(x - x_i) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{\text{lat}}(x) + V_T(x) \right) w_0(x - x_j) \) \)

(3.8)

and \( U_{ijkl} = U_0 \int d^3x w_0^*(x - x_i) w_0^*(x - x_j) w_0(x - x_k) w_0(x - x_l) \).

(3.9)

It can act on a Fock state \(|n_1, n_2, \ldots, n_M\rangle\) where the \( n_i \) denote the number of particles located at site \( i \) in a lattice with \( M \) sites.

For reasonably deep lattices (\( V_0 \gtrsim 5E_R \)) the off-site interaction elements, i.e. \( U_{ijkl} \) with at least one of the indices not equal to the others, and the non neighboring tunneling elements, i.e. \( J_{ij} \) with \( i \neq j \pm 1 \), are negligibly small compared to the on-site interaction elements \( U_{i,j,j} = U \) and the tunneling between nearest neighbours. Thus, by considering only on-site interactions and tunneling between neighbouring pairs \( (i,j) \), the Bose-Hubbard Hamiltonian is gained,

\[ \hat{H}_{BH} = -\sum_{(i,j)} J_{ij} \hat{a}_i^\dagger \hat{a}_j + U \sum_j \hat{a}_j^\dagger \hat{a}_j \hat{a}_j + \sum_j \epsilon_j \hat{a}_j^\dagger \hat{a}_j \]

(3.10)

with the energy offset \( \epsilon_j = V_T(x_j) \) being caused by the trapping potential.

The principle of this model is illustrated schematically in figure 3.1 showing two sites containing one and two particles, respectively. Due to the repulsive on-site interaction energy \( U \), the particles at the right hand site are at a slightly higher potential. Since \( U \) is related in Eq. (3.9) to the microscopic interaction strength \( U_0 \) (as seen in the GPE (2.21)) via an integral over the Wannier functions, it is not only dependent on intrinsic properties of the particles used for the condensate but also on the shape of the lattice potential.
3.3 Quantum master equation for open systems

In the Bose-Hubbard model (3.10) it is not possible to introduce the coupling to an environment by merely using some complex potential as it is done for the Gross-Pitaevskii equation in chapter 2 since this would change the meaning. A complex potential acting on the single particles would add or remove parts of their probability amplitude to and form the system. Instead a quantum master equation can be found for the density matrix $\hat{\rho}$ that uses the concept of Lindblad operators to describe the correct effects of the environment on the system coherently, i.e. the addition and removal of whole particles. The brief motivation for this description presented in this section is based on the more rigorous derivation of the model in [15].

The combined Hamiltonian of a system and an environment is given by

$$\hat{H}_{\text{tot}} = \hat{H}_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes \hat{H}_E + \hat{H}_I,$$

where $\hat{H}_S$ and $\hat{H}_E$ are the respective Hamiltonians of the system and the environment, and $\hat{H}_I$ is the Hamiltonian describing the interaction. The density matrix of the system can be gained by tracing out the environment in the total density matrix, $\hat{\rho}_S = \text{tr}_E \hat{\rho}_{\text{tot}}$.

Therefore, the equations of motion for the system are obtained by applying this partial trace to the von Neumann equation of the total system,

$$\frac{d}{dt} \hat{\rho}_S = -\frac{i}{\hbar} \text{tr}_E [\hat{H}_{\text{tot}}, \hat{\rho}_{\text{tot}}].$$

(3.12)

To turn this equation into an effective description of an open system, some simplifications must be applied. Firstly, a weak coupling of system and environment is assumed in the sense of a Born approximation. This means that the dynamics of the system is not able
The Bogoliubov back-reaction method

3.4 The Bogoliubov back-reaction method

to influence the environment significantly, and thus the environment does not show a
time dependence and system and environment stay separable,

\[ \hat{\rho}_{\text{tot}}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E. \]  

Furthermore, this relation is assumed to be fulfilled exactly for \( t = 0 \). Lastly, the
Markov approximation can be applied, which demands that the environment exhibits
short memory in the sense that all correlations in the environment decay on smaller time
scales than those relevant for the dynamics of the system.

With these assumptions it is possible to obtain a master equation for the dynamics of
the system \([43]\),

\[ \frac{d}{dt} \hat{\rho}_S = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] - \sum_j \frac{\gamma_j}{2} \left( \hat{L}_j^\dagger \hat{L}_j \hat{\rho}_S + \hat{\rho}_S \hat{L}_j^\dagger \hat{L}_j - 2 \hat{L}_j \hat{\rho}_S \hat{L}_j^\dagger \right), \]

that takes the effects of the environment into account via the Lindblad operators \( \hat{L}_j \). This
second operator term is often expressed in literature using the Lindblad superoperator

\[ \mathcal{L}(\hat{L}_j)\hat{\rho} = \frac{1}{2} \left( \hat{L}_j^\dagger \hat{L}_j \hat{\rho} + \hat{\rho} \hat{L}_j^\dagger \hat{L}_j - 2 \hat{L}_j \hat{\rho} \hat{L}_j^\dagger \right). \]

The choice of the \( \hat{L}_j \) determines the type of interaction while their associated rates \( \gamma_j \)
describe its strength. A possible choice is for example \( \hat{L}_j = \hat{a}_j^\dagger \hat{a}_j \), which represents
phase noise affecting the system \([16]\). However, the two most important instances of
interactions that can be treated with this formalism are localized particle gain and loss
described by the creation operator \( \hat{L}_j = \hat{a}_j^\dagger \) and the annihilation operator \( \hat{L}_j = \hat{a}_j \),
respectively, with the latter being the one most relevant in this work.

Localized particle loss of this type was already realized with a steady beam of electrons
produced by a commercial electron microscope \([17]\). In an optical lattice, loss described
by \( \hat{L}_j = \hat{a}_j \) is implemented by focusing the electron beam on site \( j \) such that it can
ionize or excite particles located at that site and thereby let them escape the potential.
This technique causes almost no heating of the condensate as a side effect of the particle
dissipation and therefore offers a feasible way to realize particle loss as described by the
superoperator \( \mathcal{L}(\hat{a}_j) \).

3.4 The Bogoliubov back-reaction method

Since the Bose-Hubbard model treats the complete many-body dynamics of a system, its
dimension grows rapidly with the number of sites \( M \) and particles \( N \). If \( N \) is constant
the size of the Fock base necessary to describe the system completely is given by

\[ D(N, M) = \frac{(N + M - 1)!}{N!(M - 1)!} = \frac{(N + 1) \cdots (N + M - 1)}{(M - 1)!}. \]
This relation is the result of the simple combinatorial problem of how many different ways there are for choosing \( N \) times one out of \( M \) elements while repetitions are allowed. The dimension scales as \( D(N, M) = O(N^{M-1}) \), which renders systems with high particle numbers often computationally inaccessible, especially if the number of sites is high as well. For open systems, where \( N \) is no longer constant, the necessary dimension to be considered becomes even higher. If the number of particles at each site is allowed to be between 0 and some upper limit \( N_{\text{max}} \) the dimension of the system is \( N_{\text{max}}^M \).

Therefore, in order to gain at least some insight into the many-body dynamics of relatively big systems, an approximation of the Bose-Hubbard model has to be found that is computationally less demanding but still goes beyond the mean-field approach. This can be achieved with the Bogoliubov back-reaction (BBR) method, which was developed for a closed two-site system by Anglin and Vardi [39] but can be extended for an open system with an arbitrary number of sites [44]. Instead of the dynamics of the whole density matrix \( \hat{\rho} \), it calculates the time evolution of the SPD matrix \( \sigma_{jk} \) from Eq. (2.6).

Starting point for this ansatz is the master equation (3.14) for a one-dimensional lattice with the Bose-Hubbard Hamiltonian (3.10) and with a superoperator for particle gain, particle loss and phase noise acting on each site,

\[
\frac{d}{dt} \hat{\rho} = -i[H_{BH}, \hat{\rho}] - \sum_j \left( \frac{1}{2} \left( \gamma_{\text{loss},j} \mathcal{L}(\hat{a}_j)\hat{\rho} + \gamma_{\text{gain},j} \mathcal{L}(\hat{a}_j^\dagger)\hat{\rho} + \kappa_j \mathcal{L}(\hat{a}_j^\dagger \hat{a}_j)\hat{\rho} \right) \cdot \right) ,
\]

(3.17)

Here and in the following \( \hbar \) is set to one for simplicity (i.e. natural units). The time dependence of the elements of the SPD matrix \( \sigma_{jk} \) is given by

\[
\frac{d}{dt} \sigma_{jk} = \frac{d}{dt} \text{tr}(\hat{a}_j^\dagger \hat{a}_k \hat{\rho}) = \text{tr}\left( \hat{a}_j^\dagger \hat{a}_k \frac{d}{dt} \hat{\rho} \right)
\]

(3.18)

and inserting Eq. (3.17) yields

\[
\frac{d}{dt} \sigma_{jk} = i(-J_j \sigma_{j+1,k} - J_{j-1} \sigma_{j-1,k} + J_k \sigma_{j,k+1} + J_{k-1} \sigma_{j,k-1}) + iU(\Delta_{jjkk} + \sigma_{jj} + \Delta_{jkkk} + \sigma_{kk} \sigma_{jk}) - \frac{1}{2}(\gamma_{\text{loss},j} + \gamma_{\text{loss},k}) \sigma_{jk} + \frac{1}{2}(\gamma_{\text{gain},j} + \gamma_{\text{gain},k})(\sigma_{jk} + \delta_{jk}) - \kappa(1 - \delta_{jk}) \sigma_{jk} + i(\epsilon_j - \epsilon_k) \sigma_{jk}.
\]

(3.19)

This is not a closed set of equations but the elements of the SPD matrix couple via the microscopic interaction strength \( U \) to the covariances \( \Delta_{jklm} = \langle \hat{a}_{j}^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_m \rangle - \langle \hat{a}_{j}^\dagger \hat{a}_k \rangle \langle \hat{a}_j^\dagger \hat{a}_m \rangle \).

In this context the elements of the SPD matrix \( \langle \hat{a}_{j}^\dagger \hat{a}_k \rangle \) are also called first-order moments and the expectation values of the two-particle operators \( \langle \hat{a}_{j}^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_m \rangle \) are referred to as second-order moments.
For a constant macroscopic interaction strength \( g = U(N-1) \) the covariances can be neglected in the mean-field limit \( N \to \infty \) because they scale linearly with the particle number while the products \( \sigma_{jk} \sigma_{lm} \) scale quadratically, and Eq. (3.19) becomes a closed set. The interaction strengths of the BH model \( g \) and \( U \) are not to be confused with the interaction strengths \( g_0 \) and \( U_0 \) of the GPE in Eq. (2.21) and (2.22), which have slightly different units and are related to the two former parameters via Eq. (3.9). In the mean-field limit and in the absence of phase noise (\( \kappa = 0 \)) the evolution equations can be shown to be equivalent to a discretized, dimensionless version of the GPE (2.22),

\[
i \frac{d}{dt} c_k = -J_k c_{k+1} - J_{k-1} c_{k-1} + g|c_k|^2 c_k + \epsilon_k c_k + \frac{i}{2}(\gamma_{\text{gain},k} - \gamma_{\text{loss},k})c_k, \tag{3.20}
\]

by the identification \( \sigma_{jk} = N c_j^* c_k \) of the SPD matrix elements with the complex mean-field coefficients \( c_k = \phi(r_k) \).

