Neutral impurities immersed
in Bose–Einstein condensates

Martin Ulrich Bruderer
Lincoln College, Oxford

A thesis submitted to the Mathematical and Physical Sciences Division
for the degree of Doctor of Philosophy in the University of Oxford

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Abstract

Ultra-cold atomic gases are formidable systems to investigate fundamental phenomena occurring in many-body quantum physics. In combination with scattering resonances and optical potentials, degenerate quantum gases provide new insight into strongly correlated systems and their characteristic properties. Notably, the admixture of impurity atoms to a Bose–Einstein condensate (BEC) has recently extended the physics of ultra-cold atoms into the area of quantum impurity problems.

In this thesis we investigate the effect of a BEC on the internal and external degrees of freedom of immersed impurity atoms, which may be confined to an additional trapping potential. We develop effective models for the impurities in the sense that the effects caused by the BEC enter as external parameters only. These models exhibit many interesting physical phenomena and provide an opportunity for a systematic and controlled study of the interplay between coherent, incoherent and dissipative processes.
To start, we consider the internal degrees of freedom of a single trapped impurity, namely two internal states $|0\rangle$ and $|1\rangle$, where only state $|1\rangle$ couples to the BEC. A direct relation between the dephasing of the internal states of the impurity and the temporal phase fluctuations of the BEC is established. In reference to this relation we suggest a scheme to probe BEC phase fluctuations via dephasing measurements of the internal states. In particular, the scheme allows us to trace the dependence of the phase fluctuations on the trapping geometry of the BEC.

Subsequently, we study the transport properties of impurities trapped in a tight optical lattice. Within a regime where the impurity–BEC interaction is dominant, we derive an extended Hubbard model describing the dynamics of the impurities in terms of polarons, i.e. impurities dressed by a coherent state of Bogoliubov phonons. The extended Hubbard model naturally incorporates a phonon-mediated impurity–impurity interaction, which can lead to the aggregation of polarons into stable clusters. Moreover, by using a generalized master equation based on this microscopic model we show that inelastic and dissipative phonon scattering results in (i) a crossover from coherent to incoherent transport of impurities with increasing BEC temperature and (ii) the emergence of a net atomic current across a tilted optical lattice. The dependence of the atomic current on the lattice tilt changes from ohmic conductance to negative differential conductance and is accurately described by an Esaki–Tsu-type relation.

We then examine the interaction-induced localization, the so-called self-trapping, of a single impurity atom for attractive and repulsive impurity–BEC interactions. Within the framework of a Hartree description of the BEC we show that — unlike repulsive impurities — attractive impurities have a singular ground state in 3D and shrink to a point-like state in 2D as the coupling approaches a critical value. We find that the density of the BEC increases markedly in the
vicinity of attractive impurities in 1D and 2D, which strongly enhances inelastic collisions between atoms in the BEC.

Finally, we analyze the interaction between the impurities and the BEC in the weak-coupling regime. This approach allows us to calculate the effective mass of self-trapped impurities and the phonon-mediated impurity–impurity interaction for finite impurity hopping. In addition, we discuss the effect of incoherent collisions of impurities with the BEC background and, in particular, the deceleration of supersonic impurities due to the emission of phonons.
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Chapter 1

Introduction

Introduction

The remarkable progress in trapping and cooling atoms during the past years has opened up exciting possibilities of advancing our understanding of ultra-cold many-body quantum systems [1]. Notably, since the experimental realization of Bose–Einstein condensates (BEC) with ultra-cold dilute gases, which per se are not strongly interacting [2], several new developments made it possible to realize strongly correlated systems and explore their characteristic properties. The most direct way to reach the strong coupling regime in dilute gases is to exploit the internal structure of the atoms via Feshbach resonances [3, 4], which allows one to tune the atomic interactions, for example, by applying an external magnetic field. An alternative method of enhancing the interactions between the atoms is to utilize optical potentials [5] either to reduce the effective dimensionality of the system [6–8] or to generate strong periodic potentials through optical lattices [9].

A closely intertwined development, namely the effort towards the deterministic preparation, manipulation and detection of single atoms, has been strongly motivated by the prospect of quantum information processing in ultra-cold systems [10, 11]. As an example, the controlled preparation and in situ imaging of single atoms in a three-dimensional optical lattice has recently been demonstrated [12]. Moreover, the enhanced interaction of atoms with optical modes
inside high-finesse cavities can be exploited to detect and manipulate single atoms [13, 14]. The cavity approach has already been used to investigate the properties of an atom laser [15] and a BEC inside a cavity [16]. Thus, even if the actual implementation of a cold-atom quantum computer is very challenging, the related efforts may open up the possibility to explore the dynamics of ultra-cold impurity atoms immersed in a BEC [16–18]. This evolution is particularly interesting in the light of the recent success in the production of quantum degenerate atomic mixtures [19–21], and the admixture of bosonic and fermionic impurity atoms to a BEC [22–24] has definitely extended the physics of ultra-cold atoms into the area of quantum impurity problems.

In view of these recent developments we focus in this thesis on the effect of a BEC on the internal and external degrees of freedom of neutral impurity atoms. More precisely, we consider atoms of species $A$, possibly trapped by an external potential, which are immersed in a BEC of species $B$. It is assumed that species $A$ and $B$ are subject to a density–density interaction characterized by their scattering properties. Our intention is to develop effective models for the dynamics of the impurities in the sense that the effects caused by the BEC enter as external parameters only. As we shall see, these models exhibit many interesting physical phenomena, as for example self-trapping of impurities, and offer an opportunity for a systematic and controlled study of the interplay between coherent, incoherent and dissipative processes.

As a starting point we study the effect of the BEC on the internal states of a single impurity confined to a trapping potential in chapter 2. Specifically, we analyze the consequences of a nonsymmetric interaction between the internal states of a static impurity and the BEC. As an idealization, we consider two internal states $|0\rangle$ and $|1\rangle$ of the impurity, where only the state $|1\rangle$ interacts with the atoms in the BEC. The choice of this model is partly motivated by the
prospect of using immersed impurity atoms for quantum information processing, where the BEC serves simultaneously as a coolant for the qubits [25] and as the medium for qubit interactions [26]. As a result, we show that the dephasing between the two states is directly related to the phase fluctuations of the BEC. Based on this relation we then propose a scheme to probe the phase fluctuations and the temperature of the BEC via a measurement of the dephasing between the states $|0\rangle$ and $|1\rangle$ in a Ramsey-type experiment. Despite the fact that the nonsymmetric couplings required for the states $|0\rangle$ and $|1\rangle$ seem not to occur naturally, there are promising candidates for the realization of our scheme, such as a $^{40}$K atom immersed in a $^{87}$Rb condensate. The various Feshbach resonances between the $^{87}$Rb atoms and the $^{40}$K impurity in different hyperfine states would lead to highly nonsymmetric couplings for carefully adjusted magnetic fields [27].

In the main part of this thesis, namely in chapters 3 and 4, we investigate the effect of a BEC on the external degrees of freedom of impurities and, in particular, on their transport properties. At the root of this problem is the following question: How does a bosonic quantum field coupled to impurity particles affect their motion? The answer to this question was shown to be essential for the understanding of the electron–phonon interaction in solids [28] and the motion of impurities in superfluid helium [29].

Of course, the physics of BECs and superfluid helium is closely related [30], and therefore one might expect that phenomena, which occur in a helium system, such as an increased effective impurity mass [31], phonon mediated impurity interactions [32] and self-trapping [33], should also be observable in a BEC. However, it turns out that they are hardly detectable for moderate impurity–BEC interactions given that the gas parameter* has very different values for the two

*The gas parameter is given by $(na_s^2)^{1/2}$, where $n$ is a typical value of the particle density and $a_s$ is the s-wave scattering length between the particles.
Introduction

systems [34]. We show how this difficulty can be overcome by confining the impurities to an optical lattice potential. We shall see that the introduction of an optical lattice into the system significantly enhances the influence of the BEC on the dynamics of the impurity.

The model that we develop describes the immersed impurities in terms of polarons, i.e. particles dressed by a correlated cloud of phonons [28]. The concept of polarons has been successfully applied in solid state physics [35] and, for example, motivated the search for high-temperature superconductors [36]. In the context of ultra-cold atomic physics, it was shown recently that the rich phase diagram of Bose–Fermi mixtures can be understood in terms of polarons [37–39]. We show in the course of this thesis that the impurities in the optical lattice are accurately described by an extended Bose–Hubbard model for polarons, where the phonons correspond to the low energy excitations of the BEC [40]. It is based on this model that we investigate the transport properties of the impurities.

In chapter 3 we discuss the competition between coherent and incoherent effects of the BEC on the impurities in the optical lattice, which result in an observable crossover from coherent to diffusive hopping with increasing temperature of the BEC. It is shown that at zero temperature the impurities evolve coherently with a reduced hopping rate due to the ‘drag’ of the phonon cloud, which might be detected in a similar way as the reduced tunnelling in a modulated lattice [41, 42]. At finite temperatures, however, the BEC changes its state during a hopping event, which results in a diffusive motion of the impurities. This effect is reminiscent of the observed transition from normal to anomalous diffusion of atoms in a one-dimensional optical lattice [43–46], where, however, the diffusive motion of the atoms is caused by photon (not phonon) emission.

Further, we indicate that for sufficiently low temperatures of the BEC the polarons tend to aggregate in small clusters due to the phonon mediated impurity–
impurity interaction appearing in the extended Bose–Hubbard model. In practice, these clusters consist of two or three impurities located on adjacent lattice sites and build compound particles comparable to the repulsively bound atom pairs in optical lattices that were observed recently [47].

In chapter 4 we extend our result to the case of a tilted optical lattice. The transport of atoms in tilted optical lattices has constantly attracted interest and fundamental quantum mechanical processes in periodic potentials such as Bloch oscillations [48, 49], Landau–Zener tunnelling [50] and photon assisted tunnelling [42, 51, 52] have been demonstrated. Our main motivation is the observation of incoherent transport of impurities in tilted periodic potentials caused by collisions with a non-degenerate bosonic bath [53]. We demonstrate that the incoherent phonon collisions provide the necessary dissipative process required for the emergence of a net current of impurity atoms across the lattice. Interestingly, the dependence of the net current on the lattice tilt follows an Esaki–Tsu-type relation [54–56], i.e. the system goes through a transition from an ohmic conductor to an insulator for increasing lattice tilt. A clear signature of this transition has so far only been observed in semiconductor superlattices [57, 58].

Chapter 5 is devoted to the self-trapping problem. It is well known that a single atom can get trapped in the local distortion of the BEC that is induced by the impurity–BEC interaction if the resulting potential well is deep enough to compensate for the kinetic energy cost [29]. This self-trapping effect — unlike in a BEC [59, 60] — arises naturally in liquid helium [29, 33]. We show that the nonlinearity of the Gross–Pitaevskii equation [61] becomes essential for strong attractive and repulsive impurity–BEC coupling. In particular, an attractive coupling can lead to a highly localized ground state of the impurity and a strong increase of the BEC density in the vicinity of the impurity. These experimentally relevant effects, which might result in a loss of the BEC atoms [62] or the impurity,
are not captured by the usual perturbation approach [59, 60].

In chapter 6 we analyze the interaction between the impurities and the BEC in the weak-coupling regime by considering a variant of the well-known Fröhlich polaron model [35, 63, 64]. We determine the effective mass of a loosely localized, self-trapped impurity whose ground state has been found in chapter 5. Furthermore, we calculate the corrections due to finite impurity hopping to the phonon-mediated impurity–impurity interaction, which was obtained in chapter 4, but only for static impurities. Finally, we briefly discuss the effect of incoherent collisions of impurities with the BEC background [65] and investigate the deceleration of supersonic impurities caused by the emission of phonons [66]. We conclude the thesis with a discussion of open problems and potential future directions for research related to impurities immersed in degenerate quantum gases.
Chapter 2

Probing BEC phase fluctuations with atomic quantum dots

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We consider the dephasing of two internal states \( |0\rangle \) and \( |1\rangle \) of a trapped impurity atom, a so-called atomic quantum dot (AQD), where only state \( |1\rangle \) couples to a Bose–Einstein condensate (BEC). A direct relation between the dephasing of the internal states of the AQD and the temporal phase fluctuations of the BEC is established. Based on this relation we suggest a scheme to probe BEC phase fluctuations nondestructively via dephasing measurements of the AQD. In particular, the scheme allows us to trace the dependence of the phase fluctuations on the trapping geometry of the BEC.

2.1 Introduction

The coherence properties of Bose–Einstein condensates (BECs) have attracted considerable theoretical and experimental interest since the first experimental realisation of BECs in trapped ultracold clouds of alkali atoms [67, 68]. Part of this interest is due to the importance of coherence effects for the conceptual understanding of BECs and their use as a source of coherent matter waves. In par-
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ticular, the absence of spatial coherence in low dimensional BECs, which exhibit strong spatial and temporal phase fluctuations, has been investigated theoretically [69–71] and demonstrated for one dimensional condensates [72, 73]. Moreover, temporal first and second order phase coherence of an atom laser beam extracted from a BEC has been observed [15, 74]. However, to our knowledge, temporal phase fluctuations in a BEC have not yet been measured directly, despite the fact that they ultimately limit the coherence time of an atom laser beam.

In this paper, we propose a scheme to measure temporal phase fluctuations of the BEC based on a single trapped impurity atom coupled to the BEC, hereafter called an atomic quantum dot (AQD) [75]. More specifically, we consider an AQD with two internal states $|0\rangle$ and $|1\rangle$, where we assume for simplicity that only state $|1\rangle$ undergoes collisional (s-wave scattering) interactions with the BEC. This setup could be implemented using spin-dependent optical potentials [76], where the impurity atom, trapped separately [77–79], and the BEC atoms correspond to different internal atomic states. The collisional properties of the AQD can, to a good approximation, be engineered by means of optical Feshbach resonances [80], which allow us to change the atomic scattering length locally over a wide range and are available even when no magnetic Feshbach resonance exists.

By identifying the combined system of the AQD and the BEC with an exactly solvable independent boson model [28, 81, 82], we show that the dephasing of the internal states due to the asymmetric interaction with the BEC is directly related to the temporal phase fluctuations. This dephasing can be detected under reasonable experimental conditions, for example, in a Ramsey type experiment [83], and hence it is possible to use the AQD to probe BEC phase fluctuations. Since the phase fluctuations depend strongly on the temperature and the density of states of the BEC, determined by the trapping geometry, the proposed scheme allows us to measure the BEC temperature and to observe the crossover
between different effective BEC dimensions, notably transitions from 3D to lower
dimensions. Our scheme is nondestructive and hence it is possible, in principle,
to investigate the dependence of phase fluctuations on the BEC dimension and
temperature for a single copy of a BEC.

Probing a BEC with an AQD was proposed recently in [75] and in a different
context in [84]. However, in [75] two states corresponding to the presence of a
single atom in the trap or its absence were considered, as opposed to internal atom
states. More importantly, in addition to the collisional interactions the impurity
atom was coupled to the BEC via a Raman transition, allowing the realisation
of an independent boson model with tunable coupling. In particular, Recati et al
[75] proposed to measure the Luttinger liquid parameter $K$ by observing the
dynamics of the independent boson model for different coupling strengths.

Other schemes based on interactions between impurity atoms and BECs have
been proposed recently. In [85], for example, an impurity was used to imple-
ment a single atom transistor, whereas in [26] a quantum gate exploiting phonon-
mediated interactions between two impurities was investigated. Single atom cool-
ing in a BEC was considered in [25] where some aspects of dephasing of a two
state system (qubit) due to BEC fluctuations were addressed. Whereas their
treatment focused on a three-dimensional BEC and was based on a master equa-
tion approach, in our work we use an analytical approach similar to dephasing
calculations for semiconductor quantum dots [86, 87].

The paper is organized as follows. In section 2 we introduce our model for the
AQD coupled to the BEC and identify it with an exactly solvable independent
boson model, which enables us to establish a relation between the temporal phase
fluctuations of the BEC and the dephasing of the AQD. We first consider an
effective $D$-dimensional BEC, which is strongly confined in $(3 - D)$ directions
and, as an ideal case, assumed to be homogeneous along the loosely confined
directions. Later we discuss corrections to this zero potential approximation due to a shallow trap potential. In section 3 we show by means of a concrete example how dephasing depends on the interaction time $\tau$ between the AQD and the BEC, the condensate temperature $T$ and the effective condensate dimension $D$. Section 4 addresses corrections to our results due to an imperfect measurement of the AQD state. We conclude in section 5.

2.2 Model

We consider the system of an AQD coupled to a BEC in thermal equilibrium with temperature $T$. The BEC is confined in a harmonic trapping potential

$$V_{\text{trap}}(\mathbf{r}) = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right),$$

(2.1)

with $\mathbf{r} = (x, y, z)$ the position vector and $m$ the mass of the condensate atoms. The trap frequencies $\omega_x$, $\omega_y$ and $\omega_z$ assume the value(s) $\omega_\perp$ or $\omega$, where $\omega_\perp \gg \omega$ is the trap frequency in the strongly confined (transverse) direction(s) and $\omega$ the trap frequency in the loosely confined direction(s). Depending on the number of strongly confined directions — none, one or two — the BEC is either 3D or assumes effective 2D or 1D character, provided that thermal excitations are suppressed, i.e. $k_B T \ll \hbar \omega_\perp$, and that the interaction energy of the weakly interacting BEC does not exceed the transverse energy, i.e. $mc^2 \ll \hbar \omega_\perp$, with $k_B$ Boltzmann’s constant and $c$ the speed of sound. In directions that are loosely confined the extension of the trap potential is assumed to be much larger than the length scale $\sigma$ set by the AQD size, so that it is justified to approximate the potential by zero, as discussed at the end of this section. We consider the case where the spectrum of the BEC excitations, as compared to the impurity spectrum, is practically continuous.
2.2. Model

The AQD consists of an impurity atom in the ground state of a harmonic trap potential centered at $r_0$ and is described by the wave function $\psi_\sigma(r - r_0)$. We assume that $\psi_\sigma(r - r_0)$ takes the form of the BEC density profile in the strongly confined direction(s) and has ground state size $\sigma$ in the loosely confined direction(s). For example in case of a 1D condensate

$$\psi_\sigma(r - r_0) \propto \frac{1}{\sqrt{a_\perp^2 \sigma}} \exp \left[ -\left( \frac{x - x_0}{\sqrt{2} a_\perp} \right)^2 - \left( \frac{y - y_0}{\sqrt{2} a_\perp} \right)^2 - \left( \frac{z - z_0}{\sqrt{2} \sigma} \right)^2 \right], \quad (2.2)$$

with the harmonic oscillator length $a_\perp \ll \sigma$. We further assume that the impurity atom has two internal states $|0\rangle$ and $|1\rangle$, and undergoes s-wave scattering interactions with the BEC atoms only in state $|1\rangle$.

2.2.1 Dephasing in the zero potential approximation

The total Hamiltonian of the system can be written as

$$H_{\text{tot}} = H_A + H_B + H_I, \quad (2.3)$$

where $H_A = \hbar \Omega |1\rangle \langle 1|$, with level splitting $\hbar \Omega$, is the Hamiltonian for the AQD, $H_B$ is the Hamiltonian for the BEC, and $H_I$ describes the interaction between the AQD and the BEC. Provided that $\sigma/l \gg 1$, with $l$ the average interparticle distance in the BEC, we can represent the $D$-dimensional (quasi)condensate in terms of the phase operator $\hat{\phi}(\mathbf{x})$ and number density operator $\hat{n}_{\text{tot}}(\mathbf{x}) = n_0 + \hat{n}(\mathbf{x})$. Here, $n_0 = l^{-D}$ is the equilibrium density of the BEC, $\hat{n}(\mathbf{x})$ is the density fluctuation operator and $\mathbf{x}$ a $D$-dimensional vector describing the position in the loosely confined direction(s). We describe the dynamics of the BEC by a low-
energy effective Hamiltonian [30, 88]

\[ H_B = \frac{1}{2} \int d^D x \left( \frac{\hbar^2}{m} n_0 (\nabla \hat{\phi})^2(x) + g \hat{n}^2(x) \right), \tag{2.4} \]

where the interaction coupling constant is defined by \( g \equiv mc^2/n_0^* \). We shall see that the use of this model is fully justified, even though it exhibits only Bogoliubov excitations with a linear dispersion relation \( \omega_k = ck \), henceforth called phonons.

The canonically conjugate field operators \( \hat{\phi}(x) \) and \( \hat{n}(x) \) can be expanded as plane waves

\[
\hat{\phi}(x) = \frac{1}{\sqrt{2L^D}} \sum_k A_k^{-1} (\hat{b}_k \exp[i k \cdot x] + \text{h.c.}), \tag{2.5}
\]

\[
\hat{n}(x) = i \frac{1}{\sqrt{2L^D}} \sum_k A_k (\hat{b}_k \exp[i k \cdot x] - \text{h.c.}), \tag{2.6}
\]

where \( \hat{b}_k^\dagger \) and \( \hat{b}_k \) are bosonic phonon creation and annihilation operators and \( L^D \) is the sample size. With the amplitudes \( A_k = \sqrt{\hbar \omega_k/g} \) the Hamiltonian (2.4) takes the familiar form

\[ H_B = \sum_k \hbar \omega_k (\hat{b}_k^\dagger \hat{b}_k + \frac{1}{2}). \tag{2.7} \]

The coupling between AQD and the BEC occurs in the form of a density–density interaction

\[ H_I = \kappa |1 \rangle \langle 1 | \int d^D x |\tilde{\psi}_\sigma(x - x_0)|^2 \hat{n}_{tot}(x), \tag{2.8} \]

where \( \tilde{\psi}_\sigma(x - x_0) \) is the AQD wave function integrated over the transverse direction(s), and \( \kappa \) the coupling constant, which can be positive or negative. To avoid notable deviations of the BEC density from \( n_0 \) in the vicinity of the AQD we require \( |\kappa| \sim g \) [90, 91]. The interaction Hamiltonian \( H_I \) acts on the relative phase of the two internal states, but does not change their population. This effect

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*We neglect the weak dependence of \( c \) on the dimensionality of the BEC [89] for simplicity.
is customarily called pure dephasing.