To go beyond the mean-field description, it is necessary to consider the dynamics of the covariances. For this, the time dependence of the second-order moments can be obtained analogously to Eq (3.18) through the master equation (3.14),

\[
\frac{d}{dt} \langle \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_m \rangle = \text{tr} \left( \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_m \frac{d}{dt} \hat{\rho} \right). \tag{3.21}
\]

Doing this shows that the second-order moments couple to the expectation values of the three-particle operators \( \langle \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_m \hat{a}_s \rangle \). A generalized principal can be found that the evolution equations of each order also contain elements of the next-higher order, which is referred to as the BBGKY (Bogoliubov–Born–Green–Kirkwood–Yvon) hierarchy [39]. For a system of \( N \) particles this hierarchy continues in principle till the \( N \)-th order and therefore has to be truncated to obtain a closed set of equations. Approximating the third-order moments as

\[
\langle \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_m \hat{a}_s \rangle \approx \langle \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_m \rangle \langle \hat{a}_s \rangle + \langle \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l^{\dagger} \hat{a}_s \rangle \langle \hat{a}_j^{\dagger} \hat{a}_m \rangle - 2 \langle \hat{a}_j^{\dagger} \hat{a}_k \rangle \langle \hat{a}_j^{\dagger} \hat{a}_m \hat{a}_s \rangle \tag{3.22}
\]

and thereby truncating after the second order is known as the Bogoliubov back-reaction method. Applying this approximation to (3.21) yields together with (3.19) the BBR
evolution equations for the covariances,

\[
\frac{d}{dt} \Delta_{jklm} = i(-J_j \Delta_{j+1klm} - J_{j-1} \Delta_{j-1klm} + J_k \Delta_{jk+1lm} + J_{k-1} \Delta_{jk-1lm} \\
- J_l \Delta_{jkl+1m} - J_{l-1} \Delta_{jkl-1m} + J_m \Delta_{jklm+1} + J_{m-1} \Delta_{jklm-1}) \\
+ iU[\Delta_{jklm}(\sigma_{jj} - \sigma_{kk} + \sigma_{ll} + \sigma_{mm}) \\
+ \Delta_{jmlm}\sigma_{jk} - \Delta_{klmm}\sigma_{jk} + \Delta_{jklm}\sigma_{jm} - \Delta_{jklm}\sigma_{jm}] \\
- 2(\gamma_{loss,j} + \gamma_{loss,k} + \gamma_{loss,l} + \gamma_{loss,m})\Delta_{jklm} + \delta_{kl}\gamma_{loss,k}\sigma_{jm} \\
+ \frac{1}{2}(\gamma_{gain,j} + \gamma_{gain,k} + \gamma_{gain,l} + \gamma_{gain,m})\Delta_{jklm} + \delta_{jm}\gamma_{gain,j}(\sigma_{lk} + \delta_{kl}) \\
- \kappa [(\delta_{km} + \delta_{jl} - \delta_{jm} - 2\delta_{kl})(\Delta_{jklm} + \sigma_{jk}\sigma_{lm}) + (2 - \delta_{jk} - \delta_{lm})\Delta_{jklm}] \\
+ i(\epsilon_j - \epsilon_k + \epsilon_l - \epsilon_m)\Delta_{jklm}.
\]

A detailed calculation of this term and the first-order equations (3.19) can be found in the appendix of [28].

If all fist- and second-order elements in Eq. (3.19) and (3.23) were independent, the BBR method would consist of \(M^2 + M^4\) complex equations for a system of \(M\) lattice sites. However, since the SPD matrix is hermitian, \(\sigma_{jk} = \sigma_{kj}^*\), it has only \(M^2\) independent real entries. The covariances exhibit two symmetries,

\[
\Delta_{jklm} = \Delta_{lmjk} - \delta_{jm}\sigma_{lk} + \delta_{kl}\sigma_{jm} \\
\Delta_{jklm} = \Delta_{*mlkj},
\]

which can be shown to reduce the number of independent covariances to \(\frac{1}{2}(M^4 + M^2)\) real elements [45]. The number of equations in the BBR method is therefore independent of the number of particles and of only fourth order in the number of sites.

Since the BBR method is only of one order higher than the mean-field in the BBGKY hierarchy it is not assumed to be accurate in regimes far off the mean-field limit, i.e. for small particle numbers. It can be shown that the hierarchy converges in orders of the proportion of particles that do not share the same mean-field state [46]. This implies that the method remains accurate if the system stays close to a pure BEC, i.e. if the SPD matrix of the system possesses only one large eigenvalue. However, there is no general criterion determining the accuracy of the method. A typical behavior of the method observed in simulation [19] is to stay in good agreement with the full many-body dynamics up to a certain point in the time development but diverge drastically for large time scales.

There are two scenarios in which the BBR method becomes particularly useful. If for a small total particle number \(N\), where the BH model is computationally accessible, the results of the BBR method are close to the full dynamics, the method can be used to calculate the behavior for higher particle numbers since the quality of the approximation increases with the particle number in case of a constant macroscopic interaction.
3.5 Relating mean-field and many-particle description

Since the discretized GPE (3.20) has only \( M \) complex components, it is comparatively easy to calculate its ground state. In many cases this is a feasible way to find a suitable initial state for the many-body description of the system. To be able to use this approach, a mean-field state described by the \( M \) mean-field coefficients \( c_j \) has to be expressed in the Fock base of the BH model.

The operator creating a particle in the mean field state \( \phi = (c_1, c_2, \ldots)^T \) can be written as

\[
\hat{b}^j = \sum_{j=1}^{M} c_j \hat{a}_j^\dagger
\]  

(3.26)

with \( \hat{a}_j \) being the operator creating a particle at site \( j \). Since all \( N \) particles in the system share the same mean fielded state, the many particle state of the system reads

\[
|\phi, N \rangle = \frac{1}{\sqrt{N!}} \left( \hat{b}^j \right)^N |0 \rangle = \frac{1}{\sqrt{N!}} \left( \sum_{j=1}^{M} c_j \hat{a}_j^\dagger \right)^N |0 \rangle .
\]  

(3.27)

Applying the multinomial theorem on this expression yields the mean filed state in the Fock base

\[
|\phi, N \rangle = \frac{1}{\sqrt{N!}} \sum_{n_1 + \ldots + n_M = N} \frac{N!}{n_1! \cdots n_M!} c_1^{n_1} \cdots c_M^{n_M} (a_1^\dagger)^{n_1} \cdots (a_M^\dagger)^{n_M} |0 \rangle
\]  

(3.28)

Here the coefficients \( n_j \) with \( j \in \{1, \ldots, M\} \) denote the number of particles at site \( j \) and the sum spans over all possible configurations of the coefficients that preserve the total number of particles, \( \sum_{j=1}^{M} n_j = N \).

To now further relate the mean-field coefficients to the first- and second-order moments of the BBR method, first the action of the annihilation operator on the state has to be considered,

\[
\hat{a}_j |\phi, N \rangle = \sum_{n_1 + \ldots + n_M = N} \sqrt{\frac{N!}{n_1! \cdots n_M!}} c_1^{n_1} \cdots c_M^{n_M} \sqrt{n_j} |n_1, \ldots, n_j - 1, \ldots, n_M \rangle .
\]  

(3.29)
The standard form of the Fock base is restored by performing the index shift \( n_j \to n_j' + 1 \) which yields

\[
\hat{a}_j |\phi, N \rangle = \sum_{n_1 + \cdots + n_M = N} \left( \frac{N!}{n_1! \cdots (n_j' + 1)! \cdots n_M!} \right) c_1^{n_1} \cdots c_j^{n_j' + 1} \cdots c_M^{n_M} \sqrt{n_j' + 1 |n_1, \ldots, n_M}
\]

\[
= \sqrt{N} c_j \sum_{n_1 + \cdots + n_M = N-1} \left( \frac{(N-1)!}{n_1! \cdots n_M!} \right) c_1^{n_1} \cdots c_M^{n_M} |n_1, \ldots, n_M\rangle
\]

\[
= \sqrt{N} c_j |\phi, N - 1 \rangle .
\]

(3.30)

With this relation the SPD matrix elements (first-order moments) corresponding to the mean-field state are found to be

\[
\sigma_{jk} = \langle \phi, N | \hat{a}_j \hat{a}_k | \phi, N \rangle = N c_j^* c_k
\]

(3.31)
since the Fock representation \( |\phi, N \rangle \) is normalized to one. The second-order moments amount to

\[
\langle \phi, N | \hat{a}_j \hat{a}_k \hat{a}_l \hat{a}_m | \phi, N \rangle = \langle \phi, N | \hat{a}_j (\hat{a}_k^+ \hat{a}_l^+ \hat{a}_m + \delta_{lk}) \hat{a}_m | \phi, N \rangle
\]

\[
= N c_j^* c_m \langle \phi, N - 1 | \hat{a}_j^+ \hat{a}_k | \phi, N - 1 \rangle + \delta_{lk} N c_j^* c_m
\]

(3.32)

\[
= N(N-1) c_j^* c_k c_l^* c_m + \delta_{lk} N c_j^* c_m.
\]

With these expressions the term for the covariances is given by

\[
\Delta_{jklm} = \langle \phi, N | \hat{a}_j \hat{a}_k \hat{a}_l^+ \hat{a}_m | \phi, N \rangle - \langle \phi, N | \hat{a}_j \hat{a}_k | \phi, N \rangle \langle \phi, N | \hat{a}_l^+ \hat{a}_m | \phi, N \rangle
\]

\[
= N(\delta_{kl} c_j^* c_m - c_j^* c_k c_l^* c_m),
\]

(3.33)

which is again linear in the particle number, as the expression for the first-order moments.
4 Dynamics of coupled Bose-Einstein condensates

The central question under investigation in this chapter is to what extend the many-particle dynamics of two coupled BECs shows a behavior similar to that of a BEC in a simple open system. In this context, a special focus is set on the time evolution of the coherence of the condensates as expressed by the purity $P$ (2.14).

To be able to treat the computationally expensive full many-body dynamics, the simplest setup possible allowing for the description of two coupled condensates is chosen. Therefore, an optical lattice of six sites is proposed as shown in figure 4.1, consisting of two three-site subsystems. While the sites of each subsystem are joined together via the tunneling strength $J_1$ in the BH model, the two subsystems are coupled to each other at both outer sites with a different strength $J_2$. This scheme is similar to periodic boundary conditions.

The situation considered in this work is as follows: Initially the condensates in both subsystems are isolated from another since they are separated by a large potential barrier

![Diagram](image)

Figure 4.1: Schematic representation of the setup: Two coupled three-site subsystems forming a six-site Hermitian system.
(i.e. \( J_2 = 0 \)). This means there is no phase coherence between the two BECs. In this stage the condensates can be described by the ground state of a discrete three-site GPE. At \( t = 0 \) the potential wall is lowered at the outer sites such that \( J_2 \) becomes finite and a dynamics is induced. For this approach the lowest possible number of sites in each subsystem is three because for two-site subsystems no dynamical behavior could be generated by coupling them together if they are in their respective stationary ground states before the coupling. This is since for a two-site subsystem all particles would be evenly distributed between both sites in a stationary initial state and therefore no dynamics could occur when the periodic boundary conditions are applied.

The maximum value of the number of particles in the system \( N \) that can be considered in a simulation of the BH model is strongly limited by the high dimension of the Fock base \( D \) as given in Eq. (3.16). For numerical calculations the state of the system has to be implemented as a vector of size \( D \) and the Hamiltonian as a sparse matrix of size \( D^2 \). Although the state vector is sufficient to calculate the particle number expectation values for each site (i.e. the diagonal elements of the SPD matrix) another operator of dimension \( D^2 \) is needed in the memory of the computing device for each of the 15 unique off-diagonal elements of the SPD matrix \( \sigma_{jk} = \langle \hat{a}_j^\dagger \hat{a}_k \rangle \). Propagating the state of the system with a simple Runge-Kutta algorithm, the computation time can be kept within reasonable limits by implementing the vector-matrix multiplications on a GPU instead of a CPU, and thus executing many calculations in parallel. With this approach the limiting factor for the maximal dimension of the system is the memory size of the GPU. Using the CUSP library for sparse linear algebra within the parallel computing framework CUDA, it was possible to simulate the BH model for a maximum of \( N = 70 \) particles (\( D \approx 1.7 \times 10^7 \)) on a graphics card with 6 GB RAM.

The BBR method was used extensively in the course of this work to get a fast approximation of various results before calculating the time-costly full dynamics with the BH model. However, being an inaccurate approximation, the method was not relevant for obtaining the final data presented in this chapter. Still some of its results will be discussed in comparison with the values of the BH model to get an understanding of the accuracy of the method.

For simplicity and numerical practicability dimensionless natural units are used in the following, which render the parameters \( J_{ij} \) and \( U \) in Eq. 3.10 dimensionless as well. Section 4.5 shows how the dimensionless units can be related to their physical counterparts again in order to quantify the results obtained in this chapter.

### 4.1 Construction of the initial state

It is not feasible to try to calculate an initial state for the many-particle dynamics of the system by e.g. searching for a stationary state in the BH model. This is not only because the system of equations in the BH model is of a very high dimension that varies with the total number of particles \( N \). In addition to that, the initial state should also
4.1 Construction of the initial state

represent a fully coherent pure condensate in each subsystem to be able to study the effects of the coupling on the coherence. Therefore a mean-field state is chosen as the initial state of the many-body system, which is pure a priori. To obtain the initial state the discrete dimensionless GPE (3.20) for three sites is considered in the stationary case,

$$
\begin{align*}
\mu c_1 &= g|c_1|^2 c_1 - J_1 c_2, \\
\mu c_2 &= g|c_2|^2 c_2 - J_1 c_1 - J_1 c_3, \\
\mu c_3 &= g|c_3|^2 c_3 - J_1 c_2.
\end{align*}
$$

(4.1)

The ground state of this system of equations is calculated numerically under the condition $|c_1|^2 + |c_2|^2 + |c_3|^2 = \frac{1}{2}$ using Powell’s method as implemented in the MINPACK library. By normalizing to $\frac{1}{2}$ rather than to 1 two sets of these ground states can be combined to form the initial state of the six-site system, which is therefore of norm one. All three mean-field coefficients of the ground state can be chosen real and in all cases the relations $c_1 = c_3$ and $c_1 < c_2$ have to hold. The values of the coefficients depend solely on the ratio $g/J_1$ and some exemplary sets of approximate numerical values are given in table 4.1. If not specified otherwise the choice of parameters used in this chapter is $g = J_1 = 1$.

However, since in mean-field state there is always a defined phase difference between every site, it is not possible to describe the initial state of the whole six-site system by simply combining two sets of the coefficients to a mean-field state of the form $\phi = \{c_1, c_2, c_3, c_4, c_5, c_6\}^T$ (with $c_1 = c_3 = c_4 = c_6$ and $c_2 = c_5$). Applying Eq. (3.28) in a straightforward manner to obtain the initial Fock state for the BH model or Eq. (3.31) and (3.32) to obtain the SPD matrix elements and the covariances for the BBR method would construct one single BEC spanning coherently over all six sites of the system. Describing two separated (i.e. phase-incoherent) subsystems, there cannot be a defined phase difference between them. Instead, the correct way to describe two separate condensates in the Fock base with exactly half of the total number of particles in each subsystem is given by the direct product,

$$
|\psi\rangle = \{|c_1, c_2, c_3\}, N/2\rangle \otimes \{|c_4, c_5, c_6\}, N/2\rangle \\
= \sum_{n_1+n_2+n_3=N/2}^{N} \sum_{n_4+n_5+n_6=N/2}^{N} \frac{(N/2)!}{n_1!n_2!n_3!} \frac{(N/2)!}{n_4!n_5!n_6!} \sqrt{2} \sqrt{\frac{N}{n_1!n_2!n_3!}} \sqrt{\frac{N}{n_4!n_5!n_6!}} c_1^{n_1} c_2^{n_2} c_3^{n_3} \cdots c_5^{n_5} c_6^{n_6} |n_1, \ldots, n_6\rangle.
$$

(4.2)

Table 4.1: Values of the mean-field coefficients. The default choice of parameters in this chapter is $g = J_1 = 1$.

<table>
<thead>
<tr>
<th>$g/J_1$</th>
<th>0.1</th>
<th>0.2</th>
<th>0.5</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{1,3}$</td>
<td>0.35432</td>
<td>0.35507</td>
<td>0.35720</td>
<td><strong>0.36038</strong></td>
<td>0.36567</td>
<td>0.37619</td>
<td>0.38544</td>
</tr>
<tr>
<td>$c_2$</td>
<td>0.49891</td>
<td>0.49784</td>
<td>0.49479</td>
<td><strong>0.49015</strong></td>
<td>0.48225</td>
<td>0.46578</td>
<td>0.45041</td>
</tr>
</tbody>
</table>
In this expression the sum spans over all Fock states for which exactly \( N/2 \) particles are in site 1-3 and \( N/2 \) particles are in site 4-6, as opposed to the sum in Eq. (3.28), which includes all states that fulfill \( \sum_{j=1}^{M} n_j = N \). The additional factor of \( \sqrt{2}^N \) is due to the fact that the norm of the three mean-field coefficients belonging to each subsystem is only \( \frac{1}{2} \). With this approach the two condensates do not have any phase coherence initially.

The values of the first-order moments and covariances that form the corresponding initial state of the BBR method can still be obtained with Eq. (3.31) and (3.32) if incoherence between the subsystems is established by neglecting certain elements. This is done by only granting a value to those elements for which all indices belong either exclusively to the first subsystem (i.e. \( \in \{1, 2, 3\} \)) or the second subsystem (i.e. \( \in \{4, 5, 6\} \)). If all other elements that have indices of both subsystems are set to zero, there is no coherence between the subsystems and the BECs in this description are completely separated initially.

The focus of interest in this chapter is on analyzing the behavior of the system caused by a coupling of the subsystems. Therefore, the system should be quasi stationary in the case of the no coupling (\( J_2 = 0 \)), such that for a finite \( J_2 \) the dynamics can in fact be attributed to the coupling. To verify that the mean-field ground state of the GPE is not subject to any strong dynamics in the many-body description, the time evolution of the particle number expectation value of the central site \( \langle n_2 \rangle \) is calculated for \( J_2 = 0 \) and different values of the total particle number \( N \) and is plotted as \( \langle n_2 \rangle / N \) in figure 4.2. Although there are slight oscillations of the particle number visible in the BH model, their time average equals the initial level and their amplitude is less than two percent of that value for \( N = 20 \) and less than one percent for \( N = 70 \). The oscillations are subject to a beat frequency that gets lower with increasing particle number.

The results obtained with the BBR method clearly show the limits of the approximation as discussed in section 3.4. Although the high frequency oscillations of the BH model are well reproduced in the beginning, the envelope function keeps on increasing such that the results differ drastically form the desired behavior already after a short time, especially for \( N = 20 \). For higher particle numbers, however, the quality of the approximation improves strongly and it stays in relatively good agreement with the BH results on a longer time scale.

Figure 4.3 shows the purity of the SPD matrix (2.14) corresponding to this time evolution. In the BH model the purity stays practically one, which means the condensate does not deteriorate even on a long time scale. This is also the approximate behavior of the BBR method for \( N = 70 \), although for smaller particles numbers the purity begins to deviate from unity after some time and assumes even values greater than one, which are unphysical. This is only possible because the time evolution of the BBR method is not exactly unitary anymore since the higher orders of the BBGKY hierarchy truncated.
4.1 Construction of the initial state

Figure 4.2: Evolution of $\langle n_2 \rangle / N$ for the GPE ground state in the BH model and with the BBR method for $J_2 = 0$ and different values of the particle number $N$. Although the GPE ground state is not entirely stationary in the BH model the dynamics shows only oscillations with a small amplitude, especially for $N = 70$. For low particle numbers the BBR method becomes inaccurate already on small timescales.

Figure 4.3: Evolution of the purity of the subsystem for the same situation as in figure 4.2. The system stays pure in the BH model. For small particle numbers the BBR method can yield unphysical values greater than one on a long timescale.
4.2 Time development of the particle number expectation values

The expectation values of the number operator $\langle \hat{n}_j \rangle = \langle \hat{a}_j^\dagger \hat{a}_j \rangle$ for each site (referred to as filling level in the following) are central quantities in analyzing the dynamical behavior. Because of the symmetry of the system under investigation, there are only two independent particle number expectation values. Both subsystems are identical, start in the same state, and the initial state itself is symmetric in the sense that the mean-field coefficients of the outer sites of each subsystem calculated with Eq. 4.2 are equal. Therefore, the outer sites always show the same expectation values and a decrease in the particle number expectation value of the outer sites always has to be accompanied by an increase in the expectation value of the central site.

The dynamics of the system is to a large extend determined by the choice of the tunneling parameter $J_2$, that defines the strength of the coupling between the two subsystems. To find a choice of $J_2$ that enables a rich dynamical behavior the long-term time depen-

![Figure 4.4: Time evolution of the filling level at the outer sites (lower curves) and central site (upper curves) for $g = J_1 = 1$ and for different values of the coupling tunneling strength $J_2$. While for $J_2 = J_1 = 1$ the system gravitates towards a state of an equal average filling level at all sites, for unequal values of the tunneling constants the average filling levels stay different at the outer sites and the central site. The dynamics are less pronounced for $J = 0.5$ than for $J = 2$, where strong oscillations are stimulated in the filling levels. For the higher particle number of $N = 70$ the system is more stable and the oscillations at $J_2 = 2$ stay relatively constant in amplitude on a long timescale.](image-url)
4.2 Time development of the particle number expectation values

dence of the filling levels is compared for different values of the coupling strength, as displayed in figure 4.4. Here, the curves starting at a higher initial filling level represent the central site of each subsystem, while the initially lower curves represent the outer sites. In the left plot for a particle number of $N = 40$ one can see clearly that the filling levels of all sites approach a common average value for $J_2 = J_1 = 1$. On the other hand, for both cases where the tunneling constants are not equal, the central and outer sites maintain a difference in their average filling level. In the case that the coupling within each subsystem is stronger than between the subsystems ($J_2 = 0.5$) the actual dynamics is not very pronounced, while in the opposite case ($J_2 = 2$) the filling levels are subject to oscillations of a higher amplitude. With $N = 70$ particles in the system the dynamics gets more stable. For $J_2 = 2$ the amplitude of the oscillations stays high and relatively constant between $20 \lesssim t \lesssim 60$ after an on-set period.

Due to these properties of the dynamics for $J_2 = 2J_1 = 2$, this choice of the tunneling strength is suitable for a more extensive analysis. Figure 4.5 shows the time development again for $g = 1$ and $N = 70$ in the interval $0 \leq t \leq 25$. The solid lines of the BH model are compared to the approximate values of the BBR method represented by dashed lines. Oscillations in the filling levels develop during an on-set period and stay relatively stable throughout the rest of the interval. Due to the symmetry of the system, there is a phase difference of exactly $\pi$ between the oscillations of the filling level of the central site and those of the outer sites. The BBR method is able to produce the same behavior qualitatively. This changes, however, in the subsequent interval $25 \leq t \leq 50$ displayed in figure 4.6. Although the oscillations stay almost constant in frequency and amplitude in the BH model, the harmonic shape of the oscillations breaks down in the BBR method and its results deviate drastically from the full many-body dynamics. These results support the findings of [19], where the BBR method was observed to reproduce the correct behavior quantitatively until a certain point in time evolution, and deviate strongly from it after. This deviation of the BBR values manifested itself in the form of a beat frequency that did not occur in the oscillating behavior of the full BH dynamics, which is similar to the development of the oscillations in figure 4.6.

To illustrate the effect of the macroscopic nonlinear interaction strength $g$ on the dynamics, the time dependency of the central site filling level is compared for three different values of $g$ in figure 4.7. As already displayed in figures 4.5 and 4.6 the filling level shows steady oscillations for $g = 1$ that vary only slightly in amplitude after the on-set period. For the smaller value $g = 0.2$ the initial increase of the amplitude becomes slower and steadier but the behavior is eventually very similar. However, the situation is entirely different for the higher value of the nonlinearity $g = 2$. Here, the variations of the amplitude are very pronounced and almost chaotic in nature, and the average of the amplitude is significantly smaller than for both lower values of $g$. Therefore, if the system is required to exhibit a stable and controllable dynamics, the value of the nonlinearity has to be chosen low enough such that it does not dominate the behavior of the system. In a experiment this can be done using Feshbach resonances, as mentioned in section 2.3.
Figure 4.5: Time development of the filling levels for $N = 70$, $g = J_1 = 1$ and $J_2 = 2$. The solid lines represent the full dynamics of the BH model while the dashed lines are the approximation obtained with the BBR method. Relatively stable oscillations are established after some onset period. Due to the symmetry of the system, there is a phase difference of $\pi$ between the central site and the outer sites. The BBR method is able to qualitatively reproduce the behavior of the BH model.

Figure 4.6: Same plot as in figure 4.5 for the subsequent interval $25 \leq t \leq 50$. While the oscillations of the filling levels stay stable in the BH model, the BBR method shows a behavior similar to a beat frequency.
4.3 Evolution of the coherence

A primary objective of this work is to investigate whether the Hermitian system of two coupled BECs can show a behavior similar to an open system with respect to the time evolution of the coherence in the system. For a discretized version of the \( \mathcal{PT} \)-symmetric double well presented in section 2.5, purity oscillations have been reported to occur \([19, 40]\) in the presence of a coupling to an external environment. Purity oscillations are the phenomenon of strong loss and subsequent restoration of the coherence in the system quantified by the purity of the SPD matrix (2.14) in a periodic fashion. This means that the particles in the system leave their shared condensate state but get restored to an almost fully coherent BEC shortly after. For open systems this phenomenon is mostly governed by the strength of the coupling to the environment.