The total Hamiltonian can be identified with an independent boson model, which is known to have an exact analytic solution [28, 81, 82]. Inserting the explicit expression (2.6) for \( \hat{n}(x) \) into equation (2.8) we can rewrite the total Hamiltonian as

\[
H_{\text{tot}} = (\kappa n_0 + \hbar \Omega) |1\rangle\langle 1| + \sum_k \left( g_k \hat{b}_k^\dagger + g_k^* \hat{b}_k \right) |1\rangle\langle 1| + \sum_k \hbar \omega_k (\hat{b}_k^\dagger \hat{b}_k + \frac{1}{2}),
\]

(2.9)

where \( \kappa n_0 \) is the mean field shift. The coupling coefficients \( g_k \), which contain the specific characteristics of the system, are given by

\[
g_k = - \frac{i\kappa}{\sqrt{2L^D}} A_k f_k,
\]

(2.10)

with the Fourier transform of the AQD density

\[
f_k = \int d^D x \left| \psi_\sigma(x - x_0) \right|^2 \exp \left[ -i k \cdot x \right].
\]

(2.11)

As can be seen from expression (2.9) the effect of the AQD in state \( |1\rangle \) is to give rise to a displaced harmonic oscillator Hamiltonian for each phonon mode. This problem is identical with the problem of a charged harmonic oscillator in a uniform electric field and can be solved by shifting each phonon mode to its new equilibrium position [28]. As a consequence the AQD does not change the phonon frequencies and hence the phase fluctuations are the same in the presence of the AQD as in its absence.

The state of the system is described by the density matrix \( \rho_{\text{tot}}(t) \). We assume that the AQD is in state \( |0\rangle \) for \( t < 0 \) and in a superposition of \( |0\rangle \) and \( |1\rangle \) at \( t = 0 \), which can be achieved, for example, by applying a short laser pulse. Hence
the density matrix \( \rho_{\text{tot}}(t) \) at time \( t = 0 \) is of the form

\[
\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_B, \quad \rho_B = \frac{1}{Z_B} \exp\left[-H_B/(k_B T)\right],
\]

where \( \rho(0) \) is the density matrix for the AQD and \( \rho_B \) the density matrix of the BEC in thermal equilibrium, with \( Z_B \) the BEC partition function. After a change to the interaction picture the time evolution operator of the total system takes the form [82]

\[
U(t) = \exp \left[ |1\rangle \langle 1| \sum_k \left( \beta_k \hat{b}_k^\dagger - \beta_k^* \hat{b}_k \right) \right],
\]

with \( \beta_k = g_k (1 - \exp[i \omega_k t])/(\hbar \omega_k) \). The reduced density matrix of the AQD can be determined from the relation \( \rho(t) = \text{Tr}_B \{ U(t) \rho_{\text{tot}}(0) U^{-1}(t) \} \), where \( \text{Tr}_B \) is the trace over the BEC. The coherence properties of the AQD are governed by the off-diagonal matrix elements

\[
\rho_{10}(t) = \rho_{01}(t) = \rho_{10}(0) e^{-\gamma(t)},
\]

with the dephasing function

\[
\gamma(t) = -\ln \left\langle \exp \left[ \sum_k \left( \beta_k \hat{b}_k^\dagger - \beta_k^* \hat{b}_k \right) \right] \right\rangle,
\]

where angular brackets denote the expectation value with respect to the thermal distribution \( \rho_B \).

The dephasing function \( \gamma(t) \) can be expressed in terms of the phase operator in the interaction picture \( \hat{\phi}(x) t = \exp[i H_B t/\hbar] \hat{\phi}(x) \exp[-i H_B t/\hbar] \). We introduce
the coarse-grained phase operator averaged over the AQD size $\sigma$

$$\hat{\phi}(x, t) \equiv \int d^D x |\bar{\psi}_\sigma(x - x_0)|^2 \hat{\phi}(x, t)$$ (2.16)

and the phase difference $\delta \hat{\phi}_\sigma(x_0, t) \equiv \hat{\phi}_\sigma(x_0, t) - \hat{\phi}_\sigma(x_0, 0)$ to rewrite the phase coherence as

$$e^{-\gamma(t)} = \exp \left[ \frac{\kappa}{g} \delta \hat{\phi}_\sigma(x_0, t) \right]$$ (2.17)

$$= \exp \left[ -\frac{1}{2} \left( \frac{\kappa}{g} \right)^2 \langle (\delta \hat{\phi}_\sigma)^2(x_0, t) \rangle \right], \quad (2.18)$$

where the second equality can be proven by direct expansion of the exponentials [28]. Thus we have established a direct relation between the dephasing of the AQD and the temporal phase fluctuations of the BEC averaged over the AQD size $\sigma$. Moreover, the phase coherence (2.18) is closely related to the correlation function $\langle \Psi^\dagger(x, t) \Psi(x', t') \rangle$, with $\Psi(x, t)$ the bosonic field operator describing the BEC in the Heisenberg representation. In the long-wave approximation, where the density fluctuations are highly suppressed, we have [30, 88]

$$\langle \Psi^\dagger(x_0, t) \Psi(x_0, 0) \rangle \approx n_0 \exp \left[ -\frac{1}{2} \langle (\delta \hat{\phi})^2(x_0, t) \rangle \right]. \quad (2.19)$$

Therefore expression (2.18) can be interpreted as a smoothed out temporal correlation function of the BEC field operator $\Psi(x, t)$ provided that $\kappa = g$.

To further investigate the effect of the BEC phase fluctuations on the AQD we require an explicit expression for the dephasing function $\gamma(t)$ depending on the parameters of our system. For this purpose we express the dephasing function
\( \gamma(t) \) in terms of the coupling coefficients \( g_k \) \[82\]

\[
\gamma(t) = \sum_k |g_k|^2 \coth \left( \frac{\hbar \omega_k}{2k_B T} \right) \frac{1 - \cos(\omega_k t)}{(\hbar \omega_k)^2} \quad (2.20)
\]

and take the thermodynamic limit of \( \gamma(t) \), which amounts to the replacement \( \sum_k \to \int_0^\infty dk \, g(k) \), with the density of states \( g(k) = S_D L^D k^{D-1} \), \( S_D \equiv D/[2^D \pi^{D/2} \Gamma(D/2 + 1)] \) and \( \Gamma(x) \) the gamma function. Substituting expression (2.10) for \( g_k \) we find

\[
\gamma(t) = \frac{S_D k^2}{2g} \int_0^\infty dk \, k^{D-1} |f_k|^2 \coth \left( \frac{\hbar \omega_k}{2k_B T} \right) \frac{1 - \cos(\omega_k t)}{\hbar \omega_k} . \quad (2.21)
\]

The integral is well defined due to the factor \( |f_k|^2 = \exp\left[-\sigma^2 k^2/2\right] \), which provides a natural upper cut-off. Since for typical experimental parameters \( \xi/l \sim 1 \), with \( \xi \sim \hbar/(mc) \) the healing length, the condition \( \sigma/l \gg 1 \) implies that \( \sigma \gg \xi \). Thus the upper cut-off at \( k \sim 1/\sigma \) is still in the phonon regime, which justifies the use of the effective Hamiltonian (2.4).

### 2.2.2 Corrections due to a shallow potential

We now give the conditions under which the effects of a shallow trap on result (2.21) are negligible in the thermodynamic limit. This limit is taken such that \( \omega \propto 1/R \), with \( R \) the radius of the BEC, to ensure that the BEC density at the center of the trap remains finite. To determine the trap-induced corrections to the density of states and the phonon wave functions, which affect \( f_k \) defined by (2.11), we use a semi-classical approach based on the classical Hamiltonian \[92\]

\[
H(p, x) = c(x)|p| + V(x) , \quad (2.22)
\]
with \( c(x) = c(1-x^2/R^2)^{1/2} \) the position dependent speed of sound, \( p \) the phonon momentum and \( V(x) = m\omega^2x^2/2 \) the shallow trap potential. The range of phonon energies \( \varepsilon \) relevant for the AQD dephasing is \( \hbar\omega/2 < \varepsilon < \hbar c/\sigma \), where the lower bound goes to zero in the thermodynamic limit.

Given the semi-classical phonon wave functions, we find that corrections to \( f_k \) are negligible if \( \sigma \ll L_\varepsilon \), with \( L_\varepsilon = \sqrt{2\varepsilon/(m\omega^2)} \) the classical harmonic oscillator amplitude. For the density of states \( g(\varepsilon) \) we use the semi-classical expression

\[
g(\varepsilon) = \frac{1}{(2\pi\hbar)^D} \int d^Dx \int d^Dp \, \delta\left(\varepsilon - H(p, x)\right) \tag{2.23}
\]

to obtain \( g(\varepsilon) \propto L_\varepsilon^D \varepsilon^{D-1} \left[1 + \mathcal{O}(L_\varepsilon/R)\right] \). Thus in the regime where \( \sigma \ll L_\varepsilon \ll R \) and after the substitutions \( L \rightarrow L_\varepsilon \) and \( \hbar \omega_k \rightarrow \varepsilon \) we have

\[
\gamma(t) \propto \frac{\kappa^2}{g} \int_0^\infty d\varepsilon \, \varepsilon^{D-1} |f_\varepsilon|^2 \coth\left(\frac{\varepsilon}{2k_BT}\right) \frac{1 - \cos(\varepsilon t/\hbar)}{\varepsilon}, \tag{2.24}
\]

which up to numerical constants is identical to expression (2.21). The conditions on \( L_\varepsilon \), together with the bounds of the phonon spectrum, imply that the dephasing in a shallow trap does not differ from the homogeneous case if \( \xi \ll \sigma \ll a_\omega \), with \( a_\omega = \sqrt{\hbar/(m\omega)} \) the harmonic oscillator length.

### 2.3 Application

In this section we discuss by means of a concrete example\(^\dagger\) how the AQD dephasing depends on the interaction time \( \tau \), the condensate temperature \( T \) and the effective condensate dimension \( D \). To find the phase coherence \( e^{-\gamma(\tau)} \) we have evaluated the integral (2.21) numerically (shown in figures 1, 2 and 3) and

---

\(^\dagger\)For the numerical values of the system parameters see the caption of figure (2.1).
\(^\dagger\)A discussion of a similar model in the context of quantum information processing can be found in [82].
Figure 2.1. The phase coherence $e^{-\gamma(\tau)}$ as a function of the interaction time $\tau$. In the regime $\tau \gg \sigma/c$ the phase coherence approaches a non-zero value in 3D (solid), falls off as a power law in 2D (dashed) and shows exponential decay in 1D (dotted). The system parameters were set to $m = 10^{-25}$kg, $l = 5 \times 10^{-7}$m, $c = 10^{-3}$ms$^{-1}$, $T = 2 \times 10^{-7}$K, $\sigma = 10^{-6}$m and $\kappa = g$.

analytically in the high temperature regime $k_B T \gg \hbar c/\sigma$.

Figure (2.1) shows the phase coherence $e^{-\gamma(\tau)}$ as function of the interaction time $\tau$. The evolution of the phase coherence is split into two regimes separated by the typical dephasing time $\sigma/c \sim 10^{-3}$s, which can be viewed as the time it takes a phonon to pass through the AQD. It follows from the analytic calculations that the asymptotic behaviour of $e^{-\gamma(\tau)}$ for times $\tau \gg \sigma/c$ is

$$e^{-\gamma(\tau)} = C_T \exp \left[ -\left(\frac{\kappa}{g}\right)^2 \frac{mc k_B T}{2\hbar^2 n_0} \tau \right] \quad \text{for} \quad D = 1$$

$$e^{-\gamma(\tau)} = C_T' \left(\frac{\sigma c T}{\sigma c T}\right)^\nu \quad \text{for} \quad D = 2 \quad (2.25)$$

$$e^{-\gamma(\tau)} = \exp \left[ -\left(\frac{\kappa}{g}\right)^2 \frac{m k_B T}{(2\pi)^{3/2}\hbar^2 n_0 \sigma} \right] \quad \text{for} \quad D = 3$$

where $\nu = (\kappa/g)^2 m k_B T/(2\pi\hbar^2 n_0)$ and $C_T, C'_T$ are temperature dependent con-
2.3. Application

constants. Thus the phase coherence tends asymptotically to a non-zero value in 3D, falls off as a power law in 2D and shows exponential decay in 1D. This result reflects the fact that the physics of 1D and 2D condensates differs significantly from that of a 3D condensate. Given the relation between the phase coherence and the BEC correlations, discussed in section 2.1, we note that the results for the phase coherence are consistent with findings for temporal and spatial coherence properties of the BEC [30, 88], where in the latter case the distance $|\mathbf{x}|$ has to be identified with $c\tau$.

In particular in 3D the dephasing of the AQD is incomplete under reasonable experimental conditions due to the suppressed influence of low frequency fluctuations, which has been noted in the context of quantum information processing [25, 82]. However, the residual coherence of the AQD will eventually disappear due to processes as, for example, inelastic phonon scattering [25], which are not taken into account in our model. We also point out that, in contrast to the remnant coherence of the AQD, the typical dephasing time does not depend on the coupling constant $\kappa$.

The fact that phase fluctuations depend strongly on the density of states, or equivalently the dimension of the BEC, allows us to observe the crossover between different effective dimensions, especially transitions from 3D to lower dimensions. Figure (2.2) shows the phase coherence $e^{-\gamma(\tau)}$ as a function of the dimension $D$ for the interaction times $\tau_1 = \sigma/c$, $\tau_2 = 2\sigma/c$ and $\tau_3 = 10\sigma/c$. The phase coherence $e^{-\gamma(\tau)}$ drops significantly as the BEC excitations in the strongly confined direction(s) are frozen out. Therefore we expect that the change of phase fluctuations depending on the effective dimension should be experimentally observable.

In addition, the AQD can be used to measure the BEC temperature since the dephasing function $\gamma(\tau)$ is approximately proportional to the temperature
The phase coherence $e^{-\gamma(\tau)}$ as a function of the effective condensate dimension $D$ for the interaction times $\tau_1 = \sigma/c$ (dotted), $\tau_2 = 2\sigma/c$ (dashed) and $\tau_3 = 10\sigma/c$ (solid). The phase coherence drops significantly while the BEC excitations in the strongly confined directions are frozen out. The plot was produced with the same set of parameters as in figure (2.1).

Figure 2.2. The phase coherence $e^{-\gamma(\tau)}$ as a function of the effective condensate dimension $D$ for the interaction times $\tau_1 = \sigma/c$ (dotted), $\tau_2 = 2\sigma/c$ (dashed) and $\tau_3 = 10\sigma/c$ (solid). The phase coherence drops significantly while the BEC excitations in the strongly confined directions are frozen out. The plot was produced with the same set of parameters as in figure (2.1).

$T$ according to equation (2.25). Figure (2.3) shows the relation between the phase coherence $e^{-\gamma(\tau)}$ and the BEC temperature $T$ in all three dimensions for the interaction times $\tau_1 = \sigma/c$, $\tau_2 = 2\sigma/c$ and $\tau_3 = 10\sigma/c$. In 1D and 2D the interaction time $\tau$ can be chosen to assure that the AQD dephasing changes significantly with temperature, whereas in 3D the interaction time $\tau$ has little influence on the thermal sensitivity of the AQD.

In the high temperature regime $k_B T \gg \hbar c/\sigma$ the phase coherence is reduced mainly due to thermal phonons. However, even at zero temperature coherence is lost due to purely quantum fluctuations. This loss of coherence takes place on the same time scale as in the high temperature regime, but is incomplete in both 3D and 2D, which can be seen by evaluating the integral (2.21) in the limit $t \gg \sigma/c$ with $T = 0$. 
Figure 2.3. The phase coherence $e^{-\gamma(\tau)}$ as a function of temperature $T$ for interaction times $\tau_1 = \sigma/c$ (dotted), $\tau_2 = 2\sigma/c$ (dashed) and $\tau_3 = 10\sigma/c$ (solid). In 1D and 2D the interaction time $\tau$ can be chosen to assure that dephasing changes significantly with temperature, whereas in 3D dephasing is independent of $\tau$ for $\tau \gg \sigma/c$. The plot was produced with the same set of parameters as in figure (2.1), except for the temperature.
2.4 Measurement of the internal states

The AQD dephasing can be detected in a Ramsey type experiment [83]: The AQD is prepared in state $|0\rangle$ and hence initially decoupled from the BEC. A first $\pi/2$-pulse at $t = 0$ changes the state to a superposition $(|0\rangle + |1\rangle)/\sqrt{2}$ and a spin-echo-type $\pi$-pulse at $t = \tau/2$ neutralizes the mean field shift. After a second $\pi/2$-pulse at $t = \tau$ the AQD is found in state $|1\rangle$ with probability

$$P(|1\rangle) = \frac{1}{2}(1 - e^{-\gamma(\tau)}).$$ (2.26)

However, this result is altered by decay of state $|1\rangle$ into state $|0\rangle$, atom loss, imperfect (noisy) detection of state $|1\rangle$, and additional dephasing due to environmental noise. We subsume these processes into three phenomenological constants, namely the detection probability $P_d$, the probability of a spurious detection $P_s$, and the dephasing rate $\gamma_d$, which can all be determined experimentally. Taking these effects into account we find an effective probability $\tilde{P}$ to detect state $|1\rangle$

$$\tilde{P}(|1\rangle) = \frac{1}{2}P_d (1 - e^{-\gamma(\tau) - \gamma_d \tau}) + P_s$$ (2.27)

and the visibility $V \equiv (\tilde{P}_{\text{max}} - \tilde{P}_{\text{min}})/(\tilde{P}_{\text{max}} + \tilde{P}_{\text{min}})$ in the limit $\gamma_d \tau \ll 1$ is given by

$$V = \frac{1 - \gamma_d \tau}{1 + \gamma_d \tau + 4 \frac{P_s}{P_d}},$$ (2.28)

where $\tilde{P}_{\text{max}}$ and $\tilde{P}_{\text{min}}$ correspond respectively to $\tilde{P}(|1\rangle)$ in the case of complete dephasing and no dephasing due to phase fluctuations. Kuhr et al [93] recently demonstrated state-selective preparation and detection of the atomic hyperfine state for single cesium atoms stored in a red-detuned dipole trap. They showed that dephasing times of 146ms and ratios $P_s/P_d$ of the order of $5 \times 10^{-2}$ are...
achievable. If we choose $\gamma_d = 10s^{-1}$, $\tau = 10\text{ms}$ and $P_s/P_d = 5 \times 10^{-2}$ we find a visibility of $V = 69\%$, which shows that our scheme is feasible even in the presence of additional dephasing due to environmental noise.

2.5 Conclusion

We have shown that the dephasing of the internal states of an AQD coupled to a BEC is directly related to the temporal phase fluctuations of the BEC. Based on this relation we have suggested a scheme to probe BEC phase fluctuations nondestructively via measurements of the AQD coherences, for example, in a Ramsey type experiment. It was shown that the scheme works for a BEC with reasonable experimental parameters even in the presence of additional dephasing due to environmental noise. In particular, the scheme allows us to trace the dependence of the phase fluctuations on the trapping geometry of the BEC and to measure the BEC temperature.

Our scheme is applicable even if the BEC is trapped in not strongly confined directions provided that the trapping potential is sufficiently shallow. We expect that the observed dephasing will be qualitatively different from our results only if the AQD size $\sigma$ is comparable to the classical harmonic oscillator amplitude $L_x \sim 1/\omega$. In addition, our findings indicate that the use of AQDs for quantum information processing, proposed recently in [25, 26], may be constrained because of the unfavorable coherence properties of low dimensional BECs.

The results in [82] suggest a natural extension of our work to entangled states between several AQDs, which might lead to a probe with higher sensitivity. However, the experimental requirements for the state-selective preparation and detection of entangled states are considerably higher than for a single AQD, which has to be considered in the analysis of an extended scheme.
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We investigate the effects of a nearly uniform Bose–Einstein condensate (BEC) on the properties of immersed trapped impurity atoms. Using a weak-coupling expansion in the BEC–impurity interaction strength, we derive a model describing polarons, i.e., impurities dressed by a coherent state of Bogoliubov phonons, and apply it to ultracold bosonic atoms in an optical lattice. We show that, with increasing BEC temperature, the transport properties of the impurities change from coherent to diffusive. Furthermore, stable polaron clusters are formed via a phonon-mediated off-site attraction.

3.1 Introduction

The lack of lattice phonons is a distinguishing feature of optical lattices, i.e., conservative optical potentials formed by counterpropagating laser beams, and contributes to the excellent coherence properties of atoms trapped in them [5]. However, some of the most interesting phenomena in condensed matter physics involve phonons, and thus it is also desirable to introduce them in a controlled way into optical lattices. Recently, it has been shown that immersing an optical lattice
into a Bose–Einstein condensate (BEC) leads to interband phonons, which can be used to load and cool atoms to extremely low temperatures [94]. Here, we instead concentrate on the dynamics within the lowest Bloch band of an immersed lattice, and show how intraband phonons lead to the formation of polarons [28, 95]. This has a profound effect on lattice transport properties, inducing a crossover from coherent to incoherent hopping as the BEC temperature increases. Furthermore, polarons aggregate on adjacent lattice sites into stable clusters, which are not prone to loss from inelastic collisions. Since these phenomena are relevant to the physics of conduction in solids, introducing phonons into an optical lattice system may lead to a better understanding of high-temperature superconductivity [95, 96] and charge transport in organic molecules [97]. Additionally, this setup may allow the investigation of the dynamics of classically indistinguishable particles [98].