Therefore, the time evolution of the coherence within each subsystem is compared for different strengths of the coupling of the condensates as mediated by the tunneling constant \( J_2 \). This is displayed in figure 4.8, where \( P \) does not denote the purity of the whole six-site system but only the purity of a subsystem (which is of course identical for both subsystems). To calculated this quantity with Eq. (2.11) the three-dimensional SPD matrix of one of the subsystems is used, which consists of those elements of the full SPD matrix that belong to one subsystem only. For example in the case of the first
subsystem one has to choose the elements $\sigma_{jk}$ with $j, k \in \{1, 2, 3\}$. Since the subsystems are initially prepared in a mean-field state, and therefore in a pure condensate, all curves in the figure have to start at $P = 1$ for $t = 0$. As time progresses the purity does in fact undergo oscillations, whose amplitude is strongly determined by the strength of the coupling. For $J_2 = 0.5$ the minimum of the first oscillation is still higher than $P = 0.9$ while the corresponding minimum for $J_2 = 2$ is at $P \approx 0.35$. Increasing the coupling even further to $J_2 = 3$ does only result in a slight initial increase of the amplitude. This minimal improvement goes along with an unwanted strong overall decrease of the purity over time. In addition, the almost harmonic shape that the oscillations posses for smaller values of $J_2$ is lost.

The thin dashed lines in the figure represent the approximation obtained with the BBR method, which is effectively capable of reproducing the oscillations. However, the quality of the approximation decreases over time, especially for $J_2 = 0.5$ and $J_2 = 2$. It
is notable that the BBR method yields better results for $J_2 = 2$ than for the two lower values of $J_2$ since the approximation of the BH model with the BBR method should be particularly valid when the covariances are close to zero, i.e. when the condensate is pure. Nevertheless it is of a high quality in the case of $J_2 = 3$, where the purity oscillates heavily.

The rapid loss and subsequent restoration of the coherence is a phenomenon generally exclusive to open systems, where it can be linked directly to the coupling to an environment [19, 40]. For the coupled Hermitian system presented in this chapter it was only possible to describe such purity oscillations by evaluating the purity for the two subsystems individually. That is, for one subsystem the other assumes the role of the environment. For the overall purity of the six-site system, however, a behavior typical for closed Hermitian systems is found. Figure 4.9 shows the time dependence of this total purity $P_{\text{tot}}$ for the same parameters as in figure 4.5 and 4.6. Since the initial state of the system consists of two completely separated and incoherent BECs the purity starts only at $P_{\text{tot}} = 0.4$, which corresponds to an SPD matrix with two nonzero eigenvalues of magnitude $N/2$. Over time the purity decreases slowly (although not necessarily monotonously), which can be attributed to the fact that there are much more accessible states of low purity than of high purity, and thus it is statistically more probable to find

![Figure 4.9](image)

**Figure 4.9:** (a): Time dependence of the total purity of the coupled six-site system. Since there exist two separated and incoherent condensates initially, $P_{\text{tot}}$ assumes a value much lower than one already for $t = 0$. Over time, the total purity deteriorates further for statistical reasons. (b): Long-term time evolution of the purity from figure 4.5. Although the oscillations of the purity are very stable, their amplitude and average value decrease significantly on longer timescales.
the system in an impure state after some time. An overall deterioration of the purity is observable also in the long-term time development of the subsystems, as is displayed in figure 4.9 (b), where on a long time scale the amplitude as well as the average value of the oscillations decrease.

That the stability of the purity oscillations is compromised in a system in which the nonlinear interaction term is dominant, can be seen in figure 4.10. Here the purity of the subsystem is plotted for the same parameters as in figure 4.7. Although the oscillations initially overlap for all three choices of the macroscopic interaction strength, for \( g = 2 \) they begin to decrease drastically in amplitude after only two periods and become insignificant after \( t \approx 10 \). In this regime of a relatively strong nonlinear interaction strength the approximation of the BBR method, represented with dashed lines, is of poor quality already after a short time. This is the expected behavior of the BBR method since the approximated covariances couple to the elements of the SPD matrix.
in Eq. (3.19) via the microscopic interaction strength \( U \propto g \), and therefore the quality of the approximation has to decrease with increasing \( g \).

The comparison of BH values with the BBR values in the time developments in figures 4.5, 4.6, 4.8 and 4.10 shows that the BBR method is generally able reproduce the qualitative behavior of the BH model for a limited time span, and in case of the purity even a quantitative agreement of the values is observed. However, the point in time evolution after which the BBR method does not deliver a good approximation of the BH dynamics anymore varies strongly with the system parameters used. Although it is evident and theoretically understood that the approximation gets worse for higher values of the nonlinearity \( g \), it is not possible to derive a criterion determining this point in time evolution a priori. Still both in this work and in [19] the breaking-down of the BBR method as an approximation of the BH model was accompanied by the inception of a beat-frequency-like behavior in the BBR dynamics as seen in figure 4.6. If the BBR method is used to calculate the dynamics of a system in a regime in which the full BH model is not computationally accessible, the occurrence of such a behavior might present an indication that the approximation is no longer valid.

### 4.4 Observing the purity

The coherence of the atoms in a BEC as measured by the purity plays a crucial role in interference experiments. As demonstrated in e.g. [47], the potential barrier between two lattice sites can be turned off, which results in the atoms of each site expanding and ultimately interfering. An interference pattern can be visualized with a laser and detected using a CCD camera. For a system of low coherence these interference patterns will be different each time the interference experiment is executed because in this case there is no defined phase between the atoms of each site. However, if the system is coherent and there is a defined phase relation between the atoms of both sites, the interference pattern will be identical if the experiment is repeated under the same conditions. This behavior is expressed in the average contrast of the interference pattern. For an interference experiment between two sites, where the particle density at position \( r \) and time \( t \) can be described by \( \hat{n}(r,t) \), the average contrast is defined as

\[
\nu(t) = \frac{\langle n \rangle_{\text{max}} - \langle n \rangle_{\text{min}}}{\langle n \rangle_{\text{max}} + \langle n \rangle_{\text{min}}},
\]

where \( \langle n \rangle_{\text{max}} \) and \( \langle n \rangle_{\text{min}} \) are the maximal and minimal values that the particle density expectation value assumes in the imaged area at time \( t \). For the pattern created by the atoms of two neighboring sites \( j \) and \( k \) this term can be expressed in terms of the elements of the SPD matrix \([40]\),

\[
\nu_{jk} = \frac{2|\langle \hat{a}_j^\dagger \hat{a}_k \rangle|}{\langle \hat{a}_j^\dagger \hat{a}_j \rangle + \langle \hat{a}_k^\dagger \hat{a}_k \rangle} \in [0, 1].
\]

37
A detailed derivation of this expression is found in [28]. The coherence between both sites is quantified with the two-site purity
\[ P_{jk} = \frac{\langle \hat{a}_j^\dagger \hat{a}_j \rangle + 4 \langle \hat{a}_j^\dagger \hat{a}_k \rangle - 2 \langle \hat{a}_j^\dagger \hat{a}_k \rangle \langle \hat{a}_j^\dagger \hat{a}_k \rangle}{\left( \langle \hat{a}_j^\dagger \hat{a}_j \rangle + \langle \hat{a}_k^\dagger \hat{a}_k \rangle \right)^2}, \] (4.5)
which is gained by considering only the matrix elements of site \( j \) and \( k \) in (2.11). Together with the squared particle imbalance
\[ I_{jk} = \left( \frac{\langle \hat{a}_j^\dagger \hat{a}_j \rangle - \langle \hat{a}_k^\dagger \hat{a}_k \rangle}{\langle \hat{a}_j^\dagger \hat{a}_j \rangle + \langle \hat{a}_k^\dagger \hat{a}_k \rangle} \right)^2 \] (4.6)
this two-site purity determines the average contrast,
\[ \nu_{jk}^2 = P_{jk} - I_{jk}. \] (4.7)
Hence, the two-site purity is equal to the squared average contrast if the filling level is identical for both sites. In general, any finite particle imbalance lowers the average contrast while the two-site purity provides an upper limit for \( \nu_{jk}^2 \).

For a system of only two sites, as e.g. in [19], the abstract purity of the system is thereby related to a quantity observable in experiment. Even though it is not possible to generalize this concept for multiple sites in an easy manner, it is still feasible for the system presented in this chapter because both outer sites of the subsystems behave identically. Thus, if a high coherence is observed between the central site and one of the outer sites, there has to be a high coherence in the subsystem as a whole.

However, for the average contrast to be largely determined by the purity, the dynamics of the particle imbalance must only play a minor role. To explore the relationship of these quantities for the system under investigation, the time development of the average contrast \( \nu_{12} \) in an interference experiment of sites 1 and 2 is compared in figure 4.11 with the particle imbalance \( I_{12} \), the two-site purity \( P_{12} \), and the overall purity of the subsystem \( P \). Right form the start of the time development, while the dynamics of the filling levels are still in their on-set phase, there are already distinct oscillation of the average contrast closely related in frequency and shape to the oscillations of the purity. Although \( \nu_{12} \) is lower than one for \( t = 0 \) unlike the purity, this small discrepancy caused by the finite particle imbalance does not effect the qualitative behavior. Furthermore, the maxima and minima of the evolving oscillations of \( I_{12} \) almost coincide with the minima and maxima of the purity, respectively. Therefore the dynamical behavior of the particle imbalance does not compromise the alignment of the oscillations of average contrast and purity, but rather reinforces it. This beneficial phase relation between the purity and the particle imbalance is due to the strict symmetries of the system and can not be expected to occur generally.

In view of the above the abstract purity of the SPD matrix becomes a quantity indirectly accessible in experiment through the rather clear relation of \( P \) and \( \nu_{12} \). The
4.5 Relation of dimensionless and physical units

The dimensionless units used in this chapter can be related to the physical units of the BH model in Eq. (3.10) by choosing a specific unit length $u_l$, which can be used to
construct the unit energy $u_E$ and unit time $u_t$. In this section all quantities in physical units are marked with a tilde,

$$\tilde{x} = x u_t, \quad \tilde{E} = E \frac{\hbar^2}{mu_t^2} = E u_E, \quad \tilde{t} = t \frac{mu_t^2}{\hbar} = t u_t.$$  \hspace{1cm} (4.8)

These relations can now be used to transform all quantities in the equations for $J_{ij}$ (3.8) and for $U$ (3.9) (now denoted as $\tilde{J}$ and $\tilde{U}$) to their dimensionless counterparts,

$$\tilde{J}_{ij} = J_{ij}/u_E, \quad \tilde{U} = U/u_E, \quad \tilde{w}_0(x) = w_0(\tilde{x}) u_t^{3/2}, \quad \tilde{V}_0(x) = V_0(u_t x)/u_E.$$ \hspace{1cm} (4.9)

Hence all quantities without tilde belong to the dimensionless version of the BH model used in this chapter. In the dimensionless case the equations for $J_{ij}$ and $U$ transform to

$$J_{ij} = \int d^3 x \tilde{w}_0^* (x - x_i) \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_0(x) + V_T(x) \right) \tilde{w}_0 (x - x_j)$$ \hspace{1cm} (4.10)

and

$$U = 4\pi a_s \frac{a_s}{t} \int d^3 x |\tilde{w}_0 (x - x_i)|^4.$$ \hspace{1cm} (4.11)

To relate the dimensionless parameters $J_1 = 1, J_2 = 2$ and $g = U(N - 1) = 1$ form the theoretical inquiry to physical quantities, a potential has to be found that, together with its Wannier functions, yields these values if inserted in the equations above. For a system with a low count of lattice sites it is feasible to approximate the Wannier function $w_0(x - x_i)$ as the local lowest energy solution of the single-particle Schrödinger equation for this potential at site $i$.

To get a first approximation of the units of the theoretical results, a potential is modeled to resemble the system in figure 4.1 as a superposition of a two-dimensional Mexican hat trapping potential, six two-dimensional Gaussian lattice sites and a harmonic trapping potential in the third dimension of space,

$$V(x) = -a(x_1^2 + x_2^2) + b(x_1^2 + x_2^2)^2 - \sum_{i=1}^{6} c e^{-d((x_1-x_{1,i})^2+(x_2-x_{2,i})^2)} + \omega x_3^2.$$ \hspace{1cm} (4.12)

The sites are located in the minimum of the Mexican hat potential $r_0 = \sqrt{a/2b}$ and distributed in a symmetric manner, such that their locations depend only on one angle $\phi$,

$$x_1 = (r_0 \cos \phi, r_0 \sin \phi, 0)^T, \quad x_2 = (r_0, 0, 0)^T, \quad x_3 = (r_0 \cos \phi, -r_0 \sin \phi, 0)^T$$

$$x_4 = -x_1, \quad x_5 = -x_2, \quad x_6 = -x_3.$$ \hspace{1cm} (4.13)

Figure 4.12 shows the potential for the first two dimensions of space and for the choice of parameters $a = 0.5, b = 0.05, c = 5, d = 2$ and $\phi = 0.71$. To calculate the integrals in Eq. (4.10) and (4.11), the functions $w_0(x - x_i)$ of a particle localized at site $i$ were
approximated as the ground state in a potential consisting only of the Mexican hat and one Gaussian minimum. These wave functions and the integrals were calculated numerically for the same parameter choice as for the potential in figure 4.12 and for $\omega = 0.1$. The unit length was chosen such that for a system of $N = 70$ rubidium atoms with a scattering length of $a_s = 5.768 \text{ nm}$ the tunneling constant $J_1 (= J_{12} = J_{23} = \ldots$ in Eq. 4.10) and the macroscopic interaction strength $g = U(N - 1)$ fulfill the relation $J_1 = g = 1$, which corresponds to the choice of parameters in most calculations in this chapter. In addition $\phi = 0.71$ and $\omega = 0.1$ were chosen such that $J_2 \approx 2J_1$ ($J_2 = J_{34} = J_{16}$). The actual value of the tunneling strength in between the subsystems for this choice of parameters is $J_2 = 2.097$. The unit length that produced these values is $u_l = 1.917 \mu m$, which yields $u_{E}/\hbar = 31.62 \text{ Hz}$ and $u_t = 5.033 \text{ ms}$. In these units, the minimum of the Mexican hat potential is at radius $r = 4.287 \mu m$ and a dimensionless time of e.g. $t = 30$ corresponds to 151 ms. With this, one period of the average contrast and the purity oscillations in figure 4.11 is approximately 9 ms long, which is a timescale that allows for easy measurements.
5 Incoherent loss in a reservoir chain

While the view in chapter 4 was on imitating some of the behavior common to open systems by considering the two parts of an Hermitian system independently, in this chapter the open Bose-Hubbard model is explored in a more straightforward fashion. A one-dimensional optical lattice is considered, the central site of which is subject to incoherent loss mediated by a Lindbald operator of the form (3.15). A similar system has already been investigated experimentally in [20, 48], where the incoherent loss was realized with a steady electron beam focused on the central site of the chain. The core idea of this setup is that, while the loss acting on the central site leads to a dissipation of particles, the other sites of the chain can act as a reservoir driving the central site similar to a gain term in an open system.

A schematic representation of the system is given in figure 5.1. In the ideal case, all but the central site are at the same constant filling level, such that the reservoir can in principle provide a steady flow of particles into the central site counterbalancing the dissipation, which is quantified by the loss parameter $\gamma$. The particle transport between the sites is conveyed through the tunneling parameter $J$, which depends on the depth of the optical lattice. The total number of sites in the system $M$ has to be chosen high in comparison to the system of the previous chapter in order to ensure that the environment provided by the reservoir remains relatively steady on a reasonable time scale. Therefore, the full many-body dynamics of the BH model is inaccessible here and

![Figure 5.1: A BEC in a one-dimensional optical lattice. The central site is subject to dissipation while the rest of the chain forms a driving reservoir providing a counteracting effective particle gain.](image-url)
Incoherent loss in a reservoir chain

Numerically less expensive approximations of the method have to be employed. In the experimental study [20] a bistable behavior of the system was observed with respect to the ratio of the filling levels of the central site and the reservoir sites. For some range of the dissipation strength $\gamma$ this ratio assumed a constant value of either exactly one or a smaller constant value depending on whether the central site was initially occupied or not. To investigate if such a behavior can also be found with the mathematical models used in this theoretical inquiry, the system is analyzed over a broad range of applied dissipation strengths $\gamma$ and for both an initially occupied central site and one that is initially fully depleted.

The structure of this chapter is as follows: Section 5.1 investigates how the parameters and initial state of the system have to be chosen such that the outer sites can act as a reservoir for the central site. In section 5.2 the discrete GPE is discussed as an approximation of the BH model and its validity is verified in a comparison with the next higher order (i.e. the BBR method) for a moderately high dimension $M$. The following section analyzes the dynamical behavior of the system with a focus on the consequences of the choice of the dissipation strength $\gamma$. The chapter is concluded with an investigation of the effects of phase noise on both the initial state and the dynamics of the system in section 5.4.

### 5.1 Initial state and parameter choice

An ideal version of the system presented in figure 5.1 would have an infinite number of reservoir sites with equal filling levels. In this case an equal distribution of the particles on the sites would, for any choice of the parameters $g$ and $J$, also be an eigenstate in the absence of dissipation, and hence all the dynamics observed in the case of a finite $\gamma$ could be ascribed to the incoherent loss. In an experiment or a simulation the number of sites in the system has to be finite and therefore the parameters of the system have to be chosen such that the ground state of the system resembles an ideal infinite chain of sites reasonably well, in particular with respect to the distribution of particles on the sites.

As in the preceding chapter, the basis for the calculation of the initial state is a time-independent version of the discrete GPE (3.20),

$$
\mu c_i = g|c_i|^2 c_i - Jc_{i+1} \quad \text{for } i = -M/2, \\
\mu c_i = g|c_i|^2 c_i - Jc_{i-1} - Jc_{i+1} \quad \text{for } i \in [-M/2 + 1, M/2 - 1], \\
\mu c_i = g|c_i|^2 c_i - Jc_{i-1} \quad \text{for } i = M/2.
$$

With this system of equations the values of the mean-field coefficients $c_i$ are again solely determined by the ratio $g/J$ and can be chosen real for the lowest energy state. Due to the finite dimension of the system, which manifests itself in the fact that there is only one tunneling term for each of the outermost sites $i = \pm M/2$ in Eq. (5.1), the filling...
level $\langle \hat{n}_i \rangle \propto |c_i|^2$ has to decrease at the fringes of the chain. The shape of this outward decrease, however, varies strongly with the ratio $g/J$.

Figure 5.2 shows the mean-field coefficients of the ground state for a system of $M = 101$ sites with $J = 1$ for different values of the macroscopic interaction strength $g$. For the relatively small value $g = 0.2$ the decrease in the filling levels happens very gradually and the ground state assumes an arc-like shape. With increasing interaction strength this drop of the mean-field coefficients’ values becomes both less pronounced close to the center and very steep at the edges. The result of this behavior is that for $g = 20$ there is a long range of sites surrounding the center that practically share the same value of $c_i$ (and hence the same filling level), and the steep drop in value is confined to about seven sites at both ends of the chain.

Since $M = 101$ is a dimension too high to computationally access the time evolution of not only the first and but also the second order of the BBGKY hierarchy (i.e. the discrete GPE and the BBR method, respectively), the ground state is calculated for the same parameters as in figure 5.2 also for the lower number of sites $M = 41$, as displayed in figure 5.3. While the shape of the ground state remains the same qualitatively, the ratio of the sites that share the same filling level is here $\approx 31/41 \approx 76\%$, which is considerably lower than for $M = 101$ with $\approx 85/101 \approx 84\%$.

To give a preliminary illustration of the consequences of both the choice of the interaction strength $g$ and the dimension of the system $M$ for the dynamics of the central site filling level $\langle \hat{n}_c \rangle$, the time development is calculated for the various ground states of figures 5.2 and 5.3 with the discrete GPE (3.20) for a dissipation strength of $\gamma = 1$. Figure 5.4 shows the time dependence of the central sites’ filling level for all previously discussed initial states. A BEC with initially $N_0 = 700M$ particles in the system is considered. Disregarding any local oscillations, the central site filling level decreases over the whole time range for the three lower values of $g$, with the decreasing behavior being more pronounced at a lower interaction strength. In the case of $g = 20$, however, corresponding to a ground state that includes a long range of sites with equal filling level, the central filling level assumes a quasi constant value over a long period of time. This is an indicator that for this value of $g$ the outer sites of the chain are able to act as a reservoir for the central site counterbalancing the dissipation caused by the particle loss $\gamma$. This quasi-constant behavior is qualitatively the same for both $M = 101$ sites and $M = 41$ sites, although for the lower dimension it already breaks down within the plotted time range.

With these results the default values of system parameters for the following thorough analysis of the filling level dynamics are chosen to be $J = 1$ and $g = 20$. If the system is to be analyzed in the case where the central site is initially unoccupied, the mean-field coefficient of the central site $c_0$ is set to zero. This is equivalent to the experimental situation where the central site is initially emptied by applying an electron beam of very high intensity over a short time span and subsequently reducing the intensity to a smaller level according to the value of the loss strength $\gamma$ desired for the investigation of the dynamics.
5 Incoherent loss in a reservoir chain

Figure 5.2: Real valued ground state of Eq. 5.1 for a chain of $M = 101$ sites with $J = 1$ and for different values of the macroscopic interaction strength $g$. Only for $g/J \gg 1$ there exists a long range of sites that share the same filling level.

Figure 5.3: Same plot as figure 5.2 but for only $M = 41$ sites. While for the larger system $\sim 85$ out of 101 sites are at the same filling level for $g = 20$ only $\sim 31$ out of 41 fall in that range.
5.2 Approximating the Bose-Hubbard model

With $M = 41$ and $M = 101$ the numbers of sites in the system used in the previous section are relatively high with regard to the strong dependence of the dimensionality of both BH model and BBR method on the site count, which is of order $O(N^{M-1})$ for the former and $O(M^4)$ for the latter, as discussed in section 3.4. Since a high number of outer sites is required for them to be able to act as a reservoir on the central site, the lowest order of the BBGKY hierarchy, the discrete GPE (3.20), has to be considered to keep the computational cost within reasonable limits. The number of equations in this approximation is only of order $O(M)$, which makes even large systems computationally accessible.

It is not possible to use the discrete GPE to simulate the system in chapter 4 because it does not allow for describing any phase incoherence between sites in the system, which made it impossible to express the required initial state. In contrast, the initial state of the system investigated in the present and the following section is a single coherent BEC.

Although there are no fundamental restrictions to use the discrete GPE to simulate the dynamics of this reservoir chain, its quality as an approximation of the BH model has still to be discussed. Being a mean-field approximation, it can be assumed to describe the dynamics of the full BH model very well in the case of a very high particle count.

Figure 5.4: Filling level of the central site $\langle \hat{n}_c \rangle$ for the various initial states from figures 5.2 and 5.3 propagated with the discrete GPE (3.20). Only for $g = 20$, where the ground state includes a long range of sites with equal filling level, $\langle \hat{n}_c \rangle$ holds a quasi constant value over a long period. The dynamics is qualitatively similar for both values of the dimension $M = 101$ (left plot) and $M = 41$ (right plot), although the constant behavior breaks down already within the displayed time range for the shorter chain.

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Although there are no fundamental restrictions to use the discrete GPE to simulate the dynamics of this reservoir chain, its quality as an approximation of the BH model has still to be discussed. Being a mean-field approximation, it can be assumed to describe the dynamics of the full BH model very well in the case of a very high particle count.
In the experimental work investigating a similar system [20], the initial number of particles per site was \( \sim 700 \), which leads to a relatively high initial total particle number \( N_0 = 700M \). To evaluate the quality of the mean-field approach in this regime, both the discrete GPE and the next higher order of the BH model, the BBR method, are used to calculate the time evolution of the system for \( M = 41 \) sites, which is a low enough site count such that the numerical cost of the BBR method is still within reasonable boundaries.

In figure 5.5 the time dependence of the central site filling level \( \langle \hat{n}_c \rangle \) is displayed for the BBR method (dashed lines) against the background of the GPE results (solid black lines) for different values of the dissipation strength \( \gamma \), with the initial state being the set of mean-field coefficients for \( g = 20 \) in figure 5.3. In the left part of the figure the time evolution of \( \langle \hat{n}_c \rangle \) is shown for the large initial value of the particle number corresponding to the experimental situation \( N_0 = 700M \). Here, the curves representing the BBR method lie exactly on top of the values of the GPE, which means that the mean-field approximation is not further improved by adding another order in the BBGKY hierarchy. This implies the hierarchy converges already with its first order. That this behavior is not found for significantly lower particle numbers can be seen in the right part of the figure, where the same calculation is displayed for \( N_0 = 5M \). In this regime the BBR results

![Figure 5.5](image_url)

Figure 5.5: Time evolution of the central site filling level \( \langle \hat{n}_c \rangle \) calculated with the BBR method (dashed lines) and the discrete GPE (solid black lines). For the high initial particle number of \( N_0 = 700M \) on the left hand side both methods yield the same results, indicating that already the first order of the BBGKY hierarchy (i.e. the GPE) converges. On the other hand, the results for the very low particle number \( N_0 = 5M \) in the right part of the figure differ significantly for the GPE and the BBR method.
5.3 Dynamics of the filling levels

Figure 5.6: Time dependence of the total number of particles in the system calculated with the BBR method (dashed lines) and the discrete GPE (solid black lines) for the same parameters as in figure 5.5. The difference of the values of GPE and BBR method for the relatively low initial value $N(0) = N_0 = 5M$ become very obvious for higher values of the dissipation strength $\gamma$, as seen on the right. For the high initial total particle number $N_0 = 700M$ on the left hand side, however, both approaches again yield the same results.

deviate form the mean-field already after a short time and even in the case without dissipation $\gamma = 0$ some dynamics can be observed where the GPE is in an eigenstate.