Experimental progress in trapping and cooling atoms has recently made a large class of interacting many-body quantum systems [99] accessible. For instance, the formation of repulsively bound atom pairs on a single site has been demonstrated [47], and strongly correlated mixtures of degenerate quantum gases have been realized [22, 23]. In such Bose–Fermi mixtures, rich phase diagrams can be expected, including charge and spin density wave phases [38, 100], pairing of fermions with bosons [37], and a supersolid phase [101]. Here we instead consider one atomic species, denoted as the impurities, confined to a trapping potential, for example an optical lattice, immersed in a nearly uniform BEC, as shown in Fig. 3.1. Based on a weak-coupling expansion in the BEC–impurity interaction strength, we derive a model in terms of polarons, which are composed of impurity atoms dressed by a coherent state of Bogoliubov phonons [28, 95]. The model also includes attractive impurity–impurity interactions mediated by the phonons [26, 32]. An essential requirement for our model is that neither
Figure 3.1. (Color online) A quantum degenerate gas confined to an optical lattice is immersed in a much larger BEC. For increasing BEC temperature $T$, a crossover from coherent to diffusive hopping, characterized by $\tilde{J}$ and $E_a$, respectively, can be observed. The phonon-induced interaction potential $V_{i,j}$ leads to the formation of off-site polaron clusters, separated by a gap $E_b$ from the continuum of unbound states.

interactions with impurities nor the trapping potential confining the impurities impairs the ability of the surrounding gas to sustain phononlike excitations. The first condition limits the number of impurity atoms [22, 23], whereas the latter requirement can be met by using a species-specific optical lattice potential [102]. Moreover, unlike in the case of self-localized impurities [103], we assume that the one-particle states of the impurities are not modified by the BEC, which can be achieved by sufficiently tight impurity trapping.

3.2 Model

The Hamiltonian of the system is composed of three parts, $\hat{H} = \hat{H}_\chi + \hat{H}_B + \hat{H}_I$, where $\hat{H}_\chi$ governs the dynamics of the impurity atoms, which can be either bosonic or fermionic. The BEC Hamiltonian $\hat{H}_B$ and the density–density interaction Hamiltonian $\hat{H}_I$ are

$$\hat{H}_B = \int \! d\mathbf{r} \, \hat{\phi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m_b} + V_{\text{ext}}(\mathbf{r}) + \frac{g}{2} \hat{\phi}^\dagger(\mathbf{r}) \hat{\phi}(\mathbf{r}) \right] \hat{\phi}(\mathbf{r}),$$
\[ \hat{H}_I = \kappa \int \text{d}r \, \hat{\chi}^\dagger (\mathbf{r}) \hat{\chi} (\mathbf{r}) \hat{\phi}^\dagger (\mathbf{r}) \hat{\phi} (\mathbf{r}), \]

where \( \hat{\chi} (\mathbf{r}) \) is the impurity field operator and \( \hat{\phi} (\mathbf{r}) \) is the condensate atom field operator satisfying the commutation relations \( [\hat{\phi} (\mathbf{r}), \hat{\phi}^\dagger (\mathbf{r}')] = \delta (\mathbf{r} - \mathbf{r}') \) and \( [\hat{\phi} (\mathbf{r}), \hat{\phi} (\mathbf{r}')] = 0 \). The coupling constants \( g > 0 \) and \( \kappa \) account for the boson–boson and impurity–boson interaction respectively, \( m_b \) is the mass of a condensate atom and \( V_{\text{ext}} (\mathbf{r}) \) a weak external trapping potential. Without yet specifying \( \hat{H}_I \) we expand \( \hat{\chi} (\mathbf{r}) = \sum_\nu \eta_\nu (\mathbf{r}) \hat{a}_\nu \), where \( \eta_\nu (\mathbf{r}) \) are a set of orthogonal mode functions of the impurities and \( \hat{a}_\nu (\hat{a}_\nu^\dagger) \) the corresponding annihilation (creation) operators, labeled by the quantum numbers \( \nu \).

A common approach to find the elementary excitations of the BEC in the presence of impurities is to solve the Gross–Pitaevskii equation (GPE) \cite{104} for the full system, i.e., for \( \kappa \neq 0 \), and to subsequently quantize small oscillations around the classical ground state. To obtain a quantum description of the impurity dynamics, we instead solve the GPE without taking \( \hat{H}_I \) into account, and express the BEC deformations around the impurities as coherent states of Bogoliubov phonons. Specifically, we write \( \hat{\phi} (\mathbf{r}) = \phi_0 (\mathbf{r}) + \delta \hat{\phi} (\mathbf{r}) \), with \( \phi_0 (\mathbf{r}) = \phi_0^\ast (\mathbf{r}) \) the solution of the GPE for \( \kappa = 0 \). Provided that the impurity–boson coupling is sufficiently weak, i.e., \( |\kappa|/gn_0 (\mathbf{r}) \xi^D (\mathbf{r}) \ll 1 \), with \( \xi (\mathbf{r}) = \hbar / \sqrt{m_b gn_0 (\mathbf{r})} \) the healing length, \( n_0 (\mathbf{r}) = \phi_0^2 (\mathbf{r}) \) and \( D \) the number of spatial dimensions, we expect that the deviation of \( \hat{\phi} (\mathbf{r}) \) from \( \phi_0 (\mathbf{r}) \) is of order \( \kappa \), i.e., \( \langle \delta \hat{\phi} (\mathbf{r}) \rangle \propto \kappa \), where \( \langle \cdot \rangle \) stands for the expectation value. We insert \( \phi_0 (\mathbf{r}) + \delta \hat{\phi} (\mathbf{r}) \) into the Hamiltonian \( \hat{H}_B + \hat{H}_I \), keep terms up to second order in \( \kappa \), and obtain the linear term \( \kappa \int \text{d}r \, \hat{\chi}^\dagger (\mathbf{r}) \hat{\chi} (\mathbf{r}) \phi_0 (\mathbf{r}) [\delta \hat{\phi}^\dagger (\mathbf{r}) + \delta \hat{\phi} (\mathbf{r})] \), in addition to the standard constant and quadratic terms in \( \delta \hat{\phi} (\mathbf{r}) \) and \( \delta \hat{\phi}^\dagger (\mathbf{r}) \), since \( \phi_0 (\mathbf{r}) \) is no longer the ground state of the system.

In order to diagonalize the quadratic terms in \( \delta \hat{\phi} (\mathbf{r}) \) and \( \delta \hat{\phi}^\dagger (\mathbf{r}) \), we use the
expansion \( \delta \hat{\phi}(\mathbf{r}) = \sum_{\mu} [u_{\mu}(\mathbf{r}) \hat{b}_\mu - v^*_{\mu}(\mathbf{r}) \hat{b}^\dagger_\mu] \), where \( u_{\mu}(\mathbf{r}) \) and \( v^*_{\mu}(\mathbf{r}) \) are the solutions of the Bogoliubov–de Gennes equations [104] for \( \kappa = 0 \), and \( \hat{b}_\mu (\hat{b}^\dagger_\mu) \) are the bosonic Bogoliubov annihilation (creation) operators, labeled by the quantum numbers \( \mu \). We assume that the mode functions \( \eta_{\nu}(\mathbf{r}) \) are localized on a length scale much smaller than is set by \( V_{\text{ext}}(\mathbf{r}) \), and that \( \int d\mathbf{r} |\eta_{\nu}(\mathbf{r})|^2 |\eta_{\tau}(\mathbf{r})|^2 \approx 0 \) for \( \nu \neq \tau \), i.e., the probability densities \( |\eta_{\nu}(\mathbf{r})|^2 \) for different mode functions deviate appreciably from zero only within mutually exclusive spatial regions. In this case \( \int d\mathbf{r} \phi_0(\mathbf{r})[u_{\mu}(\mathbf{r}) - v^*_{\mu}(\mathbf{r})] \eta_{\nu}(\mathbf{r}) \eta^*_{\nu}(\mathbf{r}) \approx 0 \) and \( \int d\mathbf{r} n_0(\mathbf{r}) \eta_{\nu}(\mathbf{r}) \eta^*_{\nu}(\mathbf{r}) \approx 0 \) hold for \( \nu \neq \tau \), and hence the nondiagonal impurity–phonon coupling is negligible. The total Hamiltonian can thus be rewritten in the form of a Hubbard–Holstein model [105] \( \hat{H} = \hat{H}_\chi + \sum_{\nu,\mu} \hbar \omega_{\mu} (M_{\nu,\mu} \hat{b}_\mu + M^*_{\nu,\mu} \hat{b}^\dagger_\mu) \hat{n}_\nu + \sum_{\nu} \bar{E}_\nu \hat{n}_\nu + \sum_{\mu} \hbar \omega_{\mu} \hat{b}^\dagger_\mu \hat{b}_\mu \), with \( \hbar \omega_{\mu} \) the energies of the Bogoliubov excitations, the number operator \( \hat{n}_\nu = \hat{a}^\dagger_\nu \hat{a}_\nu \), the dimensionless matrix elements \( M_{\nu,\mu} = (\kappa/\hbar \omega_{\mu}) \int d\mathbf{r} \phi_0(\mathbf{r})[u_{\mu}(\mathbf{r}) - v^*_{\mu}(\mathbf{r})] |\eta_{\nu}(\mathbf{r})|^2 \) and the mean field shift \( \bar{E}_\nu = \kappa \int d\mathbf{r} n_0(\mathbf{r}) |\eta_{\nu}(\mathbf{r})|^2 \). We obtain an effective Hamiltonian \( \hat{H}_{\text{eff}} \) including corrections to \( \phi_0(x) \) of order \( \kappa \) by applying the unitary Lang–Firsov transformation [28, 95] \( \hat{H}_{\text{eff}} = \hat{U} \hat{H} \hat{U}^\dagger \), with \( \hat{U} = \exp \left[ \sum_{\nu,\mu} (M^*_{\nu,\mu} \hat{b}^\dagger_\mu - M_{\nu,\mu} \hat{b}_\mu) \hat{n}_\nu \right] \), which yields

\[
\hat{H}_{\text{eff}} = \hat{U} \hat{H}_\chi \hat{U}^\dagger + \sum_\nu (\bar{E}_\nu - E_\nu) \hat{n}_\nu - \sum_\nu E_\nu \hat{n}_\nu (\hat{n}_\nu - 1) - \frac{1}{2} \sum_{\nu \neq \tau} V_{\nu,\tau} \hat{n}_\nu \hat{n}_\tau + \sum_\mu \hbar \omega_{\mu} \hat{b}^\dagger_\mu \hat{b}_\mu. \tag{3.1}
\]

The transformed impurity Hamiltonian \( \hat{U} \hat{H}_\chi \hat{U}^\dagger \) is obtained using the relation \( \hat{U} \hat{a}^\dagger_\nu \hat{U}^\dagger = \hat{a}^\dagger_\nu \hat{X}^\dagger_\nu \), where \( \hat{X}^\dagger_\nu = \exp \left[ \sum_\mu (M^*_{\nu,\mu} \hat{b}^\dagger_\mu - M_{\nu,\mu} \hat{b}_\mu) \right] \) is a Glauber displacement operator that creates a coherent phonon cloud, i.e., a BEC deformation, around the impurity. In the limit where the BEC adjusts instantaneously to the impurity configuration, polarons created by \( \hat{a}^\dagger_\nu \hat{X}^\dagger_\nu \) are the appropriate quasi-
particles, and $\hat{H}_{\text{eff}}$ describes a nonretarded interaction with the potential $V_{\nu,\tau} = \sum_\mu \hbar \omega_\mu (M_{\nu,\mu} M_{\tau,\mu}^* + M_{\tau,\mu}^* M_{\nu,\mu})$. The polaronic level shift $E_\nu = \sum_\mu \hbar \omega_\mu |M_{\nu,\mu}|^2$ is equal to the characteristic potential energy of an impurity in the deformed BEC.

We now turn to the specific case of bosons loaded into an optical lattice immersed in a homogeneous BEC [94]. In the tight-binding approximation, the impurity dynamics is well described by the Bose–Hubbard model

$$\hat{H}_\chi = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} U \sum_j \hat{n}_j \hat{n}_j - 1 + \mu \sum_j \hat{n}_j,$$

where $\mu$ describes the energy offset, $U$ the on-site interaction strength, and $J$ the hopping matrix element between adjacent sites [99, 106, 107]. The modes of the lattice atoms are Wannier functions $\eta_j(\mathbf{r})$ of the lowest Bloch band localized at site $j$, and $\langle i,j \rangle$ denotes the sum over nearest neighbors. Noting that $[\hat{U}, \hat{n}_j] = 0$, we find

$$\hat{U} \hat{H}_\chi \hat{U}^\dagger = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i)^\dagger \hat{X}_j \hat{a}_j + \frac{U}{2} \sum_j \hat{n}_j \hat{n}_j - 1 + \mu \sum_j \hat{n}_j,$$

with the corresponding matrix elements $M_{j,\mathbf{q}} = \kappa \sqrt{n_0 \varepsilon_\mathbf{q} / (\hbar \omega_\mathbf{q})^3} f_j(\mathbf{q})$, where $\mathbf{q}$ is the phonon momentum, $\varepsilon_\mathbf{q} = (\hbar \mathbf{q})^2 / 2 m_b$ the free particle energy, $\hbar \omega_\mathbf{q} = \sqrt{\varepsilon_\mathbf{q} (\varepsilon_\mathbf{q} + 2 g n_0)}$ the Bogoliubov dispersion relation, and $f_j(\mathbf{q}) = \Omega^{-1/2} \int d\mathbf{r} |\eta_j(\mathbf{r})|^2 \exp(i \mathbf{q} \cdot \mathbf{r})$, with $\Omega$ the quantization volume. We note that, for $|\mathbf{q}| \ll 1 / \xi$, we have $M_{j,\mathbf{q}} \propto f_j(\mathbf{q}) / \sqrt{|\mathbf{q}|}$, whereas for $|\mathbf{q}| \gg 1 / \xi$, one obtains $M_{j,\mathbf{q}} \propto f_j(\mathbf{q}) / q^2$.

The Hamiltonian $\hat{H}_{\text{eff}}$ describes the dynamics of hopping polarons according to an extended Hubbard model [99], provided that $c \gg \alpha J / \hbar$, with $c \sim \sqrt{g n_0 / m_b}$ the phonon velocity and $\alpha$ the lattice spacing. We gain qualitative insight into the dependence of $V_{i,j}$ and the constant polaronic level shift $E_\nu \equiv E_p$ on the system parameters by considering a one-dimensional quasi-BEC in the thermodynamic limit. We assume a sufficiently deep lattice to approximate the Wannier functions by Gaussians of width $\sigma \ll \xi$, and find $V_{i,j} = (\kappa^2 / \xi g) e^{-2|j-i|a / \xi}$ and
3.3. Coherent and diffusive transport

\[ E_p = \kappa^2 / 2\xi g. \] We note that the interaction between impurities is always attractive. More importantly, for realistic experimental parameters, \( \xi \sim a \), and hence the off-site terms \( V_{j,j+1} \propto e^{-2a/\xi} \) are non-negligible. This interaction potential is a direct consequence of the local deformation of the BEC around each impurity, as shown in Fig. 3.1. For a set of static impurities at positions \( x_j = aj \), the overall deformation of the BEC density to order \( \kappa \) is given by

\[ n(x) = n_0 + \sum_j \langle \hat{X}_j \hat{b}_q \hat{b}_q \hat{X}_j \rangle = n_0 - (\kappa / g \xi) \sum_j e^{-2|x-x_j|/\xi}. \]

3.3 Coherent and diffusive transport

We first consider coherent hopping of polarons at small BEC temperatures \( k_B T \ll E_p \), where incoherent phonon scattering is highly suppressed. Provided that \( \zeta = J / E_p \ll 1 \), we can apply the so-called strong-coupling theory [96], and treat the hopping term in Eq. (3.2) as a perturbation. Including terms of first order in \( \zeta \), we obtain the impurity Hamiltonian

\[
\hat{H}^{(1)} = -\tilde{J} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \tilde{U} \sum_j \hat{n}_j (\hat{n}_j - 1) + \tilde{\mu} \sum_j \hat{n}_j \\
- \frac{1}{2} \sum_{i \neq j} V_{i,j} \hat{n}_i \hat{n}_j,
\]

with \( \tilde{\mu} = \mu + \kappa n_0 - E_p \), \( \tilde{U} = U - 2E_p \), and \( \tilde{J} = J \langle \hat{X}_i^\dagger \hat{X}_j \rangle \). Here \( \langle \cdot \rangle \) denotes the average over the thermal phonon distribution and \( i, j \) are nearest neighbors.

We find \( \langle \hat{X}_i^\dagger \hat{X}_j \rangle = \exp \left\{ - \sum_{\mathbf{q} \neq 0} |M_{0,\mathbf{q}}|^2 [1 - \cos(\mathbf{q} \cdot \mathbf{a})](2N_q + 1) \right\} \), with \( \mathbf{a} \) the position vector connecting two nearest neighbor sites and \( N_q = (e^{\hbar \omega_q / k_B T} - 1)^{-1} \). Thus, the hopping bandwidth decreases exponentially with increasing coupling constant \( \kappa \) and temperature \( T \).

At high temperatures \( E_p \ll k_B T \ll k_B T_c \) (with \( T_c \) the critical temperature
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of the BEC) inelastic scattering, in which phonons are emitted and absorbed, becomes dominant, and thus the transport of atoms through the lattice changes from being purely coherent to incoherent. We investigate this crossover by deriving a generalized master equation (GME) for a single particle starting from \( \hat{H}_{\text{eff}} \) in Eq. (3.1). Using the Nakajima–Zwanzig projection method [108], we find that the occupation probabilities \( P_l(t) \) at site \( l \) and time \( t \) evolve according to the GME [109]

\[
\frac{\partial P_l(t)}{\partial t} = \int_0^t ds \sum_j \left[ W_{l,j}(s)P_j(t-s) - W_{j,l}(s)P_l(t-s) \right],
\]

(3.4)

where the effect of the phonon bath is encoded in the memory functions \( W_{i,j}(s) \), which are symmetric in \((i,j)\). To first order in \( \zeta \), thus keeping only nearest-neighbor correlations, we find

\[
W_{i,j}(s) = 2 \left( \frac{J}{\hbar} \right)^2 \operatorname{Re} \left\{ \exp \left\{ 2 \sum_{q \neq 0} |M_{0,q}|^2 [1 - \cos(q \cdot a)] \right\} \times \left[ (N_q + 1)(e^{i \omega_q s} - 1) + N_q(e^{-i \omega_q s} - 1) \right] \right\},
\]

(3.5)

and \( W_{i,j}(s) = 0 \) if \( i \) and \( j \) are beyond nearest neighbors. The nontrivial part of \( W_{i,j}(s) \) takes the values \( 2(J/\hbar)^2 \) at \( s = 0 \) and \( 2(\tilde{J}/\hbar)^2 \) in the limit \( s \to \infty \). In the regime \( k_B T \ll E_p \), we have \( \tilde{J} \sim J \), and the memory function \( W_{i,j}(s) \) is well approximated by \( 2(\tilde{J}/\hbar)^2 \Theta(s) \) [with \( \Theta(s) \) the Heaviside step function], which describes purely coherent hopping in agreement with \( \hat{H}^{(1)} \). For \( E_p \ll k_B T \ll k_B T_c \), we observe that \( J \ll J \), and \( W_{i,j}(s) \) drops off sufficiently fast for the Markov approximation to be valid, as illustrated in Fig. 3.2(a). In this case one can replace \( P_l(t-s) \) by \( P_l(t) \) in Eq. (3.4) and after integration over \( s \) the GME reduces to a standard Pauli master equation \( \partial_t P_l(t) = \sum_j w_{i,j}[P_j(t)-P_l(t)] \) describing purely incoherent hopping. The hopping rate is of the form \( w_{i,j} \sim \)
3.3. Coherent and diffusive transport

\( J^2 \exp(-E_a/k_B T)/(\hbar \sqrt{k_B T E_a}) \) [28, 105], where \( E_a \sim E_p \) is the activation energy.

The temperature-dependent crossover from coherent to diffusive hopping in a quasi-one-dimensional (1D) system is apparent in the evolution for a time \( \tau \sim 1/w_{i,j} \) of a particle initially localized at lattice site \( j = 0 \). The mean-squared displacement of the lattice atom, \( \overline{l^2}(t) = \sum_l l^2 P_l(t) \), can be decomposed as \( \overline{l^2}(t) = A t + B t^2 \) into incoherent and coherent contributions, characterized by the coefficients \( A \) and \( B \), respectively. The crossover takes place when incoherent and coherent contributions to \( \overline{l^2}(\tau) \) are comparable, i.e., \( \sqrt{B} = A \). Fig. 3.2(b) shows \( A \) and \( \sqrt{B} \) as functions of \( T \), where \( \overline{l^2}(t) \) was obtained by numerically solving the GME using the memory function \( W_{i,j} \) in Eq. (3.5). We find that, for a \(^{41}\text{K}-^{87}\text{Rb} \) system [20] under standard experimental conditions, the crossover takes place well below the critical temperature of the BEC (see caption of Fig. 3.2).