Figure 5.6 shows the same comparison for the total number of particles in the system $N(t)$. Although for $N(0) = N_0 = 5M$ the BBR method yields a significantly higher particle number over time than the GPE at the higher values of $\gamma$, as seen in the right part of the figure, for the much higher initial value $N_0 = 700M$ both methods produce the same values again.

These comparisons of the first and second order of the BBGKY hierarchy validate the discrete GPE as an approximation of the BH model in the regime of high particle numbers. It will therefore be used in the following to calculate the dynamics of the reservoir chain for an even higher number of sites $M$, which are numerically inaccessible with the BBR method.

5.3 Dynamics of the filling levels

With the discussion of the appropriate ground state and the quality of the discrete GPE as an approximation of the BH model in the previous sections the groundwork has been laid out for a detailed analysis of the dynamical behavior of the system. The choice of the
system parameters in this section is $g = 20$ and $J = 1$, and the number of sites is chosen to be $M = 101$, which is a significantly higher dimension than would be computationally accessible with the BBR method. Since the focus of this chapter is to explore how the outer sites can act as a reservoir on the central site, the central quantity of interest is again the central site’s filling level, which has already been introduced as the expectation value of the number operator, $\langle \hat{n}_c \rangle = \langle \hat{n}_0 \rangle$. As already indicated in the discussion of figure 5.4, the most interesting property of the situation where the outer sites constitute a reservoir providing an effective gain term for the central site is a quasi constant central filling level in the presence of a sustained current of particles through the central site. This situation corresponds to a steady state of a $\mathcal{PT}$-symmetric system as the double well in section 2.5. It arises when the current of particles tunneling into the central site is of the same magnitude as the incoherent particle loss.

Although this situation is naturally not a steady state of the whole system incorporating the reservoir, it can be understood by considering in the system of equations forming the discrete GPE (3.20) only the equation of the central site in a stationary version,

$$\mu_0 c_0 = g|c_0|^2 c_0 - J c_{-1} - J c_1 - i\frac{\gamma}{2} c_0 .$$

(5.2)

Here $\mu_0$ is not an eigenvalue of the complete GPE. In the case where the outer sites act as ideal reservoir, $c_1$ and $c_{-1}$ are of a constant equal magnitude and of equal phase, $c_{-1} = c_1 = |c_1| e^{i\varphi_1}$, such that they both provide a constant particle current into the central site of the same strength. Expressing the central mean-field constant as $c_0 = |c_0| e^{i\varphi_0}$ and the part of the equation associated with it as $(\mu_0 - g|c_0|^2 + i\gamma/2) = |\mu_0 - g|c_0|^2 + i\gamma/2| e^{i\varphi_0}$, this yields two equations relating the phases and amplitudes of central and outer sites,

$$\Delta \varphi = \varphi_1 - \varphi_0 = \varphi_\gamma - \pi ,$$

(5.3)

$$\frac{|c_0|}{|c_1|} = \frac{2J}{|\mu_0 - g|c_0|^2 + i\gamma/2|} .$$

(5.4)

Although the equation determining the ratio of magnitudes is still dependent on $|c_0|$ due to the nonlinearity, it nevertheless shows that the central site has to be at a much lower filling level than the reservoir sites in the case of a strong dissipation strength $\gamma$, while for a small value of $\gamma$ approximately equal filling levels are supported by the equation.

This quasi-constant central filling level in the presence of a loss term is discussed exemplarily for $\gamma = 1$ in figure 5.7. With the inception of the particle loss at the central site at $t = 0$ the central filling level falls quickly to an approximately constant height as the reservoir begins to provide a current counterbalancing the loss. The delayed response of the reservoir can be seen in the colored lines representing some of the outer sites of the chain. Propagating outward it reaches the end of the chain (site $\pm 50$) at $t \approx 25$. The counteraction originating form these outermost sites then takes the same amount of time to propagate back to the central site, where it interferes with the quasi-constant central filling level, superimposing non-harmonic oscillations on the lossy site.
5.3 Dynamics of the filling levels

Figure 5.7: Filling levels of the central site and various reservoir sites (indices as in figure 5.1 and average filling level $N(t)/M$ for $\gamma = 1$. The central site quickly approaches a quasi constant level that stays undisturbed in the interval $20 \lesssim t \lesssim 50$ and is afterwards superimposed by almost chaotic oscillations around that level. This overlaying disturbing behavior is due to the finite dimension of the chain: Following the inception of the loss term at $t = 0$, a delayed response propagates through the reservoir that reaches the end of the chain (site $\pm 50$) at $t \approx 25$. The counteraction created at these sites then takes the same time to travel trough the reservoir again and interferes with the constant central site filling level. Throughout the entire time interval displayed in the figure the average filling level $N(t)/M$ decreases constantly, corresponding to a steady current of particles out of the system through the central site.
Incoherent loss in a reservoir chain

The deviation form a constant central site filling level after $t \approx 50$ is therefore due to the finite dimension of the system. During the entire time interval displayed in the figure there is a constant decrease in the average filling level, $N(t)/M = \sum_i \langle \hat{n}_i \rangle / M$, which indicates a steady current of particles out of the system flowing through the central site.

Within the framework of the discrete GPE the quasi-constant value of the central site filling level arising in this system does not depend on the initial filling of the central site. Figure 5.8 shows the time dependence of $\langle \hat{n}_c \rangle$ form figure 5.7, where the central site is initially filled, compared to the same system with its central site initially unoccupied exemplarily for the loss strength $\gamma = 1$. In both situations the central filling level assumes the same value after a short time. The process of establishing this quasi-constant level is accompanied by strong oscillations in the case where the lossy site is initially unoccupied. These oscillations cause a stronger response in the reservoir than in the case where the central site is occupied initially. Therefore, the interference caused by the finite dimension of the chain, which arises in $\langle \hat{n}_c \rangle$ after $t \approx 50$, is of a larger magnitude in the initially unoccupied case.

The effect of the value of the loss strength on both the central site filling level $\langle \hat{n}_c \rangle$ and the average filling level $N(t)/M$ can be seen in figure 5.9. While the quasi-constant value assumed by $\langle \hat{n}_c \rangle$ (solid lines) decreases with increasing loss strength, the behavior of the

![Figure 5.8: Time development of the central site filling level $\langle \hat{n}_c \rangle$ for both an initially filled and an initially unoccupied lossy central site with $\gamma = 1$. In both situations the same constant level arises. In the case of an initially unoccupied central site, however, $\langle \hat{n}_c \rangle$ undergoes strong oscillations in reaching this level. Due to these oscillations causing a greater response in the reservoir than in the initially occupied case, the interference with the constant filling level after $t \approx 50$ caused by the finite dimension of the chain is of a greater magnitude.](image)
average filling level is more complex. Although there is a stronger decrease in \( N(t)/M \)
for \( \gamma = 1 \) than for the lower value of \( \gamma = 0.2 \), increasing the loss strength even further
to \( \gamma = 5 \) and \( \gamma = 20 \) leads to a continuously slighter decrease of \( N(t)/M \) and hence of
the total number of particles in the system \( N(t) \). This means the system exhibits the
counterintuitive behavior of loosing less particles over time if the loss strength \( \gamma \) is at
an exceptionally high value. The cause of this phenomenon common to dissipative BH
systems [16] is that the tunneling form sites \( \pm 1 \) into the central site gets considerably
suppressed in the presence of a strong imaginary potential acting on the center. In a
many-particle system this can be understood in terms of a quantum Zeno effect: A high
loss strength acts as a strong source of incoherence in the system corresponding to an
almost continuous measurement of the filling level of the central site. This makes it more
unlikely for a tunneling process to occur. Since the discrete GPE can only describe a fully
coherent state, here an analogy for this behavior can be found in optics that matches the
mathematical reality of this model better. If an electromagnetic wave passes from one
medium into another, a large mismatch in the real or imaginary part of the refractive
indices of the media leads to the reflection of a large part of the wave. The same is true
for a mismatch in real or imaginary part of the potential at neighboring sites, which
leads to a suppression of the tunneling processes between those sites. This behavior of
the system is in good agreement with Eq. (5.4) describing the ratio of the mean-filed
coefficients of the central site and first reservoir sites, which relate to the filling levels
through \( \langle \hat{n}_i \rangle = N|c_i|^2 \).

After the quasi-constant filling level of the central site is assumed, it stays constant
throughout the entire time interval in part (a) of the figure disregarding both the inter-
ference setting in at \( t \approx 50 \) and a very slight overlaying slope for \( \gamma = 0.2 \) and \( \gamma = 1 \). The
eventual breaking-down of this level can be observed in the long-term time development
in part (b) of the figure. The duration over which the constant level can be sustained by
the reservoir is determined by the number of sites in the chain, as already demonstrated
in figure 5.4. In an ideal reservoir chain with infinitely many sites the loss at the central
site is counterbalanced by the reservoir indefinitely.

A crucial consequence of the aforementioned Zeno effect is illustrated in figure 5.10.
It displays the number of particles \( N(t_i) \) remaining in the system at two points during
the time development, \( t_i = 50 \) and \( t_i = 100 \), in dependence of the applied dissipation
strength \( \gamma \). Only up to a critical value \( \gamma_c \approx 1.05 \) an increase in the dissipation strength
results in a lower number of particles in the system after a fixed time. This is because
for higher values of \( \gamma \) the incoherence introduced into the system by the loss term begins
to affect the transport, suppressing the tunneling of particles from the reservoir into the
central site and thereby reducing the overall loss of particles. The difference of the two
curves in the figure is the number of particles lost between \( t = 50 \) and \( t = 100 \), and can
therefore be used to quantify the particle current out of the system in dependence of
the dissipation strength. It is highest at \( \gamma_c \) and gets very low for the higher values of \( \gamma \)
displayed in part (b) of the figure.

To further investigate the effects of the incoherent loss on the particle transport be-
Figure 5.9: Comparison of the central filling level $\langle \hat{n}_c \rangle$ (solid lines) and average filling level $N(t)/M$ (dashed lines) for different values of the loss strength $\gamma$. Although a higher loss strength leads to a lower central filling level in all cases, the total amount of particles lost is lowest for the highest value of $\gamma$ due to the Zeno effect (see text). Apart from some interference the central filling level stays constant throughout the whole interval in part (a) of the figure. The long-term time evolution in (b), however, shows the eventual breakdown of this quasi-constant filling level of the central site.
5.3 Dynamics of the filling levels

Figure 5.10: Total number of particles in the system \( N(t_i) \) after \( t_i = 50 \) and \( t_i = 100 \) in dependence of the loss strength \( \gamma \). As seen in part (a) of the figure, the number of particles in the system after a fixed time decreases with increasing loss strength only until the critical value \( \gamma_c \approx 1.05 \) is reached. At higher values of \( \gamma \) the suppression of the tunneling due to the quantum Zeno effect becomes significant, leading to a smaller overall loss of particles in the system. Part (b) of the figure shows that for very strong dissipation strengths the number of particles in the system at \( t_i = 100 \) is not much lower than at \( t_i = 50 \), representing a situation in which almost no particle loss occurs.

Between reservoir and lossy site, the central filling level \( \langle \hat{n}_c \rangle \) and the filling level of the first reservoir sites \( \langle \hat{n}_{\pm 1} \rangle \) evaluated at \( t = 30 \) are compared in dependence of the applied dissipation strength \( \gamma \), which is shown in figure 5.11. This point in the time development is chosen such that the central filling level has already assumed its quasi-constant value. For low values of \( \gamma \) both the outer sites and the central site share the same filling level, which shows that particle transport into the central site can only be driven by a phase gradient rather than a difference in the occupation of the sites. This is only possible if there is absolute phase coherence between the central site and the reservoir, which is a priori true for any mean-field state described with the discrete GPE. For values of the dissipation strength greater than \( \gamma_c \) the Zeno effect reduces the coherent particle transport into the central site, and a finite difference in the filling levels is established as predicted by Eq. (5.4).