Polaron clusters

We now discuss the formation of polaron clusters for \( k_B T \lesssim E_p \), based on Hamiltonian \( \hat{H}^{(1)} \) in Eq. (3.3), and assume that the bosonic impurities are in thermal equilibrium with the BEC. At these temperatures \( V_{i,j} \), and \( \tilde{J} \) are well approximated by their \( T = 0 \) values. We consider the limit \( \tilde{U} \gg V_{j,j+1}, \tilde{U} \gg \tilde{J} \), and adiabatically eliminate configurations with multiply occupied sites. Keeping only nearest neighbor interactions, we obtain approximate expressions for the binding energy \( E_b(s) \approx (s - 1)V_{j,j+1} \) of a cluster of \( s \) polarons located in adjacent sites and the lowest energy band \( E_k(s) \approx -E_b(s) - 2\tilde{J}^s(V_{j,j+1})^{1-s} \cos(ka) \) [110], with \( k \) the quasimomentum. This band approximation is in good agreement with the

Figure 3.2. (a) Memory function $\hbar^2W_{i,j}(t)/(2J^2)$ versus time for $k_B T = 0$ (dotted line), $2E_p$ (dashed line) and $10E_p$ (full line). It drops off rapidly for $k_B T \gg E_p$, indicating the dominance of incoherent hopping. (b) Coefficients $\hbar A/J$ (dashed line) and $\hbar\sqrt{\beta}/J$ (full line) versus temperature, obtained from the numerical solution of the GME in Eq. (3.4) for an evolution time $\tau = 10\hbar/J \approx 0.8 \times 10^{-3}s$. The condition $A = \sqrt{\beta}$ is satisfied at $k_B T/E_p \approx 2.3$, with $E_p/k_B \approx 11nK$. The lattice (wavelength $\lambda = 790nm$) contains a single $^{41}K$ atom with $J = 2.45 \times 10^{-2}E_R$, $\kappa/E_R\lambda = 2.3 \times 10^{-2}$, the recoil energy $E_R = (2\pi\hbar)^2/2m_a\lambda^2$, and $m_a$ the mass of the lattice atom. The BEC consists of $^{87}Rb$ atoms with $n_0 = 5 \times 10^6m^{-1}$ and $g/E_R\lambda = 8.9 \times 10^{-3}$.

results from exact diagonalization of $\hat{H}^{(1)}$ using the full interaction potential $V_{i,j}$, as shown for three polarons in Fig. 3.3(a).

This model predicts a decreasing average cluster size with increasing temperature. For a small system with $N = 3$ polarons, we calculate the probability of finding a three-polaron cluster $P_3 = \sum \langle n_\nu \rangle$, where the sum is taken over all states with energies $\varepsilon_\nu < E_g(2) + E_g(1)$, $E_g(N)$ is the ground state energy of an $N$-polaron cluster, and the occupation probabilities are given by the Boltzmann law $\langle n_\nu \rangle \propto \exp(-\varepsilon_\nu/k_B T)$. Analogously, we determine the probability $P_2$ of finding a two-polaron cluster or bipolaron. The results are shown in Fig. 3.3(b). The
3.3. Coherent and diffusive transport

Figure 3.3. (Color online) (a) Energy spectrum of three polarons in a 1D optical lattice. The solid line shows the lowest energy band $E_3(k)$ characterizing off-site three-polaron clusters. The lattice (wavelength $\lambda = 790\text{nm}$, $M = 31$ sites, periodic boundary conditions) contains $^{133}\text{Cs}$ atoms with $J = 7.5 \times 10^{-3} E_R$, $U = 50 E_p$, and $\kappa/E_R \lambda = 1.05 \times 10^{-1}$. The BEC consists of $^{87}\text{Rb}$ atoms with $n_0 = 5 \times 10^6 \text{m}^{-1}$ and $g/E_R \lambda = 4.5 \times 10^{-2}$.

(b) Probability of finding a three-polaron cluster (solid line) or a two-polaron cluster (dashed line) versus temperature. The parameters are $g/E_R \lambda = 6.5 \times 10^{-2}$, $\kappa/E_R \lambda = 1.32 \times 10^{-1}$, $U = 2.2 E_p$, $M = 27$, and the rest as for (a).

The probability of having a three-polaron cluster goes down with increasing temperature and for $T = E_p/k_B \approx 18\text{nK}$ is essentially zero for the parameters chosen. For this three-polaron cluster, three-particle loss is negligible due to the on-site repulsion $U$. Decreasing the value of $U$ gives a significantly increased $P_2$ compared to the values shown in Fig. 3.3(b).

The clustering of polarons leads to their mutual exponential localization. This is illustrated by the density–density correlations $\langle \hat{n}_i \hat{n}_{i+j} \rangle$ for the three-polaron cluster in Fig. 3.4(a). With increasing attractive interaction $V_{i,j}$, the mutual localization gets stronger, leading to an increased broadening of the momentum distribution, as shown in Fig. 3.4(b). This allows polaron clusters to be identified
in time of flight experiments. We note that the transition from a superfluid to a Mott insulator also leads to broadening of the momentum distribution as, e.g., observed in [22, 23]. However, using Bragg spectroscopy [47] would allow the unambiguous distinction of boson clustering from this transition.

### 3.4 Conclusion

We have demonstrated that the dynamics of bosonic impurities immersed in a BEC is accurately described in terms of polarons. We found that spatial coherence is destroyed in hopping processes at large BEC temperatures while the main effect of the BEC at low temperatures is to reduce the coherent hopping rate. Furthermore the phonons induce off-site interactions which lead to the formation of stable clusters which are not affected by loss due to inelastic collisions. Using
the techniques introduced in this paper qualitatively similar phenomena can also be shown to occur for fermionic impurities. In either case these effects can be controlled by external parameters and lie within the reach of current experimental techniques.

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Chapter 4

Transport of strong-coupling polarons in optical lattices

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We study the transport of ultracold impurity atoms immersed in a Bose–Einstein condensate (BEC) and trapped in a tight optical lattice. Within the strong-coupling regime, we derive an extended Hubbard model describing the dynamics of the impurities in terms of polarons, i.e. impurities dressed by a coherent state of Bogoliubov phonons. Using a generalized master equation based on this microscopic model we show that inelastic and dissipative phonon scattering results in (i) a crossover from coherent to incoherent transport of impurities with increasing BEC temperature and (ii) the emergence of a net atomic current across a tilted optical lattice. The dependence of the atomic current on the lattice tilt changes from ohmic conductance to negative differential conductance within an experimentally accessible parameter regime. This transition is accurately described by an Esaki–Tsu-type relation with the effective relaxation time of the impurities as a temperature-dependent parameter.
4.1 Introduction

The study of impurities immersed in liquid helium in the 1960s opened a new chapter in the understanding of the structure and dynamics of a Bose-condensed fluid [29]. Two of the most prominent examples include dilute solutions of $^3\text{He}$ in superfluid $^4\text{He}$ [29, 111] and the measurement of ionic mobilities in superfluid $^4\text{He}$ [29, 112]. More recently, the experimental realization of impurities in a Bose–Einstein condensate (BEC) [113, 114] and the possibility to produce quantum degenerate atomic mixtures [19–23, 115] have generated renewed interest in the physics of impurities. Of particular importance, collisionally induced transport of impurities in an ultra-cold bosonic bath has been recently observed [53] in an experimental setup of a similar type as to the one considered in this paper.

In the context of liquid helium and Bose–Einstein condensates, a plethora of theoretical results have been obtained. Notably, the effective interaction between impurities [26, 32, 116, 117] and the effective mass of impurities [31, 118–121], both of which are induced by the condensate background, have been studied in detail. Moreover, the problem of self-trapping of static impurities has been addressed [59, 60, 91] in the framework of Gross–Pitaevskii (GP) theory [30, 61], and quantized excitations around the ground state of the self-trapped impurity and the distorted BEC have been investigated in [103].

In the present paper we study the dynamics of impurities immersed in a nearly uniform BEC, which in addition are trapped in an optical lattice potential [5, 107]. This setup has been considered in [122] by the present authors, however, we here motivate and develop the small polaron formalism in more detail and extend the results to the case of a tilted optical lattice potential, as illustrated in Fig. 4.1. In contrast to similar previously-studied systems, the presence of an optical lattice allows us to completely control the kinetic energy of the impurities. Crucially,
4.1. Introduction

Figure 4.1. Impurities described by the localized Wannier functions $\chi_j(\mathbf{r})$ are trapped in the optical lattice potential $V_L(\mathbf{r})$ and immersed in a nearly uniform BEC. A tilt imposed on the periodic potential leads to the formation of a Wannier–Stark ladder (dotted lines) with levels separated by the Bloch frequency $\omega_B$. Inelastic scattering of Bogoliubov phonons results in a net atomic current across the tilted lattice. The current depends on the effective hopping $\tilde{J}$, the level separation $\omega_B$ and the effective relaxation time of the impurities.

for impurities in the lowest Bloch band of the optical lattice the kinetic energy is considerably reduced by increasing the depth of the lattice potential [5, 107]. As a consequence, it is possible to access the so-called strong-coupling regime [96], where the interaction energy due to the coupling between the impurity and the BEC is much larger than the kinetic energy of the impurity. This regime is particularly interesting since it involves incoherent and dissipative multi-phonon processes which have a profound effect on the transport properties of the impurities.

As a starting point we investigate the problem of static impurities based on the GP approximation and by means of a Bogoliubov description of the quantized excitations [30, 123]. The main part of the paper is based on small polaron theory [28, 105, 124], where the polaron is composed of an impurity dressed by a coherent state of Bogoliubov phonons. This formalism accounts in a natural way
for the effects of the BEC background on the impurities and allows us to describe
the BEC deformation around the impurity in terms of displacement operators.
As a principal result, we obtain an extended Hubbard model [99, 125] for the
impurities, which includes the hopping of polarons and the effective impurity–
impurity interaction mediated by the BEC. Moreover, the microscopic model
is particularly suitable for the investigation of the transport of impurities from
first principles within the framework of a generalized master equation (GME)
approach [109, 126–128].

The transport properties of the impurities are considered in two distinct se-
tups. We first show that in a non-tilted optical lattice the Bogoliubov phonons
induce a crossover from coherent to incoherent hopping as the BEC temperature
increases [122]. In addition, we extend the results in [122] to the case of a tilted
optical lattice (see Fig. 4.1). We demonstrate that the inelastic phonon scat-
tering responsible for the incoherent hopping of the impurities also provides the
necessary relaxation process required for the emergence of a net atomic current
across the lattice [55]. In particular, we find that the dependence of the current
on the lattice tilt changes from ohmic conductance to negative differential con-
ductance (NDC) for sufficiently low BEC temperatures. So far, to our knowledge,
NDC has only been observed in a non-degenerate mixture of ultra-cold 40K and
87Rb atoms [53] and in semiconductor superlattices [57, 58], where the voltage–
current dependence is known to obey the Esaki–Tsu relation [54]. By exploiting
the analogy with a solid state system we show that the transition from ohmic
conductance to NDC is accurately described by a similar relation, which allows
us to determine the effective relaxation time of the impurities as a function of the
BEC temperature.

The implementation of our setup relies on recent experimental progress in
the production of quantum degenerate atomic mixtures [19–21, 115] and their
confinement in optical lattice potentials [22, 23]. As proposed in [94], the impurities in the optical lattice can be cooled to extremely low temperatures by exploiting the collisional interaction with the surrounding BEC. The tilt imposed on the lattice potential may be achieved either by accelerating the lattice [48] or superimposing an additional harmonic potential [53, 129].

An essential requirement for our model is that neither interactions with impurities nor the trapping potential confining the impurities impairs the ability of the BEC to sustain phonon-like excitations. The first condition limits the number of impurity atoms [22, 23, 130], and thus we assume that the filling factor of the lattice is much lower than one, whereas the second requirement can be met by using a species-specific optical lattice potential [102]. Unlike in the case of self-trapped impurities [59, 60, 91], we assume that the one-particle states of the impurities are not modified by the BEC, which can be achieved by sufficiently tight impurity trapping, as shown in 4.9.

The paper is organized as follows. In Section 2 we present our model. In Section 3, we motivate the small polaron formalism by considering the problem of static impurities based on the GP equation and within the framework of Bogoliubov theory. In Section 4, the full dynamics of the impurities is included. We develop the small polaron formalism in detail and derive an effective Hamiltonian for hopping impurities. In Section 5, the GME is used to investigate the transport properties of the impurity atoms. First, we discuss the crossover from coherent to incoherent hopping and subsequently study the dependence of a net atomic current across a tilted optical lattice on the system parameters. We discuss possible extensions of our model and conclude in Section 6. Throughout the paper we consider impurity hopping only along one single direction for notational convenience. However, the generalization to hopping along more than one direction is straightforward.
4.2 Model

The Hamiltonian of the system is composed of three parts $\hat{H} = \hat{H}_B + \hat{H}_\chi + \hat{H}_I$, where $\hat{H}_B$ is the Hamiltonian of the Bose-gas, $\hat{H}_\chi$ governs the dynamics of the impurity atoms and $\hat{H}_I$ describes the interactions between the impurities and the condensate atoms.

The Bose-gas is assumed to be at a temperature $T$ well below the critical temperature $T_c$, so that most of the atoms are in the Bose-condensed state. The boson–boson interaction is represented by a pseudo-potential $g\delta(r-r')$, where the coupling constant $g > 0$ depends on the s-wave scattering length of the condensate atoms. Accordingly, the grand canonical Hamiltonian $\hat{H}_B$ of the Bose-gas reads

$$\hat{H}_B = \int dr \hat{\psi}^\dagger(r) \left[ \hat{\mathcal{H}}_0 - \mu_b \right] \hat{\psi}(r) + \frac{g}{2} \int dr \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r) \hat{\psi}(r) \hat{\psi}(r), \quad (4.1)$$

where $\mu_b$ is the chemical potential and

$$\hat{\mathcal{H}}_0 = -\frac{\hbar^2}{2m_b} \nabla^2 + V_{\text{ext}}(r) \quad (4.2)$$

is the single-particle Hamiltonian of the non-interacting gas, with $m_b$ the mass of a boson and $V_{\text{ext}}(r)$ is a shallow external trapping potential. The boson field operators $\hat{\psi}^\dagger(r)$ and $\hat{\psi}(r)$ create and annihilate an atom at position $r$, respectively, and satisfy the bosonic commutation relations $[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \delta(r-r')$ and $[\hat{\psi}(r), \hat{\psi}(r')] = [\hat{\psi}^\dagger(r), \hat{\psi}^\dagger(r')] = 0$.

To be specific we consider bosonic impurity atoms with mass $m_a$ loaded into an optical lattice, which are described by the impurity field operator $\hat{\chi}(r)$. The optical lattice potential for the impurities is of the form $V_L(r) = V_x \sin^2(kx) + V_y \sin^2(ky) + V_z \sin^2(kz)$, with the wave-vector $k = 2\pi/\lambda$ and $\lambda$ the wavelength of the laser beams. The depth of the lattice $V_\ell (\ell = x, y, z)$ is determined by the
4.2. Model

intensity of the corresponding laser beam and conveniently measured in units of the recoil energy $E_R = \hbar^2 k^2 / 2m_a$. Since we are interested in the strong-coupling regime we assume that the depth of the lattice exceeds several recoil energies. As a consequence, the impurity dynamics is accurately described in the tight-binding approximation by the Bose–Hubbard model [5, 107], where the mode-functions of the impurities $\chi_j(\mathbf{r})$ are Wannier functions of the lowest Bloch band localized at site $j$, satisfying the normalization condition $\int d\mathbf{r} |\chi_j(\mathbf{r})|^2 = 1$. Accordingly, the impurity field operator is expanded as $\hat{\chi}(\mathbf{r}) = \sum_j \chi_j(\mathbf{r}) \hat{a}_j$ and the Bose–Hubbard Hamiltonian is given by

$$
\hat{H}_\chi = -J \sum_{\langle i, j \rangle} \hat{a}^\dagger_i \hat{a}_j + \frac{1}{2} U \sum_j \hat{n}_j (\hat{n}_j - 1) + \mu_a \sum_j \hat{n}_j + \hbar \omega_B \sum_j j \hat{n}_j, \quad (4.3)
$$

where $\mu_a$ is the energy offset, $U$ is the on-site interaction strength, $J$ is the hopping matrix element between adjacent sites and $\langle i, j \rangle$ denotes the sum over nearest neighbours. The operators $\hat{a}_j$ ($\hat{a}^\dagger_j$) create (annihilate) an impurity at lattice site $j$ and satisfy the bosonic commutation relations $[\hat{a}_i, \hat{a}^\dagger_j] = \delta_{i,j}$ and $[\hat{a}_i, \hat{a}_j] = [\hat{a}^\dagger_i, \hat{a}^\dagger_j] = 0$, and $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ is the number operator. The last term in Eq. $(4.3)$ was added to allow for a tilted lattice with the energy levels of the Wannier states $\chi_j(\mathbf{r})$ separated by Bloch frequency $\omega_B$, as shown in Fig. $(4.1)$.

For the lattice depths considered in this paper it is possible to expand the potential wells about their minima and approximate the Wannier functions by harmonic oscillator ground states. The oscillation frequencies of the wells are $\omega_\ell = 2\sqrt{E_R V_\ell / \hbar}$ and the spread of the mode-functions $\chi_j(\mathbf{r})$ is given by the harmonic oscillator length $\sigma_\ell = \sqrt{\hbar / m_a \omega_\ell}$. Explicitly, the Gaussian mode-function in one dimension reads

$$
\chi_{j,\sigma}(x) = (\pi \sigma^2)^{-1/4} \exp \left[ - (x - x_j)^2 / (2 \sigma^2) \right], \quad (4.4)
$$
where \( x_j = a_j \) with \( a = \lambda/2 \) being the lattice spacing. We note that the mode-functions \( \chi_{j,\sigma}(r) \) are highly localized on a scale short compared to the lattice spacing \( a \) since \( \sigma_\ell/a = (V_\ell/E_R)^{-1/4}/\pi \ll 1 \) for sufficiently deep lattices. Consistency of the tight-binding model requires that excitations into the first excited Bloch band due to Landau–Zener tunneling or on-site interactions are negligible, i.e. \( \omega_B \ll \omega_\ell \) and \( 1/2 \sum_j (n_j - 1) \ll \hbar \omega_\ell \), with \( n_j \) the occupation numbers. These inequalities are readily satisfied in practice.

The density–density interaction between the impurities and the Bose-gas atoms is again described by a pseudo-potential \( \kappa \delta(r - r') \), with \( \kappa \) the coupling constant, and the interaction Hamiltonian is of the form

\[
\hat{H}_I = \kappa \int \! dr \, \hat{\chi}(r)^\dagger \hat{\chi}(r) \hat{\psi}(r)^\dagger \hat{\psi}(r).
\]

We note that the effect of \( \hat{H}_B \) and \( \hat{H}_I \) dominate the dynamics of the system in the strong-coupling regime and hence the kinetic part in \( \hat{H}_\chi \) can be treated as a perturbation.

### 4.3 Static impurities

In a first step we investigate the interaction of static impurities with the BEC, i.e. we neglect the hopping term in \( \hat{H}_\chi \). We first derive a mean-field Hamiltonian based on the GP approximation and subsequently quantize the small-amplitude oscillations about the GP ground state using standard Bogoliubov theory [30, 123].

In the GP approximation, the bosonic field operator \( \hat{\psi}(r) \) is replaced by the classical order parameter of the condensate \( \psi(r) \). Accordingly, the impurities are described by the impurity density \( \rho_\chi(r) = \langle \hat{\chi}(r)^\dagger \hat{\chi}(r) \rangle = \sum_j n_j |\chi_j(r)|^2 \), where the average is taken over a fixed product state \( |\Upsilon\rangle \) representing a set of static
4.3. Static impurities

impurities, i.e. \( |\Psi\rangle = \prod_{\{j\}} \hat{a}_j^\dagger |0\rangle \), with \( \{j\} \) a set of occupied sites and \( |0\rangle \) the impurity vacuum. We linearize the equation for \( \psi(r) \) by considering small deviations \( \vartheta(r) = \psi(r) - \psi_0(r) \) from the ground state of the condensate \( \psi_0(r) \) in absence of impurities. This approach is valid provided that \( |\vartheta(r)|/\psi_0(r) \ll 1 \) and corresponds to an expansion of \( \hat{H}_B + \hat{H}_I \) to second order in \( \kappa \). Explicitly, by replacing \( \hat{\psi}(r) \) with \( \psi_0(r) + \vartheta(r) \) in \( \hat{H}_B + \hat{H}_I \) we obtain the GP Hamiltonian \( H_{GP} = H_{\psi_0} + H_\vartheta + H_{\text{lin}} \) with

\[
H_{\psi_0} = \int \! dr \left\{ \psi_0^*(r) H_0 \psi_0(r) - \mu_b |\psi_0(r)|^2 + \frac{g}{2} |\psi_0(r)|^4 \right\} 
+ \kappa \int \! dr \rho_\chi(r) |\psi_0(r)|^2 , \tag{4.6}
\]

\[
H_{\vartheta} = \int \! dr \left\{ \vartheta^*(r) [H_0 - \mu_b + 2g|\psi_0(r)|^2] \vartheta(r) \right\} 
+ \frac{g}{2} \int \! dr \left\{ \vartheta^*(r)[\psi_0^*(r)]^2 \vartheta^*(r) + \vartheta(r)[\psi_0^*(r)]^2 \vartheta(r) \right\} , \tag{4.7}
\]

\[
H_{\text{lin}} = \kappa \int \! dr \rho_\chi(r) [\psi_0^*(r) \vartheta^*(r) + \psi_0^*(r) \vartheta(r)] . \tag{4.8}
\]

In absence of impurities, i.e. for \( \kappa = 0 \) and \( \vartheta(r) \) identically zero, the stationary condition \( \delta H_{GP}/\delta \psi_0^*(r) = 0 \) implies that \( \psi_0(r) \) satisfies the time-independent GP equation

\[
[H_0 + g|\psi_0(r)|^2] \psi_0(r) = \mu_b \psi_0(r) . \tag{4.9}
\]

The deformed ground state of \( H_{GP} \) due to the presence of impurities is found by imposing the stationary condition \( \delta H_{GP}/\delta \vartheta^*(r) = 0 \) or equivalently

\[
[H_0 - \mu_b + 2g|\psi_0(r)|^2] \vartheta(r) + g[\psi_0(r)]^2 \vartheta^*(r) + \kappa \rho_\chi(r) \psi_0(r) = 0 , \tag{4.10}
\]

which is the Bogoliubov–de Gennes equation \([30, 123]\) for the zero-frequency
For the case of a homogeneous BEC, the effect of the impurities on the ground state of the condensate can be expressed in terms of Green’s functions [59, 60, 103]. If we assume for simplicity that both $\psi_0(r)$ and $\vartheta(r)$ are real then Eq. (4.10) reduces to the modified Helmholtz equation

$$\left[ \nabla^2 - \left( \frac{2}{\xi} \right)^2 \right] \vartheta(r) = \frac{2\kappa}{g \sqrt{n_0 \xi^D}} \rho_{\chi}(r),$$

(4.11)

where $\xi = \hbar / \sqrt{m_0 g n_0}$ is the healing length, $D$ is the number of spatial dimensions, and $n_0 = |\psi_0|^2$ is the condensate density. The solution of Eq. (4.11) is found to be [131]

$$\vartheta(r) = -\frac{\kappa}{g \sqrt{n_0 \xi D}} \int \! dr' \, G(r - r') \rho_{\chi}(r'),$$

(4.12)

where the Green’s functions are

$$G_{1D}(r) = \frac{1}{2} \exp(-2|r|/\xi),$$

(4.13)

$$G_{2D}(r) = \frac{1}{\pi} K_0(2|r|/\xi),$$

(4.14)

$$G_{3D}(r) = \frac{1}{2\pi} \frac{\exp(-2|r|/\xi)}{|r|/\xi},$$

(4.15)

with $K_0(x)$ the modified Bessel function of the second kind. Thus, independent of the dimension $D$ of the system, the BEC deformation induced by the impurities falls off exponentially on a length scale set by $\xi$, as illustrated in Fig. (4.2).

It follows from Eq. (4.12) that for occupation numbers $n_j \sim 1$ the condition $|\vartheta(r)|/\psi_0(r) \ll 1$ is equivalent to

$$\alpha = \frac{|\kappa|}{g} \left( \frac{d}{\xi} \right)^D \ll 1,$$

(4.16)

with $d = n_0^{-1/D}$ the average separation of the condensate atoms. The
4.3. Static impurities

Figure 4.2. The order parameter $\psi(r)$ of a two-dimensional homogeneous condensate deformed by two highly localized impurities with $\kappa > 0$ according to Eq. (4.12). The deformation of the BEC results in an effective interaction potential $V_{i,j}$ between the impurities at lattice sites $i$ and $j$. The range of the potential is characterized by the healing length $\xi$, which is comparable to the lattice spacing $a$ for realistic experimental parameters.

generalization of this condition to the non-homogeneous case is $\alpha(r) = (|\kappa|/g)d(r)/\xi(r)^D \ll 1$ under the assumption that the BEC is nearly uniform. We note that $\alpha(r) \propto n_0(r)^{(D-2)/2}$, and hence $\alpha(r)$ diverges in 1D as $n_0(r) \rightarrow 0$, e.g. near the boundary of the condensate. However, this is consistent with the GP approach, which is no longer applicable in the dilute limit $\xi(r)/d(r) \ll 1$ of a 1D Bose-gas [30].

The change in energy of the BEC due to the impurities is found by inserting the formal solution for $\vartheta(r)$ in Eq. (4.12) into $H_{GP}$. Provided that $\vartheta(r)$ satisfies Eq. (4.10) the identity $H_{lin} + 2H_\vartheta = 0$, or equivalently $H_{GP} = H_{\psi_0} + \frac{1}{2}H_{lin}$, holds.
Using the latter expression for $H_{GP}$ we find

$$H_{GP} = \sum_j (\tilde{E} - E_j) n_j - \sum_j E_j n_j (n_j - 1) - \frac{1}{2} \sum_{i \neq j} \mathcal{V}_{i,j} n_i n_j,$$  \hspace{1cm} (4.17)

where $\tilde{E} = \kappa n_0$ is the first order contribution to the mean-field shift. In Eq. (4.17) we have neglected constant terms which do not depend on the impurity configuration, i.e. contributions containing $\psi_0(r)$ only. The off-site interaction potential between the impurities is given by

$$\mathcal{V}_{i,j} = \frac{2 \kappa^2}{g \xi_D} \int dr dr' |\chi_i(r)|^2 \mathcal{G}(r-r') |\chi_j(r')|^2,$$ \hspace{1cm} (4.18)

and $E_j = \frac{1}{2} \mathcal{V}_{j,j}$ is the potential energy of an impurity, both resulting from the deformation of the condensate, as illustrated in Fig. (4.2).

In order to quantize the GP solution we consider small excitations $\hat{\zeta}(r)$ of the system, which obey bosonic commutation relations, around the static GP ground state $\psi_0(r) + \vartheta(r)$ of the condensate [30, 123]. This corresponds to an expansion of the bosonic field operator as $\hat{\psi}(r) = \psi_0(r) + \vartheta(r) + \hat{\zeta}(r)$. The Hamiltonian $\hat{H}_\zeta$ governing the evolution of $\hat{\zeta}(r)$ can be obtained by substituting $\vartheta(r) + \hat{\zeta}(r)$ for $\vartheta(r)$ in $H_{GP}$. By collecting the terms containing $\hat{\zeta}(r)$ and $\hat{\zeta}^\dagger(r)$ we find

$$\hat{H}_\zeta = \int dr \left\{ \hat{\zeta}^\dagger(r) \left[ H_0 - \mu_b + 2g|\psi_0(r)|^2 \right] \hat{\zeta}(r) \right\} + \frac{g}{2} \int dr \left\{ \hat{\zeta}^\dagger(r)[\psi_0(r)]^2 \hat{\zeta}^\dagger(r) + \hat{\zeta}(r)[\psi_0^*(r)]^2 \hat{\zeta}(r) \right\},$$  \hspace{1cm} (4.19)

where the linear terms in $\hat{\zeta}(r)$ and $\hat{\zeta}^\dagger(r)$ vanish identically since $\vartheta(r)$ satisfies Eq. (4.10). The Hamiltonian $\hat{H}_\zeta$ in Eq. (4.19) can be diagonalized by the standard
**4.3. Static impurities**

Bogoliubov transformation \([30, 123]\)

\[
\hat{\zeta}(\mathbf{r}) = \sum_\nu \left[ u_\nu(\mathbf{r}) \hat{\beta}_\nu + v_\nu^*(\mathbf{r}) \hat{\beta}_\nu^\dagger \right].
\] (4.20)

Here, \(u_\nu(\mathbf{r})\) and \(v_\nu^*(\mathbf{r})\) are complex functions and the operators \(\hat{\beta}_\nu^\dagger\) (\(\hat{\beta}_\nu\)) create (annihilate) a Bogoliubov quasi-particle, with quantum numbers \(\nu\), and satisfy bosonic commutation relations. The Bogoliubov transformation in Eq. (4.20) reduces the Hamiltonian \(\hat{H}_\zeta\) to a collection of noninteracting quasi-particles provided that the coefficients \(u_\nu(\mathbf{r})\) and \(v_\nu(\mathbf{r})\) obey the Bogoliubov–de Gennes equations \([30, 123]\)

\[
\begin{align*}
[H_0 - \mu_b + 2g|\psi_0(\mathbf{r})|^2] u_\nu(\mathbf{r}) + g|\psi_0(\mathbf{r})|^2 v_\nu(\mathbf{r}) &= \hbar \omega_\nu u_\nu(\mathbf{r}) \quad (4.21) \\
[H_0 - \mu_b + 2g|\psi_0^*(\mathbf{r})|^2] v_\nu(\mathbf{r}) + g|\psi_0^*(\mathbf{r})|^2 u_\nu(\mathbf{r}) &= -\hbar \omega_\nu v_\nu(\mathbf{r}), \quad (4.22)
\end{align*}
\]

with the spectrum \(\hbar \omega_\nu\). Under the condition that Eqs. (4.21) are satisfied one finds that \(\hat{H}_\zeta\) takes the form \(\hat{H}_\zeta = \sum_\nu \hbar \omega_\nu \hat{\beta}_\nu^\dagger \hat{\beta}_\nu\), where constant terms depending on \(\psi_0(\mathbf{r})\) and \(v_\nu(\mathbf{r})\) only were neglected*.

Consequently, the total Hamiltonian \(\hat{H}_{\text{stat}}\) of the BEC and the static impurities is composed of three parts

\[
\hat{H}_{\text{stat}} = \hat{H}_\zeta + H_{\text{GP}} + \langle \hat{H}_\chi \rangle,
\] (4.23)

where \(\hat{H}_\zeta\) governs the dynamics of the Bogoliubov quasi-particles and \(H_{\text{GP}}\) is the GP ground state energy, which for the case of a homogeneous BEC takes the simple form in Eq. (4.17). The third term \(\langle \hat{H}_\chi \rangle\) represents the average value of \(\hat{H}_\chi\) with respect to the fixed product state \(|\Upsilon\rangle\) introduced earlier with \(n_j\) impurities.

*The details of establishing the above form of \(\hat{H}_\zeta\) are contained in Ref. [123].
at each site $j$, giving explicitly

$$\langle \hat{H}_\chi \rangle = \frac{1}{2} U \sum_j n_j(n_j - 1) + \mu_a \sum_j n_j + \hbar \omega_B \sum_j j n_j. \quad (4.24)$$

The ground state of the system corresponds to the Bogoliubov vacuum defined by $\hat{\beta}_\nu |\text{vac}\rangle = 0$.

### 4.4 Hopping impurities in the polaron picture

Given the Hamiltonian $\hat{H}_{\text{stat}}$ derived in the previous section it is straightforward to determine the ground state energy for a set of static impurities. However, an analysis of the full dynamics of the impurities requires an alternative description in terms of polarons, i.e. impurities dressed by a coherent state of Bogoliubov quasi-particles. In this picture small polaron theory allows us, for example, to calculate the effective hopping matrix element for the impurities, which takes the BEC background into account.

Our approach is based on the observation that the Hamiltonian $\hat{H}_\zeta$ of the quantized excitations and consequently the Bogoliubov–de Gennes equations (4.21) are independent of $\rho_\chi(r)$. In other words, the effect of the impurities is only to shift the equilibrium position of the modes $\hat{\beta}_\nu$ without changing the spectrum $\hbar \omega_\nu$. Therefore it is possible to first expand the bosonic field operator as $\hat{\psi}(r) = \psi_0(r) + \hat{\vartheta}(r)$, with $\hat{\vartheta}(r) = \vartheta(r) + \hat{\zeta}(r)$, subsequently express $\hat{\vartheta}(r)$ in terms of Bogoliubov modes about the state $\psi_0(r)$ and finally shift their equilibrium positions in order to (approximately) minimize the total energy of the system.

Similarly to the case of static impurities, we first replace $\hat{\psi}(r)$ with $\psi_0(r) + \hat{\vartheta}(r)$
in $\hat{H}_B + \hat{H}_I$ to obtain the Hamiltonian $\hat{H}_{GP} = \hat{H}_{\psi_0} + \hat{H}_\theta + \hat{H}_{\text{lin}}$ with

$$
\hat{H}_{\psi_0} = \int \mathrm{d}r \left\{ \psi_0^*(\mathbf{r})H_0\psi_0(\mathbf{r}) - \mu_b|\psi_0(\mathbf{r})|^2 + \frac{g}{2}|\psi_0(\mathbf{r})|^4 \right\} + \kappa \int \mathrm{d}r \, \hat{\chi}^\dagger(\mathbf{r})\hat{\chi}(\mathbf{r})|\psi_0(\mathbf{r})|^2,
$$

(4.25)

$$
\hat{H}_\theta = \int \mathrm{d}r \left\{ \hat{\vartheta}^\dagger(\mathbf{r}) \left[ H_0 - \mu_b + 2g|\psi_0(\mathbf{r})|^2 \right] \hat{\vartheta}(\mathbf{r}) \right\} + \frac{g}{2} \int \mathrm{d}r \left\{ \hat{\vartheta}^\dagger(\mathbf{r})[\psi_0(\mathbf{r})]^2\hat{\vartheta}^\dagger(\mathbf{r}) + \hat{\vartheta}(\mathbf{r})[\psi_0^*(\mathbf{r})]^2\hat{\vartheta}(\mathbf{r}) \right\},
$$

(4.26)

$$
\hat{H}_{\text{lin}} = \kappa \int \mathrm{d}r \, \hat{\chi}(\mathbf{r})^\dagger \hat{\chi}(\mathbf{r}) \left[ \psi_0^*(\mathbf{r})\hat{\vartheta}(\mathbf{r}) + \psi_0(\mathbf{r})\hat{\vartheta}^\dagger(\mathbf{r}) \right].
$$

(4.27)

We note that now $\hat{H}_{GP}$ contains the density operator $\hat{\chi}^\dagger(\mathbf{r})\hat{\chi}(\mathbf{r})$ instead of $\rho_{\chi}(\mathbf{r})$ in order to take into account the full dynamics of the impurities. The expansion of $\hat{\vartheta}(\mathbf{r})$ in terms of Bogoliubov modes reads

$$
\hat{\vartheta}(\mathbf{r}) = \sum_\nu \left[ u_\nu(\mathbf{r})\hat{b}_\nu + v_\nu^*(\mathbf{r})\hat{b}_\nu^\dagger \right],
$$

(4.28)

where the spectrum $\hbar\omega_\nu$ and coefficients $u_\nu(\mathbf{r})$ and $v_\nu(\mathbf{r})$ are determined by Eqs. (4.21). The bosonic operators $\hat{b}_\nu^\dagger$ ($\hat{b}_\nu$) create (annihilate) a Bogoliubov excitation around the ground state of the condensate $\psi_0(\mathbf{r})$ in absence of impurities, and thus, importantly, do not annihilate the vacuum $|\text{vac}\rangle$ defined in the previous section, i.e. $\hat{b}_\nu |\text{vac}\rangle \neq 0$. By substituting the expansion in Eq. (4.28) for $\hat{\vartheta}(\mathbf{r})$ in the Hamiltonian $\hat{H}_{GP}$ and using the identity $\hat{\chi}^\dagger(\mathbf{r})\hat{\chi}(\mathbf{r}) = \sum_{i,j} \chi_i^*(\mathbf{r})\chi_j(\mathbf{r})\hat{a}_i^\dagger\hat{a}_j$ we find that up to constant terms\(^1\)

$$
\hat{H}_{\psi_0} = \sum_{i,j} \tilde{\mathcal{E}}_{i,j} \hat{a}_i^\dagger\hat{a}_j,
$$

(4.29)

\(^1\)As for $\hat{H}_\xi$, the details of establishing the above form of $\hat{H}_\theta$ are contained in Ref. [123].
\[ \hat{H}_\theta = \sum_\nu \hbar \omega_\nu \hat{b}_\nu \hat{b}_\nu, \]  
\[ \hat{H}_{\text{lin}} = \sum_{i,j,\nu} \hbar \omega_\nu \left[ M_{i,j,\nu} \hat{b}_\nu + M_{i,j,\nu}^* \hat{b}_\nu^\dagger \right] \hat{a}_i^\dagger \hat{a}_j, \]  
with the matrix elements
\[ \bar{E}_{i,j} = \kappa \int dr \, n_0(r) \chi_i^*(r) \chi_j(r), \]
\[ M_{i,j,\nu} = \frac{\kappa}{\hbar \omega_\nu} \int dr \, \psi_0(r) \left[ u_\nu(r) + v_\nu(r) \right] \chi_i^*(r) \chi_j(r), \]
where we assumed for simplicity that \( \psi_0(r) \) is real. The non-local couplings \( M_{i,j,\nu} \) and \( \bar{E}_{i,j} \) with \( i \neq j \) resulting from the off-diagonal elements in \( \chi_i^*(r) \chi_j(r) \) are highly suppressed because the product of two mode-functions \( \chi_i(r) \) and \( \chi_j(r) \) with \( i \neq j \) is exponentially small. As a consequence, the evolution of the BEC and the impurities, including the full impurity Hamiltonian \( \hat{H}_\chi \), is accurately described by the Hubbard–Holstein Hamiltonian \[ \hat{H}_\text{hol} = \hat{H}_\chi + \sum_{j,\nu} \hbar \omega_\nu \left[ M_{j,\nu} \hat{b}_\nu + M_{j,\nu}^* \hat{b}_\nu^\dagger \right] \hat{n}_j + \sum_j \bar{E}_j \hat{n}_j + \sum_\nu \hbar \omega_\nu \hat{b}_\nu^\dagger \hat{b}_\nu, \]  
where we discarded the non-local couplings and introduced \( \bar{E}_j = \bar{E}_{j,j} \) and \( M_{j,\nu} = M_{j,j,\nu} \).

Since we intend to treat the dynamics of the impurities as a perturbation we shift the operators \( \hat{b}_\nu \) and \( \hat{b}_\nu^\dagger \) in such a way that \( \hat{H}_\text{hol} \) in Eq. (4.34) is diagonal, i.e. the total energy of the system is exactly minimized, for the case \( J = 0 \). This is achieved by the unitary Lang–Firsov transformation [28, 124]
\[ \hat{U} = \exp \left[ \sum_{j,\nu} \left( M_{j,\nu}^* \hat{b}_\nu^\dagger - M_{j,\nu} \hat{b}_\nu \right) \hat{n}_j \right], \]
from which it follows that by applying the Baker–Campbell–Hausdorff formula [132] \( \hat{U} \hat{b}_\nu^\dagger \hat{U}^\dagger = \hat{b}_\nu^\dagger - M_{j,\nu} \hat{n}_j \), \( \hat{U} \hat{n}_j \hat{U}^\dagger = \hat{n}_j \) and \( \hat{U} \hat{a}_j^\dagger \hat{U}^\dagger = \hat{a}_j^\dagger \hat{X}_j^\dagger \), with
\[
\hat{X}_j^\dagger = \exp \left[ \sum_\nu \left( M_{j,\nu}^* \hat{b}_\nu^\dagger - M_{j,\nu} \hat{b}_\nu \right) \right]. \tag{4.36}
\]

The operator \( \hat{X}_j^\dagger \) is the sought after displacement operator that creates a coherent state of Bogoliubov quasi-particles, i.e. a condensate deformation around the impurity. As a result, the transformed Hamiltonian \( \hat{H}_{LF} = \hat{U} \hat{H}_{hol} \hat{U}^\dagger \) is given by
\[
\hat{H}_{LF} = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i \dagger)(\hat{X}_j \hat{a}_j \dagger) + \frac{1}{2} \sum_j \hat{U}_j \hat{n}_j (\hat{n}_j - 1) + \sum_j \hat{\mu}_j \hat{n}_j
+ \hbar \omega_B \sum_j j \hat{n}_j - \frac{1}{2} \sum_{i \neq j} V_{i,j} \hat{n}_i \hat{n}_j + \sum_\nu \hbar \omega_\nu \hat{b}_\nu^\dagger \hat{b}_\nu, \tag{4.37}
\]
with the effective energy offset \( \hat{\mu}_j = \mu_a + \hat{E}_j - E_j \), the effective on-site interaction strength \( \hat{U}_j = U - 2E_j \), the interaction potential \( V_{i,j} = \sum_\nu \hbar \omega_\nu (M_{i,\nu}^* M_{j,\nu} + M_{i,\nu}^* M_{j,\nu}) \), and \( E_j = \frac{1}{2} V_{j,j} \) the so-called polaronic level shift [28, 124].

In the case of static impurities and, more generally, in the limit \( \zeta = J/E_j \ll 1 \), the polarons created by \( \hat{a}_j^\dagger \hat{X}_j^\dagger \) are the appropriate quasi-particles. Consequently, the Hamiltonian in Eq. (4.37) describes the dynamics of hopping polarons according to an extended Hubbard model [99, 125] with a non-retarded interaction potential \( V_{i,j} \). The contributions to \( \hat{H}_{LF} \) are qualitatively the same as for static impurities, except for the additional hopping term. In the thermodynamic limit, the interaction potential \( V_{i,j} \) and the polaronic level shift \( E_j \) are identical, respectively, to their GP counterparts \( V_{i,j} \) and \( \mathcal{E}_j \). The reason for the simple connection between GP theory and small polaron results is that both involve a linearization of the equations describing the condensate. It should be noted that
the interaction potential $V_{i,j}$ and the polaronic level shift $E_j$ can also be obtained exactly from $\hat{H}_{\text{hol}}$ by applying standard Rayleigh–Schrödinger perturbation theory up to second order in $\kappa$ since all higher order terms vanish. However, the merit of using the Lang–Firsov transformation lies in the fact that it yields a true many-body description of the state of the system, which would require a summation of perturbation terms to all orders in $\kappa$ [133].