The quasi-constant central filling level and the corresponding filling levels of the first reservoir sites do not depend on the initial occupation of the central site for all values of the dissipation strength \( \gamma \) shown in figure 5.11. Within the simple model of the discrete
5 Incoherent loss in a reservoir chain

Figure 5.11: Value of the quasi-constant central filling level represented by $\langle \hat{n}_c \rangle$ at $t = 30$ and the filling level at the first reservoir sites $\langle \hat{n}_{\pm 1} \rangle$ at the same point in time plotted over the loss strength $\gamma$. There is no difference in the filling levels approximately until the critical value $\gamma_c$ from figure 5.10 is reached, indicating a superfluid particle transport driven by a phase gradient. For higher values of $\gamma$ there is a finite difference in the filling levels since the incoherence introduced by the dissipation begins to suppress the tunneling into the central site.

GPE it is not possible to observe any bistability with respect to the ratio $\langle \hat{n}_c \rangle / \langle \hat{n}_{\pm 1} \rangle$ as in the experimental work [20]. Following a suggestion by the authors, the model is therefore extended to include phase noise, which can have an impact on the transport processes in a system by disturbing its coherence.

5.4 Loss of coherence in the presence of phase noise

Until now the only interaction of the system with a real environment considered in this chapter is the particle loss acting on the central site. In an experimental situation, however, phase noise interfering with the coherence of the system can play a significant role. It can originate e.g. form the occasional absorption of a photon from the optical lattice by one of the particles in the system [16].

Since the GPE (3.20) only describes the dynamics of mean-field coefficients, and hence of a pure state, it is not able to treat the incoherence introduced by phase noise. Instead the elements of the single particle density matrix $\sigma_{jk}$ can be calculated directly with equation (3.19), where the phase noise is quantified with the parameter $\kappa$. Neglecting the covariances $\Delta_{jklm}$ of the BBR method in the regime of a high particle number $N$ as discussed in section 5.2, this first order of the BBGKY hierarchy is fully equal to the...
5.4 Loss of coherence in the presence of phase noise

5.4.1 Incoherent initial state

To gain a set of first-order moments $\sigma_{jk}$ that is stationary in equation (3.19) in the absence of dissipation, and therefore presents a suitable initial state for the analysis of the dynamics, the mean-field initial state used in the previous section is first propagated with the equation in the case of $\gamma = 0$. By observing the change of the filling levels and the purity $P$ (2.14) of the system during this process, the differences of a system with and without phase noise become apparent. Figure 5.12 (a) shows the time dependence of the filling levels of the outermost sites $\langle \hat{n}_{\pm50} \rangle$ if the mean-field state is propagated in the presence of phase noise of various strengths $\kappa$. Here the observed behavior is exemplary for all sites of the system. Over time all filling levels equalize and assume the same value of $\langle \hat{n}_{i} \rangle = 700$. Although the initial increase in $\langle \hat{n}_{\pm50} \rangle$ becomes greater with increasing $\kappa$, this stationary state of equal filling is reached fastest for the intermediate value $\kappa = 0.1$. For the relatively small value $\kappa = 0.01$ the stationary state is only reached after a long time $t \approx 700$ in comparison to the timescale of the dynamics in the previous section.

The fact that the stationary state is of equal filling levels in the presence of phase noise presents a contrast to the drop of the filling levels that is observed at the outer sites for $\kappa = 0$ as seen in figure 5.2. Since a prominent feature of coherent quantum mechanical systems is that the probability density decreases at the edges of the system, this behavior suggests that the inception of phase noise introduces incoherence in the system that stimulates a more classical (i.e. less coherent) filling level dynamics. This can be understood mathematically by considering Eq. (3.19) determining the dynamics of the SPD matrix elements in the case without dissipation while neglecting the nonlinear terms $\propto U$ for simplicity. The coherence in a system is determined by the off-diagonal elements of the SPD matrix, $\sigma_{jk}$ with $j \neq k$. A system is completely incoherent if all those elements are zero. The flux of particles into a site $i$ couples via the tunneling constant $J$ to all off-diagonal elements that site $i$ shares with its neighboring sites,

$$\frac{d}{dt}\sigma_{ii} = iJ(\sigma_{ii+1} + \sigma_{i-1i} - \sigma_{i+1i} - \sigma_{i-i1}).$$  \hspace{1cm} (5.5)

Hence, there can only be particle transport in the system if it is not completely incoherent and some of these elements posses a finite value. The effect of the phase noise in Eq. (3.19), however, is to induce an exponential decay in the off-diagonal elements and therefore to drive the system to a state of complete incoherence. The off-diagonal elements of two neighboring sites $i$ and $i + 1$ can only fully decay if those sites are at the same filling level since the equations determining the dynamics of these elements include a term proportional to the filling level difference $\sigma_{ii} - \sigma_{i+1i+1}$,

$$\frac{d}{dt}\sigma_{ii+1} = iJ(\sigma_{ii} - \sigma_{i+1i+1} + \sigma_{i+2} - \sigma_{i+1i+1}) - \kappa\sigma_{ii+1}.$$

$$\hspace{1cm} (5.6)$$
5 Incoherent loss in a reservoir chain

Figure 5.12: Time evolution of the steady state of the GPE in the presence of phase noise of various strengths $\kappa$ without dissipation (i.e. $\gamma = 0$). (a): All filling levels including the outermost ones $\langle \hat{n}_{\pm 50} \rangle$ displayed in this figure approach the same value $\langle \hat{n}_i \rangle = 700$. (b): The purity $P$ of the system (2.14) starts at unity since the system is initially in a mean-field state but deteriorates over time due to the incoherence introduced by the phase noise.

Therefore, the stationary state of the first order of the BBGKY hierarchy is fully incoherent in the absence of dissipation and the particles are evenly distributed over all sites of the system.

To quantify the loss of coherence caused by the phase noise, the purity of the SPD matrix (2.14) $P$ is displayed in figure 5.12 (b). The system goes from the unity purity of the initial mean-field state to zero purity over the course of the time evolution. This process is observed for all phase noise strengths $\kappa$ while the actual value of $\kappa$ determines only its timescale.

5.4.2 Comparison of the dynamics

The effects of both the incoherent initial state and actual phase noise on the filling level dynamics in the presence of a non-vanishing dissipation $\gamma = 1$ can be seen in figure 5.13. For the small value of $\kappa = 0.01$ the phase noise is not strong enough to disturb the dynamics significantly, and the system is able to establish a quasi-constant central site filling level (solid lines) similar to the case without phase noise ($\kappa = 0$). The difference in height, shape and especially in the behavior after $t \approx 50$, when the response of the outermost site begins to interfere with the central site, can be attributed to the different initial states used, especially with regard to the initial distribution of particles in the chain. The fact that the values of the filling levels reduce gradually at the fringes of the
chain for $\kappa = 0$ and stay constant up to the last sites for $\kappa = 0.01$ leads to a higher value of the quasi-constant central filling level in the latter case. It decreases drastically once the response form the outermost sites reaches the center.

If the value of $\kappa$ is increased further, the exponential decay acting on the off-diagonal elements of the SPD matrix begins to suppress the tunneling within the chain significantly, similarly to the Zeno effect discussed in the previous section. Because of this, the transport of particles form the reservoir into the central site is inhibited and the dissipation can no longer be compensated. Therefore, the central site filling does not assume a quasi-constant value but decreases monotonously. For $\kappa = 0.5$ this inhibition of the transport processes in the chain leads already to a considerable slowing-down of the over-all loss of particles in the system as quantified by the average filling level $N(t)/M$ (dashed lines).

Since no quasi-constant filling of the central site can be established for higher values

![Figure 5.13: Filling level of the central site $\langle \hat{n}_c \rangle$ (solid lines) and average filling level $N(t)/M$ (dashed lines) for different values of the phase noise strength $\kappa$ and $\gamma = 1$. For the relatively small strength $\kappa = 0.01$ the reservoir is still able to counterbalance the dissipation and $\langle \hat{n}_c \rangle$ assumes a quasi-constant level. Its difference in shape to the results without phase noise is mostly due to the incoherent initial state used. For higher values of $\kappa$ the phase noise begins to inhibit the tunneling between sites noticeably, which leads to the reservoir not being able to compensate the dissipation anymore. Therefore, no constant central filling level is established for $\kappa = 0.1$ and $\kappa = 0.5$.](image-url)
Figure 5.14: Time dependence of the filling levels of the central site $\langle \hat{n}_c \rangle$ (solid lines) and the first reservoir sites $\langle \hat{n}_{\pm 1} \rangle$ (dashed lines) for $\gamma = 1$ in the presence of phase noise of the strength $\kappa = 0.01$. The comparison with the case of $\kappa = 0$ (figure 5.8) shows that the phase noise is able to smooth the oscillations that arise if the central site is initially unoccupied, and the quasi-constant level is reached already after a shorter time. The eventual values of both $\langle \hat{n}_c \rangle$ and $\langle \hat{n}_{\pm 1} \rangle$ do not depend on the initial filling level of the central site.

of the phase noise strength $\kappa$, the dynamical behavior is investigated further for the relatively small value of $\kappa = 0.01$. Figure 5.14 shows the time dependence of the filling levels of the central site $\langle \hat{n}_c \rangle$ (solid lines) and the first reservoir sites $\langle \hat{n}_{\pm 1} \rangle$ (dashed lines) for $\gamma = 1$ both in the case where $\langle \hat{n}_c \rangle$ is initially on the same level as the other sites and where it is initially zero. Comparing this plot to figure 5.8, which displays the same situation for $\kappa = 0$, shows that the phase noise smooths the oscillations that arise if the central site is initially unoccupied due to the damping of the off-diagonal SPD matrix elements that are associated with the particle transport. Additionally, the constant level is reached already after a shorter time span than in the case without phase noise. The system exhibits a different value of the ratio $\langle \hat{n}_c \rangle / \langle \hat{n}_{\pm 1} \rangle < 1$ in the presence of phase noise than in the coherent case of the discrete GPE in the previous section, where it assumed the value 1 for all dissipation strengths $\gamma \lesssim 1.05$. However, as in the case without phase noise, this value does not depend on the initial filling level of the central site.

### 5.4.3 Particle transport at finite $\kappa$

A central difference in the behavior of the system with and without phase noise lies in the prevalent transport processes. This becomes apparent by comparing the filling levels of the central site $\langle \hat{n}_c \rangle$ and the first reservoir sites $\langle \hat{n}_{\pm 1} \rangle$ at a point in time where
they have assumed their quasi-constant values. Figure 5.15 shows these filling levels at $t = 30$ in dependence of the applied dissipation strength $\gamma$. Here, a finite difference in the filling levels arises already for small values of $\gamma$, which becomes very pronounced as $\gamma$ increases. This presents a contrast to the situation without phase noise displayed in figure 5.11, where the central site is at the same filling level as the first reservoir sites until the Zeno effect becomes significant around $\gamma_c \approx 1.05$. This is because without phase noise the transport can be solely driven by a phase gradient. If $\kappa$ is at a finite value, however, a finite difference in the filling levels has to be established to counteract the term proportional to $\kappa$ in Eq. (5.6), which determines the dynamics of the off-diagonal SPD matrix elements responsible for the particle transport. As the current through the central site and its exponential damping due to the phase noise rise with increasing $\gamma$ (before the Zeno effect becomes significant), the difference in the filling levels has to increase as well.

As in the case without phase noise, $\langle \hat{n}_c \rangle$ and $\langle \hat{n}_{\pm 1} \rangle$ at $t = 30$ do not depend on the initial filling level of the central site as shown in figure 5.15. This shows that the bistable behavior observed in the experiment [20] cannot be found within the theoretical model used in this work. However, the value of the ratio $\langle \hat{n}_c \rangle / \langle \hat{n}_{\pm 1} \rangle$ at a given dissipation strength is greatly different depending on whether there is phase noise in the system or not.