We gain qualitative and quantitative insight into the dependence of the quantities in Eq. (4.37) on the system parameters by considering the specific case of a homogeneous BEC with the total Hamiltonian

$$\hat{H}_{LF} = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i) (\hat{X}_j \hat{a}_j) + \frac{1}{2} \hat{U} \sum_j \hat{n}_j (\hat{n}_j - 1) + \mu \sum_j \hat{n}_j + \hbar \omega_B \sum_j \hat{n}_j - \frac{1}{2} \sum_{i \neq j} V_{i,j} \hat{n}_i \hat{n}_j + \sum_q \hbar \omega_{aq} \hat{b}_{aq} \hat{b}_{aq},$$  \hfill (4.38)

with the energy offset $\tilde{\mu} = \mu_a + \kappa n_0 - E_p$, the on-site interaction strength $\tilde{U} = U - 2E_p$, the polaronic level shift $E_j \equiv E_p$ and the phonon momentum $q$. For a homogeneous BEC the Bogoliubov coefficients are of the form $u_q(r) = u_q \exp(iq \cdot r)$ and $v_q(r) = v_q \exp(iq \cdot r)$ with [30, 123]

$$u_q = \frac{1}{\sqrt{2\Omega}} \left( \varepsilon_q + \frac{gn_0}{\hbar \omega_q} + 1 \right)^{1/2} \quad \text{and} \quad v_q = -\frac{1}{\sqrt{2\Omega}} \left( \varepsilon_q + \frac{gn_0}{\hbar \omega_q} - 1 \right)^{1/2}. \hfill (4.39)$$

Here, $\varepsilon_q = (h^2q^2)/2m_b$ is the free particle energy, $\hbar \omega_q = \sqrt{\varepsilon_q (\varepsilon_q + 2gn_0)}$ is the Bogoliubov dispersion relation and $\Omega$ is the quantization volume. The corresponding matrix elements are found to be

$$M_{j,q} = \kappa \sqrt{\frac{n_0 \varepsilon_q}{(\hbar \omega_q)^3} f_j(q)}, \hfill (4.40)$$
4.4. Hopping impurities in the polaron picture

Figure 4.3. (a) The function $-G_{3D}(r, \sigma)$ plotted versus $r$ for $\sigma/\xi = 0.1$ (solid line), $\sigma/\xi = 0.15$ (dashed line), $\sigma/\xi = 0.2$ (dotted line). The potential $V(r) \propto G_{3D}(r, \sigma)$ falls off on a scale set by $\xi$ and has an increasing depth $V(0)$ with decreasing $\sigma$. (b) The function $-G(0, \sigma)$ plotted versus $\sigma$ for 3D (solid line), 2D (dashed line) and 1D (dotted line). The depth of the potential $V(0) \propto G(0, \sigma)$ and $E_p = \frac{1}{2}V(0)$ depend strongly on $\sigma$ in 3D and only weakly in 2D and 1D. The relevant range of $\sigma$ can be estimated for deep lattices by $\sigma/\xi \approx (a/\xi)/[\pi(V_{l}/E_{R})^{1/4}]$.

where

$$f_j(q) = \frac{1}{\sqrt{\Omega}} \int dr |\chi_j(r)|^2 \exp(iq \cdot r). \quad (4.41)$$

For the Gaussian mode-function $\chi_{3,\sigma}(r)$ in Eq. (4.4) the factor $f_j(q)$ takes the simple form

$$f_j(q) = \frac{1}{\sqrt{\Omega}} \prod_\ell \exp\left(-\frac{q_\ell^2 \sigma_\ell^2}{4}\right) \exp(iq \cdot r_j). \quad (4.42)$$

The $q$-dependence of the impurity–phonon coupling is $M_{j,q} \propto f_j(q)/\sqrt{|q|}$ in the long wavelength limit $|q| \ll 1/\xi$, which corresponds to a coupling to acoustic phonons in a solid state system [28], whereas in the free particle regime $|q| \gg 1/\xi$ we have $M_{j,q} \propto f_j(q)/q^2$.

The potential $V_{i,j}$ and the polaronic level shift $E_p$ reduce to a sum over all momenta $q$ and can be evaluated in the thermodynamic limit $\Omega^{-1} \sum_q \rightarrow (2\pi)^{-D} \int dq$
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where \( V_{i,j} \rightarrow \mathcal{V}_{i,j} \). In particular, for the Gaussian mode-functions \( \chi_{j, \sigma}(r) \) one finds

\[
\mathcal{V}_{i,j} = \frac{2\kappa^2}{g \xi B} G(r_i - r_j, \sigma), \tag{4.43}
\]

where the functions \( G(r, \sigma) \) are defined in 4.7 and plotted in Fig. 4.3a for a three-dimensional system. It follows from the definition of \( G(r, 0) \) that \( \mathcal{G}(r) \equiv G(r, 0) \), and hence the shape of the potential is determined by the Green’s function \( \mathcal{G}(r) \) in the limit \( \sigma \ll \xi \). The \( \sigma \)-dependence of \( G(0, \sigma) \), which determines the depth of the interaction potential \( \mathcal{V}_{i,j} \) and the level shift \( E_p = \frac{1}{2} \mathcal{V}_{j,j} \), is shown in Fig. 4.3b.

The range of the potential, characterized by the healing length \( \xi \), is comparable to the lattice spacing \( a \) for realistic experimental parameters, and hence the off-site terms \( \mathcal{V}_{j,j+1} \) are non-negligible. In particular, as shown in [122, 134], the off-site interactions can lead to the aggregation of polarons on adjacent lattice sites into stable clusters, which are not prone to loss from three-body inelastic collisions.

### 4.5 Transport

The coupling to the Bogoliubov phonons via the operators \( \hat{X}_j^\dagger \) and \( \hat{X}_j \) changes the transport properties of the impurities notably. Since we assume the filling factor of the lattice to be much lower than one we can investigate the transport properties by considering a single polaron with the Hamiltonian \( \hat{h}_0 + \hat{h}_I \) given by

\[
\hat{h}_0 = \hbar \omega_B \sum_j j \hat{n}_j + \sum_q \hbar \omega_q \hat{b}_q^\dagger \hat{b}_q, \tag{4.44}
\]

\[
\hat{h}_I = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i^\dagger)(\hat{X}_j \hat{a}_j). \tag{4.45}
\]

To start we investigate the crossover from coherent to diffusive hopping [28, 105] in a non-tilted lattice (\( \omega_B = 0 \)) and then extend the result to a tilted lattice (\( \omega_B \neq 0 \))
to demonstrate the emergence of a net atomic current across the lattice [55] due to energy dissipation into the BEC.

4.5.1 Coherent versus incoherent transport

We first consider coherent hopping of polarons at small BEC temperatures $k_B T \ll E_p$, where incoherent phonon scattering is highly suppressed. In the strong-coupling regime $\zeta = J/E_j \ll 1$, and hence the hopping term in Eq. (4.45) can be treated as a perturbation. The degeneracy of the Wannier states requires a change into the Bloch basis

$$ |k\rangle = \frac{1}{\sqrt{N}} \sum_j \exp(\mathbf{i} \mathbf{k} \cdot \mathbf{r}_j) \hat{a}_j^\dagger |0\rangle, \quad (4.46) $$

with $\mathbf{k}$ the quasi-momentum and $N$ the number of lattice sites. Applying standard perturbation theory in the Bloch basis and describing the state of the system by $|k, \{N_q\}\rangle$, where $\{N_q\}$ is the phonon configuration with phonon occupation numbers $N_q$, we find the polaron energy up to first order in $\zeta$

$$ E(k) = \tilde{\mu}_a - 2 \tilde{J} \cos(\mathbf{k} \cdot \mathbf{a}), \quad (4.47) $$

where we defined the effective hopping $\tilde{J} = J \sum_q \langle N_q | \hat{X}_j^\dagger \hat{X}_{j+1} | N_q \rangle$ and $\mathbf{a}$ is the position vector connecting two nearest neighbor sites. In particular, for the case of a thermal phonon distribution with occupation numbers $N_q = (e^{\hbar \omega_q / k_B T} - 1)^{-1}$ the effective hopping is [28, 105, 124]

$$ \tilde{J} = J \exp \left\{ - \sum_{\mathbf{q} \neq 0} |M_{0,q}|^2 \left[ 1 - \cos(\mathbf{q} \cdot \mathbf{a}) \right] (2N_q + 1) \right\}. \quad (4.48) $$

Thus, the hopping bandwidth of the polaron band is highly suppressed with increasing coupling $\kappa$ and temperature $T$. 
Figure 4.4. Coherent and diffusive hopping in a one-dimensional system: (a) The memory function $\tilde{W}_{i,j}(t)/(2J^2)$ plotted versus time for $k_B T = 0$ (dotted line), $k_B T = 5E_p$ (dashed line) and $k_B T = 15E_p$ (solid line). The memory function drops off rapidly for $k_B T \gg E_p$, indicating the dominance of incoherent hopping. (b) – (d) The evolution of the occupation probabilities $P_j(t)$ of a single impurity initially localized at site $j = 0$ according to the GME with the memory functions in (a). (b) For small temperatures $k_B T \ll E_p$ the hopping is coherent with two wave-packets moving away from $j = 0$. (d) For high temperatures $k_B T \gg E_p$ the inelastic scattering of phonons results in a diffusive motion of the impurity, where the probability $P_j(t)$ remains peaked at $j = 0$. The lattice with spacing $a = 395\text{nm}$ and $J = 2.45 \times 10^{-2}E_R$ contains a single $^{41}\text{K}$ atom. The BEC with $d = 200\text{nm}$ and $\xi = 652\text{nm}$ consists of $^{87}\text{Rb}$ atoms; $\kappa/g = 2.58$, $E_p/k_B \approx 10\text{nK}$ and $J/\hbar \approx 1.2\text{kHz}$.
At high temperatures $E_p \ll k_B T \ll k_B T_c$ inelastic scattering, in which phonons are emitted and absorbed, becomes dominant, and thus the transport of impurities through the lattice changes from being purely coherent to incoherent. While matrix elements $\langle \{N_q\} | \hat{X}_j^\dagger \hat{X}_{j+1} | \{N_q\}' \rangle$ involving two different phonon configurations $\{N_q\}$ and $\{N_q\}'$ vanish at zero temperature they can take non-zero values for $T > 0$. The condition for energy and momentum conservation during a hopping event implies that incoherent hopping is dominated by a three-phonon process that involves phonons with a linear dispersion $\hbar \omega_q = \hbar c |q|$, where $c \sim \sqrt{gn_0/m_b}$ is the speed of sound. This process is reminiscent of the well-known Beliaev decay of phonons [30].

We investigate the incoherent transport properties by using a generalized master equation (GME) [126] for the site occupation probabilities $P_j(t)$ of the impurity. This formalism has been applied to the transfer of excitons in the presence of electron–phonon coupling [109, 127] and is based on the Nakajima–Zwanzig projection method [128]. The generalized master equation is of the form

$$\frac{\partial P_j(t)}{\partial t} = \int_0^t ds \sum_i W_{i,j}(s) [P_j(t - s) - P_i(t - s)], \quad (4.49)$$

where the effect of the condensate is encoded in the memory functions $W_{i,j}(s)$. As shown in 4.8 the memory function to second order in $\zeta$ is given by

$$W_{i,j}(s) = 2\delta_{j,i\pm 1} \left(\frac{J}{\hbar}\right)^2 \Re \left[ \exp \left\{ -2 \sum_{q \neq 0} |M_{0,q}|^2 [1 - \cos(q \cdot a)] \right\} \times \left[ (N_q + 1)(1 - e^{i\omega_q s}) + N_q(1 - e^{-i\omega_q s}) \right] \exp(\pm i\omega_B s) \right]. \quad (4.50)$$

In the case $\omega_B = 0$, the nontrivial part of $W_{i,j}(s)$ takes the values $2(J/\hbar)^2$ at $s = 0$ and $2(\tilde{J}/\hbar)^2$ in the limit $s \to \infty$ due to the cancellation of highly oscillating terms,
as shown in Fig. 4.4a.

In the regime \( k_B T \ll E_p \), the effective hopping \( \tilde{J} \) is comparable to \( J \) and the memory function \( W_{i,j} \) is well approximated by \( 2(\tilde{J}/\hbar)^2 \Theta(s) \), with \( \Theta(s) \) the Heaviside step function, and thus describes purely coherent hopping. In the regime \( E_p \ll k_B T \ll k_B T_c \), processes involving thermal phonons become dominant and coherent hopping is highly suppressed, i.e. \( \tilde{J} \ll J \). In this case the memory function \( W_{i,j} \) drops off sufficiently fast for the Markov approximation to be valid, as illustrated in Fig. 4.4a. More precisely, one can replace \( P_j(t-s) \) by \( P_j(t) \) in Eq. (4.49) and after intergration over \( s \) the GME reduces to the standard Pauli master equation

\[
\frac{\partial P_i(t)}{\partial t} = \sum_j w_{i,j} \left[ P_j(t) - P_i(t) \right],
\]

where the hopping rates \( w_{i,j} \) are given by

\[
w_{i,j} = \int_0^\infty ds \left[ W_{i,j}(s) - \lim_{t\to\infty} W_{i,j}(t) \right].
\]

The Pauli master equation describes purely incoherent hopping with a thermally activated hopping rate \( w_{i,j} \) [28, 105].

The evolution of an initially localized impurity at different temperatures \( T \) for a one-dimensional \( ^{41}\text{K} - ^{87}\text{Rb} \) system [20] is shown in Figs. 4.4b – 4.4d, which were obtained by numerically solving the GME with the memory function \( W_{i,j}(s) \) in Eq. (4.50). It can be seen that for small temperatures \( k_B T \ll E_p \) the hopping is coherent with two wave-packets moving away from the initial position of the impurity atom. In contrast, for high temperatures \( k_B T \gg E_p \) inelastic scattering of phonons results in a diffusive motion of the impurity, where the probability \( P_j(t) \) remains peaked at the initial position of the impurity.

This crossover from coherent to diffusive hopping can be quantitatively an-
Figure 4.5. Analysis of the mean-square displacement $l^2(t) = \sum_l l^2 P_l(t)$, obtained from the evolution of an initially localized impurity in a one-dimensional system for the time $t_{\text{evol}} = 10 \hbar/J$ according to the GME. The mean-squared displacement was assumed to be of the form $l^2(t) = A t^\alpha$. (a) The exponent $\alpha$ versus temperature $T$ for the full evolution time (solid line) and the period $t_{\text{evol}}/2$ to $t_{\text{evol}}$ (dashed line). The drop from $\alpha \approx 2$ at zero temperature to $\alpha \approx 1$ at high temperatures $k_B T \gg E_p$ clearly indicates the crossover from coherent to diffusive transport. (b) The prefactor $A$ in units of $(J/\hbar)^\alpha$ versus temperature $T$ for the full evolution time (solid line) and the period $t_{\text{evol}}/2$ to $t_{\text{evol}}$ (dashed line). The system parameters are the same as for Fig. 4.4.

analyzed by considering the mean-squared displacement of the impurity, $l^2(t) = \sum_l l^2 P_l(t)$, which we assume to be of the form $l^2(t) = A t^\alpha$. The exponent $\alpha$ takes the value $\alpha = 2$ for a purely coherent process, whereas $\alpha = 1$ for diffusive hopping. Figure (4.5) shows $\alpha$ and $A$ in units of $(J/\hbar)^\alpha$ as functions of the BEC temperature $T$, which were obtained from the evolution (according to the GME) of an impurity initially localized at $j = 0$. We see that the exponent $\alpha$ drops from $\alpha \approx 2$ at zero temperature to $\alpha \approx 1$ at high temperatures $k_B T \gg E_p$, thereby clearly indicating the crossover from coherent to diffusive transport. We note that the transition from coherent to diffusive hopping takes place in a tempera-
ture regime accessible to experimental study and therefore, importantly, may be observable.

### 4.5.2 Atomic current across a tilted lattice

The inelastic phonon scattering responsible for the incoherent hopping of the impurities also provides the necessary relaxation process required for the emergence of a net atomic current across a tilted optical lattice. This is in contrast to coherent Bloch oscillations, which occur in an optical lattice system in absence of incoherent relaxation effects or dephasing [48]. As pointed out in [55], the dependence of the atomic current on the lattice tilt $\hbar \omega_B$ changes from ohmic conductance to NDC in agreement with the theoretical model for electron transport introduced by Esaki and Tsu [54].

To demonstrate the emergence of a net atomic current, and, in particular, to show that impurities exhibit NDC, we consider the evolution of a localized impurity atom in a one-dimensional system. With the impurity initially at site $j = 0$ we determine its average position $x_d = \sum_j a_j P_j(t_d)$ after a fixed drift time $t_d$ of the order of $\hbar / J$. This allows us to determine the drift velocity $v_d = x_d / t_d$ as a function of the lattice tilt $\hbar \omega_B$ and the temperature $T$ of the BEC. In analogy with a solid state system, the drift velocity $v_d$ and the lattice tilt $\hbar \omega_B$ correspond to the current and voltage, respectively.

Figure 4.6a shows the voltage–current relation at different temperatures $T$, which was obtained by numerically solving the GME with the memory function in Eq. (4.50). We see that for a small lattice tilt the system exhibits ohmic behavior $v_d \sim \hbar \omega_B$, whereas for a large lattice tilt the current decreases with increasing voltage as $v_d \sim 1/(\hbar \omega_B)$, i.e. the impurities feature NDC.

Following [55] we describe the voltage–current relation for the impurities by
4.5. Transport

The drift velocity $v_d$ in units of $v_0 = J \alpha / \hbar$ as a function of the lattice tilt $\hbar \omega_B / J$ for temperatures $k_B T = 0$ (+), $k_B T = 5 E_p$ (○) and $k_B T = 15 E_p$ (×) according to the GME and the best fit of the Esaki–Tsu-type relation in Eq. (4.53) (dotted lines). The dependence of the current on the tilt changes from ohmic conductance $v_d \sim \hbar \omega_B$ to negative differential conductance $v_d \sim 1 / (\hbar \omega_B)$. (b) The relaxation time $\tau$ (+) in units of $\tau_0 = \hbar / g \mu_0$ and the prefactor $\gamma$ (+) yielding the best fit of the Esaki–Tsu-type relation to the numerical results. The relaxation time $\tau$ of the impurities decreases with increasing BEC temperature $T$ and the prefactor $\gamma$ varies only slightly since the exponential temperature dependence of the current is accounted for by $\tilde{v}_0$. The system parameters are the same as for Fig. 4.4.

an Esaki–Tsu-type relation

$$v_d = 2 \gamma \tilde{v}_0 \frac{\omega_B \tau}{1 + (\omega_B \tau)^2},$$  \hspace{1cm} (4.53)

where $\tilde{v}_0 = \tilde{J} \alpha / \hbar$ the characteristic drift velocity, $\tau$ the effective relaxation time of the impurities and $\gamma$ a dimensionless prefactor. Fitting the Esaki–Tsu-type relation in Eq. (4.53) to the numerical data allows us to extract the parameters $\tau$ and $\gamma$, both depending on the BEC temperature. As can be seen in Fig. 4.6b, the
effective relaxation time $\tau$ decreases with increasing BEC temperature $T$ and is of the order of $\tau_0 = \hbar/(g n_0)$. The significance of $1/\tau$ is that of an average collision rate between the impurities and Bogoliubov excitations, which would allow us, for example, to formulate the problem of transport in terms of a classical Boltzmann equation for the distribution function of the impurities [28]. The prefactor $\gamma$ varies only slightly since the exponential dependence of the current on the temperature is accounted for by $\tilde{v}_0$. We note that independently of $\omega_B\tau$ the maximum drift velocity is given by $\gamma \tilde{v}_0$.

The Esaki–Tsu-type relation in Eq. (4.53) reflects the competition between coherent and incoherent, dissipative processes. In the collision dominated regime $\omega_B\tau \ll 1$, inelastic scattering with phonons destroys Bloch oscillations, whereas in the collisionless regime $\omega_B\tau \gg 1$ the evolution of the impurities is mainly coherent, i.e. Bloch oscillations of the impurities lead to a suppression of the net current. The crossover between the two regimes is most pronounced at zero temperature, where $\tilde{J}$ is comparable to $J$. However, the change from ohmic to negative differential conductance is identifiable even at finite temperatures and thus should be observable in an experimental setup similar to the one used in [53].

4.6 Conclusion

We have studied the transport of impurity atoms in the strong-coupling regime, where the interaction energy due to the coupling between the BEC and the impurities dominates their dynamics. Within this regime, we have formulated an extended Hubbard model describing the impurities in terms of polarons, i.e. impurities dressed by a coherent state of Bogoliubov phonons. The model accommodates hopping of polarons and the effective off-site impurity–impurity interaction mediated by the BEC.
4.6. Conclusion

Based on the extended Hubbard model we have shown from first principles that inelastic phonon scattering results in a crossover from coherent to incoherent hopping and leads to the emergence of a net atomic current across a tilted optical lattice. In particular, we have found that the dependence of the current on the lattice tilt changes from ohmic conductance to negative differential conductance for sufficiently low BEC temperatures. Notably, this transition is accurately described by an Esaki–Tsu-type relation with the effective relaxation time of the impurities as a temperature-dependent parameter.

Using the techniques introduced in this paper, qualitatively similar phenomena can also be shown to occur for fermionic impurities and, moreover, for impurities of different species [135]. For instance, in the case of two impurity species A and B with the couplings $\kappa_A > 0$ and $\kappa_B < 0$, respectively, the effective off-site impurity–impurity interaction is attractive for the same species, but repulsive for different species. In either case, observation of the phenomena reported in this paper lies within the reach of current experiments, which may give new insight into the interplay between coherent, incoherent and dissipative processes in many-body systems.

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4.7 Appendix A. Definition of the functions $G(r, \sigma)$

The function $G(r, \sigma)$, which are a generalization of the Green’s functions $G(r)$ for $\sigma > 0$, are defined by

$$G_{1D}(r, \sigma) = \frac{1}{\pi} \int_{-\infty}^{\infty} dy \frac{\cos(y|r|/\xi)}{y^2 + 4} \exp \left[ -\frac{1}{2} y^2 \left( \frac{\sigma}{\xi} \right)^2 \right], \quad (4.54)$$

$$G_{2D}(r, \sigma) = \frac{1}{\pi} \int_{0}^{\infty} dy \frac{J_0(y|r|/\xi)}{y^2 + 4} \exp \left[ -\frac{1}{2} y^2 \left( \frac{\sigma}{\xi} \right)^2 \right], \quad (4.55)$$

where $J_0(x)$ is the Bessel function of the first kind.

$$G_{3D}(r, \sigma) = \frac{1}{\pi^2} \int_{0}^{\infty} dy y^2 \frac{j_0(y|r|/\xi)}{y^2 + 4} \exp \left[ -\frac{1}{2} y^2 \left( \frac{\sigma}{\xi} \right)^2 \right], \quad (4.56)$$

where $j_0(x) = \sin(x)/x$ is the spherical Bessel function of the first kind. For the special case $r = 0$ we have with $z = \sqrt{2} \sigma/\xi$

$$G_{1D}(0, \sigma) = \frac{1}{2} \exp(z^2) \text{erfc}(z) \quad (4.57)$$

$$G_{2D}(0, \sigma) = -\frac{1}{2\pi} \exp(z^2) \text{Ei}(-z^2) \quad (4.58)$$

$$G_{3D}(0, \sigma) = \frac{1}{\pi} \left[ \frac{1}{\sqrt{\pi z}} - \exp(z^2) \text{erfc}(z) \right] \quad (4.59)$$

where erfc$(x)$ is the complementary error function and Ei$(x)$ is the exponential integral [136].
4.8 Appendix B. Derivation of the GME

The Hamiltonian for the single impurity and the BEC is

\[
\hat{h}_0 = \hbar \omega_B \sum_j \hat{n}_j + \sum_q \hbar \omega_q \hat{b}_q^\dagger \hat{b}_q
\]
\[
\hat{h}_I = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i)^\dagger (\hat{X}_j \hat{a}_j),
\]

where \( \hat{h}_0 \) is the unperturbed Hamiltonian and \( \hat{h}_I \) is treated as a perturbation in the strong-coupling regime \( \zeta \ll 1 \).

Starting point of the derivation of the GME is the Liouville–von Neumann equation [126]

\[
\frac{\partial \hat{\rho}(t)}{\partial t} = L \hat{\rho}(t),
\]

(4.60)

where \( \hat{\rho}(t) \) is the density matrix of the system expressed in the eigenbasis of \( \hat{h}_0 \). The Liouville operator \( L \) is defined by \( L = L_0 + L_I \), with \( L_0 = -i/\hbar [\hat{h}_0, \cdot \cdot \cdot] \) and \( L_I = -i/\hbar [\hat{h}_I, \cdot \cdot \cdot] \). The density matrix \( \hat{\rho}(t) \) is decomposed as \( \hat{\rho}(t) = \mathcal{P}\hat{\rho}(t) + \mathcal{Q}\hat{\rho}(t) \), where \( \mathcal{P} \) is the projection operator on the relevant part of \( \hat{\rho}(t) \) and \( \mathcal{Q} = 1 - \mathcal{P} \) the complementary projection operator to \( \mathcal{P} \). The time evolution of the relevant part \( \mathcal{P}\hat{\rho}(t) \) is governed by the Nakajima–Zwanzig equation [128]

\[
\frac{\partial \mathcal{P}\hat{\rho}(t)}{\partial t} = \mathcal{P}L\mathcal{P}\hat{\rho}(t) + \int_0^t ds \mathcal{P}\mathcal{L}\mathcal{P}\mathcal{L}_s\mathcal{Q}\mathcal{L}\mathcal{P}\hat{\rho}(t-s) + \mathcal{P}\mathcal{L}\mathcal{P}_{\mathcal{L}_0\mathcal{Q}}\hat{\rho}(0).
\]

(4.61)

Specifically, the projection operator \( \mathcal{P} \) employed in the derivation of the GME is defined by \( \mathcal{P}\hat{\rho}(t) = \hat{\rho}_B \otimes \mathcal{D}\mathcal{Tr}_B\hat{\rho}(t) \) [109, 126]. Here, \( \hat{\rho}_B \) is the density matrix of the condensate in thermal equilibrium, \( \mathcal{Tr}_B \) is the trace over the condensate degrees of freedom and \( \mathcal{D} \) is the projection operator on the diagonal part. Thus \( \hat{\rho}_A(t) = \mathcal{D}\mathcal{Tr}_B\hat{\rho}(t) \) is the diagonal part of the reduced density matrix. We note that the trace over the Bogoliubov phonon states in the definition of \( \mathcal{P} \) introduces
irreversibility into the system.

The Nakajima–Zwanzig equation can be simplified given that \( P L_0 = L_0 P = 0 \) and \( P L_I P = 0 \) for the definitions of \( L_0 \), \( L_I \) and \( P \) above. In addition, we assume that the initial density matrix of the total system has the form \( \hat{\rho}(0) = \hat{\rho}_B \otimes \hat{\rho}_A(0) \) so that \( Q\hat{\rho}(0) = 0 \), and hence the inhomogeneous term in Eq. (4.61) vanishes. Taking these simplification into account and using \( \text{Tr}_B P\hat{\rho} = \hat{\rho}_A \) we find from Eq. (4.61) that \( \hat{\rho}_A(t) \) evolves according to

\[
\frac{\partial}{\partial t} \hat{\rho}_A(t) = \int_0^t ds K(s) \hat{\rho}_A(t - s) \tag{4.62}
\]

with the memory kernel

\[
K(s) = D\text{Tr}_B \left[ L_I e^{L_0 s + Q L_I s} L_I \hat{\rho}_B(0) \right]. \tag{4.63}
\]

The memory kernel to second order in \( \zeta \), i.e. dropping \( L_I \) in the exponent in Eq. (4.63), can be expressed in tetradic form as [109, 128]

\[
K_{ii,jj}^0(s) = \frac{2}{\hbar^2} Z_B^{-1} \sum_{\{N_q\},\{N_q\}'} e^{-\hbar\omega_{\{N_q\}}/k_B T} |\langle i, \{N_q\}'|\hat{h}_I|j, \{N_q\}\rangle|^2 \\
\times \cos \left[(\Omega_{i,j} + \hbar\omega_{\{N_q\}}) t\right], \tag{4.64}
\]

with the partition function of the condensate

\[
Z_B = \sum_{\{N_q\}} e^{-\hbar\omega_{\{N_q\}}/k_B T}, \tag{4.65}
\]

and where \( \hbar\Omega_{i,j} \) is the energy difference between the impurity configurations \( i \) and \( j \), and \( \hbar\omega_{\{N_q\}} \) is the energy of the phonon configuration \( \{N_q\} \).

The explicit expression for the memory function \( W_{i,j}(s) = K_{ii,jj}^0(s) \) for the Hamiltonian \( \hat{h}_0 + \hat{h}_I \) has been evaluated in [109, 127] based on Eq. (4.63), however,
we here give an alternative derivation of \( W_{i,j}(s) \) starting from Eq. (4.64). The evaluation of \( K_{ii,jj}^{q}(s) \) in Eq. (4.64) can be separated into a phonon part and an impurity part, where the latter is given by

\[
J^2 \sum_k |\langle i| \hat{a}_k^\dagger \hat{a}_{k \pm 1}|j \rangle|^2 e^{-i\Omega_{i,j} t} = J^2 \delta_{j,j \pm 1} e^{\pm i\omega_B t}.
\] (4.66)

Thus, for the phonon part we only have to consider operators of the form \( \hat{X}_j^\dagger \hat{X}_{j \pm 1} \), which can be written in terms of displacement operators

\[
\hat{X}_j^\dagger \hat{X}_{j \pm 1} = \prod_q D(\beta_{j,q}) e^{i\Phi_{j,q}},
\] (4.67)

with \( \beta_{j,q} = M_{j,q}^* - M_{j \pm 1,q}^* \) and \( \Phi_{j,q} \) the corresponding phase. This allows us to treat each phonon mode in Eq. (4.64) separately, and the problem reduces to the summation

\[
\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} e^{-n\hbar\omega_q/k_B T} |\langle m| D(\beta_{j,q}) |n \rangle|^2 e^{i\omega_q t(m-n)},
\] (4.68)

where \( m \) and \( n \) are phonon occupation numbers of the mode \( \omega_q \). The matrix elements of the displacement operator in the Fock basis are [132]

\[
\langle m| D(\beta) |n \rangle = \sqrt{\frac{m!}{n!}} \beta^{m-n} e^{-|\beta|^2/2} L_{m-n}^{m-n}(|\beta|^2) \quad \text{for} \quad m \geq n
\]

\[
\langle m| D(\beta) |n \rangle = \sqrt{\frac{m!}{n!}} (-\beta)^{m-n} e^{-|\beta|^2/2} L_{m-n}^{m-n}(|\beta|^2) \quad \text{for} \quad n \geq m,
\] (4.69)

where \( L_n^k(x) \) are generalized Laguerre polynomials. At this point we introduce the new variables \( x = |\beta_{j,q}|^2, y = e^{i\omega_q t}, z = e^{-\hbar\omega_q/k_B T}, \) and \( l = m - n \). For the case \( m \geq n \), or equivalently \( l \geq 0 \), we find after the substitution of \( m = n + l \) that the sum in Eq. (4.68) becomes

\[
e^{-x} \sum_{l=0}^{\infty} (xy)^l \sum_{n=0}^{\infty} \frac{n!}{(n+l)!} [L_n^l(x)]^2 z^n.
\] (4.70)
To evaluate the sum over $n$ we use the fact that the following relation for generalized Laguerre polynomials holds [137]

$$
\sum_{n=0}^{\infty} \frac{L_n^\gamma(x)L_n^\gamma(y)z^n}{\Gamma(n+\gamma+1)} = \frac{(xyz)^{-\gamma/2}}{1-z} \exp\left(-z\frac{x+y}{1-z}\right) I_\gamma\left(2\sqrt{xyz}\right),
$$

(4.71)

provided that $|z| < 1$. Here, $\Gamma(x)$ is the Gamma function and $I_\gamma(x)$ are modified Bessel functions of the first kind. Using the relation in Eq. (4.71) we find that the sum over $n$ yields

$$
\frac{1}{1-z} \exp\left(-\frac{2xz}{1-z}\right) (x\sqrt{z})^{-l} I_l\left(2x\sqrt{z}\right).
$$

(4.72)

For the case $n \geq m$, or equivalently $l \leq 0$, we have to express $L_m^{n-m}(x)$ in terms of $L_m^{m-n}(x)$ in order to exploit Eq. (4.71). Using the relation

$$
L_{r-s}(x) = \frac{x^s}{(-r)^s} L_{r-s}^s(x),
$$

(4.73)

with $(x)_n = x(x+1)(x+2)\cdots(x+n-1)$ the Pochhammer symbol, we find that

$$
[L_m^{(m-n)}(x)]^2 = \frac{x^{2(m-n)}}{[(-m)_{(m-n)}]^2} [L_m^{m-n}(x)]^2,
$$

(4.74)

and since $[(-m)_{(m-n)}]^2 = [(-m)(-m+1)\cdots(-n-1)]^2 = (m!/n!)^2$ substituting $l = m - n$ in expression (4.68) yields

$$
e^{-x} \sum_{l=0}^{\infty} (xy)^l \sum_{n=0}^{\infty} \frac{n!}{(n+l)!} [L_n^l(x)]^2 z^n,
$$

(4.75)

which is identical to expression (4.70) except for the upper limit in the sum over $l$. Using relation (4.71) again and discarding the double counting of $l = 0$ we find
4.8. Appendix B. Derivation of the GME

that the total sum in Eq. (4.68) is given by

$$\frac{1}{1-z} \exp \left[ -x \left( 1 + \frac{2z}{1-z} \right) \right] \sum_{l=-\infty}^{\infty} \left( \frac{y}{\sqrt{z}} \right)^l I_l \left( \frac{2x\sqrt{z}}{1-z} \right). \quad (4.76)$$

To evaluate the sum over $l$ we use the identity [136]

$$\sum_{l=-\infty}^{\infty} I_l(x)t^l = \exp \left[ \frac{x}{2} \left( t + \frac{1}{t} \right) \right] \quad (4.77)$$

and find that Eq. (4.76) equals

$$\frac{1}{1-z} \exp \left[ -x \left( 1 + \frac{2z}{1-z} \right) \right] \exp \left[ \frac{x\sqrt{z}}{1-z} \left( \frac{y}{\sqrt{z}} + \frac{\sqrt{y}}{z} \right) \right], \quad (4.78)$$

which can be written as

$$Z_q \exp \left[ -|\beta_{j,q}|^2 \left( (N_q + 1)(1 - e^{i\omega q t}) + N_q(1 - e^{-i\omega q t}) \right) \right], \quad (4.79)$$

with $N_q = z/(1-z) = (e^{\omega_q/k_B T} - 1)^{-1}$ and $Z_q = 1/(1-z) = (1 - e^{-\omega_q/k_B T})^{-1}$. Taking the impurity part and the product of all phonon modes $q$ into account we find the complete memory function

$$W_{i,j}(s) = 2\delta_{j,i+1} \left( \frac{J}{\hbar} \right)^2 \Re \left[ \exp \left\{ -\sum_{q \neq 0} |\beta_{j,q}|^2 \right. \right.$$

$$\times \left. \left[ (N_q + 1)(1 - e^{i\omega q s}) + N_q(1 - e^{-i\omega q s}) \right] \right\} \exp(\pm i\omega_B t) \right], \quad (4.80)$$

where we used $Z_B = \prod_q Z_q$. 
4.9 Appendix C. Self-trapping

Impurities immersed in a BEC get self-trapped for sufficiently strong impurity–BEC interactions, even in the absence of an additional trapping potential [59, 60, 91]. Based on the results for static impurities in Section 4.3 we now show that for the parameter regime considered in this paper self-trapping effects can be neglected.

As pointed out by Gross [138] the coupled equations describing the impurity and the condensate in the Hartree approximation are given by

\[ \mu_b \psi(r) = -\frac{\hbar^2}{2m_b} \nabla^2 \psi(r) + g|\psi(r)|^2 \psi(r) + \kappa |\chi(r)|^2 \psi(r), \quad (4.81) \]

\[ \varepsilon \chi(r) = -\frac{\hbar^2}{2m_a} \nabla^2 \chi(r) + \kappa |\psi(r)|^2 \chi(r), \quad (4.82) \]

where \( \chi(r) \) is the wavefunction of the impurity, \( m_a \) is the impurity mass and \( \varepsilon \) the impurity energy. To determine whether the impurity localizes for given experimental parameters one has, in principle, to solve the coupled equations for \( \psi(r) \) and \( \chi(r) \) [91]. Alternatively, as suggested in [60], we use the Gaussian mode-function \( \chi_{j,\sigma}(r) \) in Eq. (4.4) as a variational wavefunction for the impurity, with the spread \( \sigma \) as a free parameter, and minimize the total energy of the system in the regime \( \alpha \ll 1 \), where the linearization of the GP equation is valid. For a homogenous condensate, the potential energy of the impurity and the BEC is \( -E_p \), and thus adding the kinetic energy of the impurity yields the total energy

\[ E(\sigma) = E_{\text{kin}}(\sigma) - E_p(\sigma) = \frac{D}{4} \frac{\hbar^2}{m_a \sigma^2} - \frac{\kappa^2}{g\xi D} G(0, \sigma). \quad (4.83) \]

The impurity localizes if \( E(\sigma) \) has a minimum for a finite value of \( \sigma \), which depends
on the dimensionless quantity

\[ \alpha' = \frac{|\kappa| m_a}{g m_b} \alpha \sim \frac{\mathcal{E}_p}{\mathcal{E}_{\text{kin}}}. \]  

(4.84)

In one dimension, we find by asymptotically expanding \( \mathcal{E}(\sigma) \) in the limit \( \sigma/\xi \gg 1 \) that there exists a self-trapping solution for arbitrarily small \( \alpha' \) and that

\[ \sigma_{1D} = \sqrt{2\pi} \frac{\xi}{\alpha'}. \]  

(4.85)

For the two-dimensional case, asymptotically expanding \( \mathcal{E}(\sigma) \) in the limit \( \sigma/\xi \gg 1 \) yields a critical value \( \alpha'_c = 2\pi \), above which self-trapping occurs. The corresponding spread of the self-trapping solution \( \sigma_{2D} \) diverges close to \( \alpha'_c \), which validates the asymptotic expansion of \( \mathcal{E}(\sigma) \). In three dimensions, numerical minimization of \( \mathcal{E}(\sigma) \) shows that the critical value is \( \alpha'_c \approx 31.7 \), and the corresponding self-trapped state is highly localized with \( \sigma_{3D} \approx 0.87 \xi \).

According to Eq. (4.85) the spread of the self-trapping solution exceeds several lattice spacings for the parameter regime considered in this paper. In other words, the spread \( \sigma_{1D} \) is much larger than the harmonic oscillator length \( \sigma_\ell \) in practice, and hence self-trapping effects are indeed small.
Chapter 5

Self-trapping of an impurity in a Bose–Einstein condensate: Strong attractive and repulsive coupling

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We study the interaction-induced localization — the so-called self-trapping — of a neutral impurity atom immersed in a homogeneous Bose–Einstein condensate (BEC). Based on a Hartree description of the BEC we show that — unlike repulsive impurities — attractive impurities have a singular ground state in 3d and shrink to a point-like state in 2d as the coupling approaches a critical value \( \beta^* \). Moreover, we find that the density of the BEC increases markedly in the vicinity of attractive impurities in 1d and 2d, which strongly enhances inelastic collisions between atoms in the BEC. These collisions result in a loss of BEC atoms and possibly of the localized impurity itself.
5.1 Introduction

Impurities immersed in liquid helium have proven to be a valuable tool for probing the structure and dynamics of a Bose-condensed fluid [29]. An example is the use of impurities for the direct visualization of quantized vortices in superfluid $^4$He [139]. Recently, the experimental realization of impurities in a BEC [113, 114] and the possibility to produce quantum degenerate atomic mixtures [22, 23] have generated renewed interest in the physics of impurities. In particular, it was pointed out that single atoms can get trapped in the localized distortion of the BEC that is induced by the impurity–BEC interaction [59, 60, 91, 103, 140]. More precisely, the impurity becomes self-trapped if its interaction with the BEC is sufficiently strong to compensate for the high kinetic energy of a localized state, an effect akin to the self-trapping of impurities in liquid helium [29].

However, there are two fundamental differences between liquid helium and a BEC. First, for typical experimental parameters the healing length of a BEC is three orders of magnitude larger than for liquid helium [34], and thus the so-called 'bubble' model [141] cannot be applied. A second important difference is that the impurity–BEC interactions are tunable by an external magnetic field in the vicinity of Feshbach resonances [27, 142]. In view of recent experimental progress [1] it thus seems possible to investigate the self-trapping problem in the same physical system over a wide range of interaction strengths — for both attractive and repulsive impurities.

In the present paper we study the self-trapping properties of impurities for strong attractive and repulsive impurity–BEC coupling within the framework of a Hartree description of the BEC. This necessitates the use of an essentially non-perturbative approach, which is in contrast to previous analytical studies [59, 60, 103] where the effect of the impurities on the BEC was treated as
a small perturbation. We first consider the effect of a highly localized $\delta$-impurity on the BEC in one dimension. This approach indicates that the density of the BEC is substantially increased in the vicinity of an attractive impurity, which enhances inelastic collisions and may result in the loss of the impurity atom. In addition, we bring forward a scaling argument to show that attractive impurity–BEC interactions can lead to a point-like ground state of the impurity in 2d and 3d. Specifically, the ground state is singular for arbitrarily small attractive coupling in 3d, which seemingly contradicts the known perturbative results. Finally, in order to extend our analytical findings we present numerical results stemming from the exact solutions for the ground state of the system, where unlike in previous numerical studies [91, 140] neither the impurity nor the BEC are subject to an external trapping potential.

Our analysis of the self-trapping problem is based on the model suggested by Gross [29, 138] describing the impurity wave-function $\chi(x, t)$ interacting with the condensate wave-function $\psi(x, t)$ in the Hartree approximation. The model is given by the coupled equations

\begin{align}
    i\hbar \partial_t \psi &= -\frac{\hbar^2}{2m_b} \nabla^2 \psi + \kappa |\chi|^2 \psi + g|\psi|^2 \psi, \\
    i\hbar \partial_t \chi &= -\frac{\hbar^2}{2m_a} \nabla^2 \chi + \kappa |\psi|^2 \chi,
\end{align}

where the impurity–BEC interaction and the repulsive interaction among the BEC atoms have been approximated by the contact potentials $\kappa \delta(x - x')$ and $g\delta(x - x')$, respectively. Here, $m_a$ is the mass of the impurity, $m_b$ is the mass of a boson in the BEC and the coupling constants $\kappa$ and $g > 0$ depend on the respective s-wave scattering lengths [143, 144]. The functions $\psi(x, t)$ and $\chi(x, t)$
are normalized as

\[ \int \! \mathrm{d}x |\psi(x)|^2 = N \quad \text{and} \quad \int \! \mathrm{d}x |\chi(x)|^2 = 1, \quad (5.3) \]

where \( N \) is number of atoms in the BEC. We tacitly assume that the properties of
the BEC, e.g. the density far away from the impurity, are fixed. The interaction
strength \( \kappa \) on the other hand is considered to be an adjustable parameter, since
it may be easily changed in experiments.

As a starting point we briefly review and systematically extend the pertur-
bative results on the self-trapping problem [59, 60, 103] based on a variational
approach. This method, however, yields results that are of second order in \( \kappa \), and
hence is not adequate to capture the differences between attractive and repulsive
impurities. In the main part of the paper, we present our non-perturbative and
numerical results in order to reveal these fundamental differences. Finally, we
conclude with a discussion of the physical implications of our findings.