Figure 5.15: Filling level of the central site $\langle \hat{n}_c \rangle$ and the first reservoir sites $\langle \hat{n}_{\pm 1} \rangle$ at $t = 30$ for $\kappa = 0.01$ plotted over the loss strength $\gamma$. In contrast to the same situation without phase noise shown in figure 5.11 a finite difference in the filling levels arises already for small dissipation strengths $\gamma$. This is because in the presence of phase noise the transport cannot be driven solely by a phase gradient but a difference in the filling levels has to be established to counteract the term proportional to $\kappa$ in Eq. (5.6), which determines the dynamics of the off-diagonal SPD matrix elements responsible for the particle transport.
not. This suggests that the incoherent particle loss realized with an electron beam might also act as a phase-noise-like source of incoherence that has a more significant impact on the system if the central site is initially not at the same filling level as the reservoir. If and how the incoherence introduced into the system through the dissipation depends on the initial filling of the central site is to be investigated in a future work.

This particle transport driven by a difference in the filling levels of neighboring sites shows a slightly different response to an increase in the dissipation strength than the phase gradient driven transport in the case without phase noise. Figure 5.16 shows the remaining number of particles in the system $N(t_i)$ at $t_i = 50$ and $t_i = 100$ for $\kappa = 0.01$ in dependence of the dissipation strength $\gamma$. Qualitatively, the development is similar to the behavior without phase noise displayed in figure 5.10. For small values of $\gamma$ increasing the dissipation strength leads to a smaller number of particles remaining in the system, while at higher values of $\gamma$ the Zeno effect due to the incoherent nature of the dissipation becomes significant. It suppresses the tunneling into the central site and therefore reduces the overall particle loss. However, in the presence of phase noise the

![Figure 5.16: Number of particles remaining in the system $N(t_i)$ at $t_i = 50$ and $t_i = 100$ for $\kappa = 0.01$ in dependence of the dissipation strength $\gamma$. The development is qualitatively similar to the case without phase noise as seen in figure 5.10. The tunneling into the central site is suppressed by the Zeno effect for high values of $\gamma$ leading to a smaller number of particles leaving the system at higher dissipation strengths. However, the minimum of the curves is at a higher value than $\gamma_c$ in the presence of phase noise. This suggests that the transport originating from a difference in the filling levels of neighboring sites is less prone to the Zeno effect than the phase gradient driven transport for $\kappa = 0.$](image)
minimum of the curves is at a higher value than the critical loss strength $\gamma_c$ in figure 5.10. This suggests that the phase gradient driven transport prevalent in the absence of phase noise is more prone to the Zeno effect caused by the incoherent loss than the transport driven by a finite difference in the filling levels at finite values of $\kappa$. To investigate the cause of the different responses to the Zeno effect shown by these two types of particle transports might be an interesting subject for future studies.
6 Conclusions and Outlook

The central object of this thesis was to investigate how a part of a system within the Bose-Hubbard model can act as an environment for the dynamics of a subsystem. This approach presents an alternative to the indetermined implementation of an external environment as an open system. The experimental realization, especially for particle gain, requires a defined coupling. In this context two different arrangements of Bose-Einstein condensates in optical lattices were analyzed independently.

The purely Hermitian system under investigation in chapter 4 consists of a six-site optical lattice on a ring divided into two symmetric three-site subsystems. Both subsystems are initially separated in the sense that they share no phase coherence. Such a state cannot be constructed in a mean-field approach and the full Bose-Hubbard model is employed to calculated the dynamics for $N = 70$ particles in the system.

By coupling the subsystems together at both outer sites at the beginning of the time evolution, an oscillating behavior is induced in the particle number expectation values. This is similar to the oscillations observed in an open system of two sites [10]. Calculating the purity of the single-particle density matrix separately for both subsystems a strong decrease and subsequent restoration of the coherence in a periodic fashion is found within each subsystem. These purity oscillations are a phenomenon previously observed in open systems in which particle gain and loss were provided by a Born-Markov environment [49].

The coherence within the subsystems is linked to the average contrast in an interference experiment between two sites. A comparison of the average contrast with the purity and the squared particle imbalance at the two sites shows that the time dependence of the contrast is largely determined by the behavior of the purity in this setup. This renders the purity a quantity observable in an experiment.

To get an approximation for the time scale on which the purity oscillations occur, the dimensionless units of the theoretical investigation are related to physical quantities with a simple ansatz for the shape of the trapping potential and the corresponding wave functions. The period of the oscillations is found to be in the range of milliseconds, which is an adequate timescale for an experimental observation.

A detailed analysis of the quality of this simple ansatz for both the trapping potential and the wave functions in view of possible improvements might be the subject of a future study. Another question for future investigation is whether a similar behavior can be observed if, instead of coupling two subsystems at both ends in a periodic fashion, a central subsystem is connected to two separate subsystems providing particle gain and
loss. Such a system has already been analyzed in the mean field [50] but a many-particle description considering the behavior of the purity is still missing.

In chapter 5 a Bose-Einstein condensate is analyzed in a one-dimensional optical lattice of \( M = 101 \) sites that is subject to particle loss localized at its center site. The system is prepared such that the outer sites constitute a reservoir providing a particle influx into the central site. Following the situation in an experimental study of a similar setup [20] the initial number of particles in the system is chosen to be \( N_0 = 700M \). A comparison between the first two orders of the BBGKY hierarchy shows that in this high particle regime the discrete Gross-Pitaevskii equation presents already a good approximation of the Bose-Hubbard model.

The dynamics shows that the reservoir is able to counterbalance the dissipation such that over a long time range a quasi-constant filling level of the central site is established, the value of which is determined by the dissipation strength \( \gamma \). Within this mean-field approach the particle transport is driven by a phase gradient and up to a critical value \( \gamma_c \) the central site is at the same filling level as the reservoir during its quasi-constant state. For larger values \( \gamma > \gamma_c \) the incoherent loss begins to suppress the coherent transport of particles into the central site similar to a Zeno effect, which leads to a smaller total number of particles lost at large dissipation strengths.

To study how the dynamics is changed in presence of phase noise acting as a source of incoherence, the time development of the single-particle density matrix elements is calculated directly with the first order of the BBGKY hierarchy, which allows for considering incoherent initial states. In the presence of strong phase noise the tunneling transport within the chain is suppressed such that the reservoir cannot counterbalance the dissipation anymore and no quasi-constant filling level is established. If the phase noise strength is of a relatively small value, the particle transport is not inhibited significantly and the quasi-constant central filling level can still be assumed. However, even for small values of \( \kappa \) the nature of this transport is inherently different to the phase gradient driven transport in the absence of phase noise. A finite phase noise strength \( \kappa \) forces the system to establish a finite difference between the filling levels of the central site \( \langle \hat{n}_c \rangle \) and those of the first reservoir sites \( \langle \hat{n}_{\pm 1} \rangle \). This difference constitutes the driving force behind the transport in the partially incoherent system.

In the experimental work [20] a bistable behavior of the ratio \( \langle \hat{n}_c \rangle / \langle \hat{n}_{\pm 1} \rangle \) was observed in the sense that it assumed the value one if the central site was initially filled and a smaller value if it was initially unoccupied for a certain range of dissipation strengths \( \gamma \). Although no bistable behavior is found in the mathematical models employed in this thesis, for \( \gamma < \gamma_c \) this ratio is equal to one in the absence of phase noise, while it is smaller than one at the same dissipation strength if phase noise is applied. Therefore it is an interesting question to investigate in a future work if the dissipation realized in the experiment by an electron beam can act as a phase-noise like source of incoherence that has a more significant impact on the system if the central site is initially not at the same filling level as the reservoir.
Furthermore, in the case that the particle transport is driven by a filling level difference, its suppression due to the Zeno effect sets in at considerably higher values of the particle loss $\gamma$ as compared to the phase-gradient driven case. To analyze the nature of both transport processes with regard to their different reactions to the tunneling suppression at high dissipation strengths, thus, presents another interesting subject for further works.
Zusammenfassung in deutscher Sprache


Die Reinheit wird als ein wichtiger Faktor für den gemittelten Kontrast in einem

Um eine Abschätzung der Zeitskala zu erhalten, auf der die Reinheitsozillationen stattfinden, werden die dimensionslosen Einheiten der theoretischen Untersuchung über einen einfachen Ansatz für das Fallenpotential und die zugehörigen Wellenfunktionen mit physikalischen Größen in Verbindung gebracht. Dadurch wird die Periodendauer der Oszillationen dem Bereich einiger Millisekunden zugeordnet, was im Experiment praktikabel ist.


Die Dynamik zeigt, dass das Reservoir in der Lage ist den Teilchenverlust in der zentralen Mulde auszugleichen, sodass sich ein quasi-konstantes Besetzungsniveau ausbildet, dessen Wert durch die Verluststärke $\gamma$ bestimmt ist. Innerhalb des Molekularfeld-Ansatzes der diskreten Gross-Pitaevskii-Gleichung ist der Teilchentransport durch einen Phasengradienten getrieben und bis zu einem kritischen Wert $\gamma_c$ weist die zentrale Mulde in ihrem quasi-konstanten Zustand das selbe Besetzungs niveau wie das Reservoir auf. Für größere Werte $\gamma > \gamma_c$ beginnt der Verlust durch einen Zeno-Effekt den kohärenten Teilchentransport in die zentrale Mulde zu unterdrücken, was dazu führt, dass bei hohen Verluststärken insgesamt weniger Teilchen das System verlassen.

Um zu untersuchen, wie sich die Dynamik in Gegenwart von Phasenrauschen verändert, wird die Zeitentwicklung der Ein-Teilchen-Dichtematrix mit der ersten Ordnung der BBGKY-Hierarchie direkt ausgerechnet, was es ermöglicht inkohärente Zustände zu betrachten. Starkes Phasenrauschen sorgt dafür, dass die Tunnelprozesse in der Kette unterdrückt werden, sodass das Reservoir den Verlust nicht mehr ausgleichen kann und
sich kein quasi-konstantes Besetzungsniveau mehr einstellt. In der Gegenwart von relativ schwachem Phasenrauschen ist der Teilchentransport nicht wesentlich behindert und der quasi-konstante Zustand der zentralen Mulde tritt weiterhin auf. Allerdings ist die Natur dieses Transports auch für schwaches Phasenrauschen maßgeblich von der des Transports im System ohne Phasenrauschen verschieden. Eine endliche Stärke des Phasenrauschens zwingt das System eine Differenz zwischen den Besetzungsniveaus der zentralen Mulde \( \langle \hat{n}_c \rangle \) und den ersten Mulden des Reservoirs \( \langle \hat{n}_{\pm 1} \rangle \) aufzubauen. Diese Besetzungszahldifferenz stellt die treibende Kraft für den Teilchentransport in dem teilweise incohärenten System dar.

In der experimentellen Arbeit [20] wurde ein bistabiles Verhalten des Verhältnisses \( \langle \hat{n}_c \rangle / \langle \hat{n}_{\pm 1} \rangle \) derart beobachtet, dass es in einem bestimmten Bereich der Verluststärke den Wert eins annahm, wenn die zentrale Mulde anfänglich gefüllt war und einen geringeren Wert, wenn sie zu Beginn entleert gewesen ist. Auch wenn keine Bistabilität in den mathematischen Modellen dieser Masterarbeit gefunden werden konnte, ist dieses Verhältnis für \( \gamma < \gamma_c \) in der Abwesenheit von Phasenrauschen gleich eins und nimmt einen kleineren Wert an, wenn im System Phasenrauschen einer endlichen Stärke auftritt. Eine interessante Frage für zukünftige Untersuchungen ist deshalb, ob der von einem Elektronenstrahl hervorgerufene Teilchenverlust wie Phasenrauschen als eine Quelle der Incohärenz wirken kann, die einen stärkeren Effekt hat, wenn die zentrale Mulde und das Reservoir unterschiedliche Besetzungsniveaus aufweisen.

Darüber hinaus wird der von dem Besetzungsniveauunterschied getriebene Teilchentransport erst für deutlich höhere Verluststärken \( \gamma > \gamma_c \) merklich vom Zeno-Effekt unterdrückt als in dem von einem Phasengradienten getriebenen Fall. Daher ist eine weitere interessante Fragestellung für zukünftige Arbeiten, zu untersuchen was die Ursache der unterschiedlichen Reaktion der beiden Transportprozesse auf den Teilchenverlust ist.
Bibliography


Danksagung

Erklärung

Ich versichere,

• dass ich diese Masterarbeit selbständig verfasst habe,

• dass ich keine anderen als die angegebenen Quellen benutzt und alle wörtlich oder sinngemäß aus anderen Werken übernommenen Aussagen als solche gekennzeichnet habe,

• dass die eingereichte Arbeit weder vollständig noch in wesentlichen Teilen Gegenstand eines anderen Prüfungsverfahrens gewesen ist,

• und dass das elektronische Exemplar mit den anderen Exemplaren übereinstimmt.

Stuttgart, den 2. Mai 2017

Jonathan Stysch