### 5.2 Perturbative results

To start we reformulate Eqs. (5.1) and (5.2) in terms of dimensionless quantities
for a homogeneous BEC with density \( n_0 \). The two relevant length scales in the
model are the healing length \( \xi = \hbar / \sqrt{\gamma n_0 m_b} \) and the average separation of the
condensate atoms \( s = n_0^{-1/d} \), where \( d \) is the dimension of the system. Introducing
the dimensionless quantities \( \tilde{x} = x / \xi \), \( \tilde{\psi} = \psi s^{d/2} \) and \( \tilde{\chi} = \chi \xi^{d/2} \) one obtains the
time-independent equations

\[ \tilde{\psi} = -\frac{1}{2} \nabla^2 \tilde{\psi} + \beta \gamma d |\tilde{\chi}|^2 \tilde{\psi} + |\tilde{\psi}|^2 \tilde{\psi}, \quad (5.4) \]

\[ \epsilon \tilde{\chi} = -\frac{\alpha}{2} \nabla^2 \tilde{\chi} + \beta |\tilde{\psi}|^2 \tilde{\chi}. \quad (5.5) \]
Here, $\alpha = m_b/m_a$ is the mass ratio, $\beta = \kappa/g$ is the relative coupling strength, $\gamma = s/\xi$ and $\varepsilon$ is the energy of the impurity. The energy of the condensate $E_{\text{bec}}$, the interaction energy $E_{\text{int}}$ and the kinetic energy of the impurity $E_{\text{kin}}$ are given by

\begin{align*}
E_{\text{bec}} &= \gamma^{-d} \int \! \! \int d^d \mathbf{x} \left( \frac{1}{2} |\nabla \psi|^2 - |\psi|^2 + \frac{1}{2} |\psi|^4 \right), \\
E_{\text{int}} &= \beta \int \! \! \int d^d \mathbf{x} |\chi|^2 |\psi|^2, \\
E_{\text{kin}} &= \frac{\alpha}{2} \int \! \! \int d^d \mathbf{x} |\nabla \chi|^2,
\end{align*}

where all energies are measured in units of $g n_0$ and we dropped the tilde for notational convenience, as in the remainder of the paper. Equations (5.4) and (5.5) have a trivial solution with $|\psi|^2 = 1$ and $\varepsilon = \beta$, which corresponds to a delocalized impurity.

### 5.2.1 Thomas–Fermi approximation

If the density of the BEC changes smoothly we can apply the Thomas–Fermi approximation, i.e. neglect the term $\nabla^2 \psi$ in Eq. (5.4). In this regime we immediately find that $|\chi(\mathbf{x})|^2 = 1 - \beta \gamma^d |\chi(\mathbf{x})|^2$, and thus $\chi(\mathbf{x})$ obeys the self-focusing nonlinear Schrödinger equation

\begin{align*}
\varepsilon' \chi &= -\frac{1}{2} \nabla^2 \chi - \zeta |\chi|^2 \chi, \\
\end{align*}

with the self-trapping parameter $\zeta = \beta^2 \gamma^d / \alpha$ and $\varepsilon' = (\varepsilon - \beta)/\alpha$. In one dimension Eq. (5.9) admits the exact solution \[ \chi(\lambda)(x) = (2\lambda)^{-1/2} \text{sech}(x/\lambda), \]
with the localization length $\lambda = 2/\zeta$ and the energy $\varepsilon' = -\zeta^2/8$. In addition, numerical solutions of Eq. (5.9) show that the wave-function of the form $\chi(\lambda)(x) = N_{\lambda} \text{sech}(|x|/\lambda)$, with $N_{\lambda}$ the normalization constant, is also an accu-
Figure 5.1. The localization length $\sigma$ (solid lines) as a function of the self-trapping parameter $\zeta$ obtained by using a Gaussian variational wavefunction. Self-trapping occurs for arbitrarily small $\zeta$ in 1d, for $\zeta > 2\pi$ in 2d and for $\zeta \gtrsim 31.7$ in 3d (vertical dashed lines). From the two self-trapping solutions for a given $\zeta$ in 3d, only the more localized state is stable.

rate approximation to the exact solution in two and three dimensions [145, 146]. However, these solutions can self-focus and become singular in finite time [145]. A comparison of the individual terms in $E_{\text{bec}} + E_{\text{int}}$ shows that the Thomas–Fermi approximation is valid for $\zeta \ll 1$, which is a rather stringent condition on the system parameters. However, the merit of Eq. (5.9) lies in the fact that it yields an almost exact wave-function for weakly localized impurities with $\ell_{\text{loc}} \gg 1$, where $\ell_{\text{loc}}$ is the localization length of the impurity. In addition, we see from the solution of Eq. (5.9) that self-trapping occurs for arbitrarily small coupling in 1d for both types of impurities.

5.2.2 Weak-coupling approximation

An alternative approach is to linearize the equation for $\psi(x)$ by considering small deformations $\delta \psi(x) = \psi(x) - 1$ of the condensate [59, 60, 103]. This corresponds
5.2. Perturbative results

To a consistent expansion of Eqs. (5.4) and (5.5) in $\beta$, which results in the linear equations

$$\left(-\frac{1}{2}\nabla^2 + 2\right)\delta\psi = -\beta\gamma^d|\chi|^2,$$

(5.10)

$$\left(-\frac{\alpha}{2}\nabla^2 + 2\beta\delta\psi\right)\chi = (\varepsilon - \beta)\chi,$$

(5.11)

where we assumed that $\delta\psi$ is real for simplicity. It can be seen from Eq. (5.10) that the linearization of Eq. (5.4) is valid in the regime $|\beta|\gamma^d/\ell_{\text{loc}} \ll 1$. The solution of Eq. (5.10) is given in terms of the Green’s function $G(x)$ satisfying the Helmholtz equation. One finds by inserting the solution of Eq. (5.10) into Eq. (5.11) that $\chi$ obeys the nonlocal nonlinear Schrödinger equation

$$\left(-\frac{1}{2}\nabla^2 - 2\zeta\int\!dx'G(x-x')|\chi(x')|^2\right)\chi = \varepsilon'\chi.$$

(5.12)

Equation (5.12) minimizes the energy functional $F[\chi] = E_{\text{kin}} + E_{\text{def}}$, with

$$E_{\text{def}} = -\beta^2\gamma^d\int\!dx\,dx'|\chi(x)|^2G(x-x')|\chi(x')|^2,$$

(5.13)

which has been discussed in the context of liquid helium by Lee and Gunn [59]. We see from Eqs. (5.8) and (5.13) that the self-trapping parameter $\zeta$ is proportional to $E_{\text{def}}/E_{\text{kin}}$, i.e. the ratio between the potential energy gained by deforming the BEC and the kinetic energy of the impurity.

In order to estimate the critical parameters for which self-trapping occurs we insert the harmonic oscillator ground state

$$\chi_\sigma(x) = (\pi\sigma^2)^{-d/4}\prod_{j=1}^{d}\exp(-x_j^2/2\sigma^2),$$

(5.14)

with $\sigma$ the harmonic oscillator length, as a variational wave-function into the
functional $F[\chi]$. The resulting energy $f(\sigma)$ is given by

$$f(\sigma) = \frac{\alpha d}{4\sigma^2} - \beta^2 \gamma^d h(\sigma),$$  \hspace{1cm} (5.15)

with the functions

$$h_{1d}(\sigma) = \frac{1}{2} \exp(2\sigma^2) \text{erfc}(\sqrt{2}\sigma),$$

$$h_{2d}(\sigma) = -\frac{1}{2\pi} \exp(2\sigma^2) \text{Ei}(-2\sigma^2),$$

$$h_{3d}(\sigma) = \frac{1}{\pi} \left[ \frac{1}{\sqrt{2\pi}\sigma} - \exp(2\sigma^2) \text{erfc}(\sqrt{2}\sigma) \right],$$

where $\text{erfc}(x)$ is the complementary error function and $\text{Ei}(x)$ the exponential integral. The impurity localizes if $f(\sigma)$ has a minimum for a finite value of $\sigma$, which depends only on the self-trapping parameter $\zeta$.

The explicit expression for $f(\sigma)$, which appears to be a novel result, allows us to determine the self-trapping threshold, i.e. the critical coupling strength above which self-trapping occurs, and the size of the self-trapped state even for highly localized self-trapping solutions as long as $|\beta|\gamma^d/\sigma^d \ll 1$. Figure (5.1) shows the localization length $\sigma$ as a function of the self-trapping parameter $\zeta$ in 1d, 2d and 3d. Specifically, in 1d we find by asymptotically expanding $f(\sigma)$ in the limit $\sigma \gg 1$ that there exists a self-trapping solution for arbitrarily small $\zeta$ with $\sigma = \sqrt{2\pi}/\zeta$. The same expansion yields a critical value $\zeta_{\text{crit}} = 2\pi$ above which self-trapping occurs in 2d. In the 3d case, numerical minimization of $f(\sigma)$ shows that the critical value is $\zeta_{\text{crit}} \approx 31.7$, where the corresponding state is highly localized with $\sigma \approx 0.87$. Interestingly, there exist two self-trapping solutions for a given $\zeta$ in 3d, however only the more localized state is stable.
5.3 Beyond perturbation theory

We now consider the self-trapping problem in the regime of strong impurity–BEC interactions, \textit{i.e.} the case of a localized self-trapping state accompanied by a possibly strong deformation of the BEC. We first illustrate the effect of higher order terms in $\beta$ for a 1d system and subsequently discuss 2d and 3d systems based on a scaling argument.

5.3.1 The $\delta$-approximation in 1d

In order to find approximate solutions of Eqs. (5.4) and (5.5) we assume that the impurity is highly localized due to the strong impurity–BEC interaction. More precisely, we consider the regime where the effect of the impurity on the BEC is essentially the same as for a $\delta$-impurity with $|\chi(x)|^2 = \delta(x)$. This approximation

Figure 5.2. (a) Deformation of the BEC for an attractive (left) and repulsive (right) $\delta$-impurity with the same interaction strength $\gamma|\beta| = 1$. (b) Deformation energy $E_{\text{def}}$ for a $\delta$-impurity as a function of the interaction strength $\beta$ (solid line) compared to the weak-coupling approximation (dashed line) for $\gamma = 0.5$. Attractive (repulsive) impurities have lower (higher) energy than predicted by the weak-coupling approximation.
is valid provided that $\ell_{\text{loc}} \ll 1$, i.e. the localization length is much smaller than the healing length of the BEC, which is achieved for sufficiently large $|\beta|$. Our approach focuses only on the deformation of the BEC caused by the impurity. Nevertheless, the $\delta$-approximation allows us to illustrate the differences between attractive and repulsive impurities, which are also present in higher dimensions.

We first calculate the condensate wave-function $\psi(x)$ in presence of a $\delta$-impurity at position $x_0$, which is determined by the equation

$$\left[-\frac{1}{2} \partial_{xx} - 1 + |\psi(x)|^2 + \beta \gamma \delta(x - x_0)\right] \psi(x) = 0,$$

with the boundary conditions $\psi(x) = 1$ and $\partial_x \psi(x) = 0$ in the limit $x \to \pm \infty$.

Using the known solutions of Eq. (5.19) for $\beta = 0$ and taking $x_0 = 0$ for simplicity we obtain $\psi(x) = \coth(|x| + c)$ and $\psi(x) = \tanh(|x| + c)$ for attractive and repulsive impurities, respectively, with $c$ a constant. Given that the derivative of $\psi(x)$ has a discontinuity at $x_0$ it follows that in both cases $1 - [\psi(x_0)]^2 = \beta \gamma \psi(x_0)$ and thus

$$\psi(x_0) = -\frac{\beta \gamma}{2} + \sqrt{1 + \left(\frac{\beta \gamma}{2}\right)^2},$$

which fixes the constant $c$. We note that $\psi(x_0) \in (0,1]$ for $\beta \geq 0$ and $\psi(x_0) \in (1,\infty)$ for $\beta < 0$. Thus the density of the condensate $n(x_0) \equiv [\psi(x_0)]^2$ at the position of the impurity $x_0$ is not bounded for attractive interactions. The enhanced deformation of the BEC due to an attractive $\delta$-impurity is already visible for a moderate interaction strength as illustrated in Fig. (5.2)a.

The solution of Eq. (5.19) allows us to determine the deformation energy $E_{\text{def}}$ to all orders of $\beta$. Using Eqs. (5.6) and (5.7) we find that for both types of impurities

$$E_{\text{def}} = \frac{4}{3} \gamma^{-1} \left\{1 - \left[1 + \left(\frac{\beta \gamma}{2}\right)^2\right]^{3/2} + \left(\frac{\beta \gamma}{2}\right)^3\right\}.$$
Figure 5.3. The localization length $\sigma$ (solid line) and the density of the condensate $n(x_0)$ (long-dashed line) at the impurity position $x_0$ as a function of the interaction strength $\beta$ in 1d. The weak-coupling approximation (dotted line) accurately reproduces $\sigma$ in the regime $|\beta|\gamma/\sigma \ll 1$. The localization length saturates to a finite value $\sigma \sim 60$ as $\beta \to 0$ because of the finite system size. The deformation of the BEC is qualitatively described by the $\delta$-approximation (short-dashed line). The inset shows the smooth transition from a sech-type ($R_{\text{fit}} = 1$) to a Gaussian ($R_{\text{fit}} = -1$) self-trapping state for repulsive impurities.

We note that the non-perturbative result for $E_{\text{def}}$ is consistent with the weak-coupling approximation since in the limit $\sigma \to 0$ we find from Eq. (5.16) that $\beta^2\gamma h_{1d}(\sigma) \to \beta^2\gamma/2$. Figure (5.2)b shows the deformation energy $E_{\text{def}}$ as a function of the interaction strength $\beta$ in comparison with the weak-coupling result. It can be seen that attractive impurities have lower energy than predicted by the weak-coupling approximation, whereas repulsive impurities have higher energy.
5.3.2 Impurity collapse

The results in the previous section indicate that the ground state of the impurity and the BEC strongly depend on the sign of $\beta$. We now show that the sign of $\beta$ has a crucial effect on the ground state in 2d and 3d by using a scaling argument based on a variational wave-function for $\psi(x)$ and $\chi(x)$.

Let us consider the total energy of the system $E_{\text{tot}} = E_{\text{bec}} + E_{\text{int}} + E_{\text{kin}}$, which is clearly bounded from below for $\beta > 0$ but not necessarily for $\beta < 0$. We now analyze the scaling of the individual terms in $E_{\text{tot}}$ depending on the localization length of the impurity and the deformation of the BEC. To this end we insert the Gaussian trial function $\chi_\sigma(x)$ for the impurity and $\psi_\sigma(x) = 1 + \delta \psi_\sigma(x)$ for the condensate into $E_{\text{tot}}$, where

$$\delta \psi_\sigma(x) = \frac{a}{\sigma^{\delta/2}} \prod_{j=1}^{d} \exp \left(-\frac{x_j^2}{b\sigma^2} \right),$$

with $a$, $b$ and $\delta$ positive constants. In what follows we are particularly interested in the limit $\sigma \to 0$ and only consider finite deformations of the BEC. Consequently, we add the constraint $\delta \leq d$ to assure that $\int \text{d}x |\delta \psi(x)|^2 \sim \sigma^{d-\delta}$ is finite. We note that $\chi_\sigma(x)$ and $\psi_\sigma(x)$ have the correct asymptotic behavior required for them to be valid physical states of the system, however, they may not be a good approximation for the ground state. We obtain that the individual energy contributions scale as $E_{\text{int}} \sim \sigma^{-\delta}$, $E_{\text{kin}} \sim \sigma^{-2}$ and

$$E_{\text{bec}} \sim c_0 \sigma^{d-\delta-2} + \sum_{j=1}^{4} c_j \sigma^{d-j\delta/2},$$

where the $c_j > 0$ depend on the system parameters.

Comparing the terms above one finds that for a three-dimensional system $E_{\text{tot}}$ is not bounded from below in the limit $\sigma \to 0$ for a fixed $\delta$, i.e. the energy of the
system becomes arbitrarily low if the impurity collapses to a point. Explicitly, in the 3d case we have $E_{\text{bec}} \sim c_0 \sigma^{1-\delta} + c_1 \sigma^{3-\delta/2} + \cdots + c_4 \sigma^{3-2\delta}$ and hence a comparison of the exponents yields that $|E_{\text{int}}| > E_{\text{kin}} + E_{\text{bec}}$ for $2 < \delta < 3$ in the limit $\sigma \to 0$. Moreover, in the same limit $\int d\mathbf{x} |\delta \psi_\sigma(\mathbf{x})|^2 \to 0$, i.e. the deformation of the BEC is vanishingly small despite the collapse of the impurity. We note that the above argument holds for arbitrarily small $\beta$, and thus the weak-coupling approximation in 3d is valid for $\beta > 0$ only since for $\beta < 0$ there is always a state of lower energy with $\sigma \to 0$.

In the 2d case it is not possible to find a value for $\delta$ such that the total energy $E_{\text{tot}}$ is dominated by $E_{\text{int}}$ in the limit $\sigma \to 0$. Nevertheless, for $\delta = 2$ we obtain $E_{\text{int}} \sim E_{\text{kin}} \sim E_{\text{bec}} \sim \sigma^{-2}$, which implies that the collapse of the impurity depends on the particular system parameters, e.g. the coupling strength $\beta$. In contrast to the 3d case this collapse is accompanied by a sizeable deformation of the BEC since $\int d\mathbf{x} |\delta \psi_\sigma(\mathbf{x})|^2$ is finite in the limit $\sigma \to 0$ for $\delta = 2$. Finally, for a one-dimensional system similar considerations lead to result that $|E_{\text{int}}| < E_{\text{kin}} + E_{\text{bec}}$ in the limit $\sigma \to 0$ for any valid $\delta$, and hence our variational approach does not predict a collapse of the impurity.

5.4 Numerical results

We have determined the ground state of the impurity and the BEC numerically by using the normalized gradient flow method [147, 148] in order to extend the analytical results. To make Eqs. (5.4) and (5.5) amenable to computational modelling we assumed that both the impurity and the condensate were enclosed in a sphere of zero potential with infinitely high potential walls at its radius $R$. The system parameters for the numerical calculations were set to $\alpha = 1.0$ and $\gamma = 0.5$, whereas $\beta$ was varied over a large range.
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Figure 5.4. The localization length $\sigma$ (solid line) and the density of the condensate $n(x_0)$ (dashed line) at the impurity position $x_0$ as a function of the interaction strength $\beta$ in 2d. The weak-coupling approximation (dotted lines) accurately predicts the self-trapping threshold at $\beta_{\text{crit}} = \sqrt{8\pi}$ (vertical dashed lines). The localization length saturates to a finite value $\sigma \sim 20$ for $|\beta| < \beta_{\text{crit}}$ because of the finite system size. Attractive impurities shrink to a point-like state and the density of the BEC $n(x_0)$ diverges as $\beta$ approaches a critical value $\beta^* \sim -10$ in agreement with our scaling argument. The behavior of $R_{\text{fit}}$ (inset) is similar to the 1d case.

A quantitative measure for the localization length $\ell_{\text{loc}}$ was found by fitting the functions $\chi_\sigma(x)$ and $\chi_\lambda(x)$ to the exact impurity wave function yielding the values $\sigma$ and $\lambda$. In addition, we compared the corresponding fitting errors $S_\sigma$ and $S_\lambda$ and evaluated the quantity $R_{\text{fit}} = (S_\sigma - S_\lambda)/(S_\sigma + S_\lambda)$. Accordingly, $R_{\text{fit}} = -1$ indicates that the self-trapped state is accurately described by a Gaussian $\chi_\sigma(x)$, whereas for $R_{\text{fit}} = 1$ the impurity is rather in a sech-type state $\chi_\lambda(x)$. One would expect that $R_{\text{fit}} \approx -1$ for a highly localized impurity with $\ell_{\text{loc}} \ll 1$ since the impurity sees only the harmonic part of the effective potential $\beta|\psi(x)|^2$. On the other hand, $R_{\text{fit}} \approx -1$ for a weakly localized impurity with $\ell_{\text{loc}} \gg 1$ according to
5.4. Numerical results

Figure 5.5. The localization length $\sigma$ (solid line) and the density of the condensate $n(x_0)$ (dashed line) at the impurity position $x_0$ as a function of the interaction strength $\beta$ in 3d. There is no well-defined ground state for $\beta < 0$ in 3d in agreement with our scaling argument. The weak-coupling approximation (dotted line) predicts a self-trapping threshold at $\beta_{\text{crit}} \simeq 15.9$ (vertical dashed line), which is lower than the numerical result $\beta_{\text{crit}} \simeq 18.8$. The localization length saturates to a finite value $\sigma \sim 10$ for $\beta < \beta_{\text{crit}}$ because of the finite system size. The convergence of the impurity wave-function to a Gaussian self-trapping state is slower than in 1d and 2d as indicated by $R_{\text{fit}}$ (inset).

As can be seen in Fig. (5.3), in the 1d case there is no self-trapping threshold in agreement with the weak-coupling result, which accurately reproduces the localization length $\sigma$ in the regime $|\beta| \gamma / \sigma \ll 1$. However, we see that for large $|\beta|$ attractive impurities are more localized than the repulsive ones. Moreover, repulsive impurities undergo a smooth transition from a sech-type to a Gaussian self-trapping state for increasing $\beta$ as indicated by $R_{\text{fit}}$. The deformation of the condensate $n(x_0)$ at the position of the impurity $x_0$ is qualitatively described...
by the $\delta$-approximation with a strong increase in the density of the BEC for attractive impurities.

In two dimensions, the impurity localizes for $|\beta| > \beta_{\text{crit}}$, where $\beta_{\text{crit}}$ is correctly predicted by the weak-coupling result, as shown in Fig. (5.4). This is not accidental since the localization length $\sigma$ diverges close to $\beta_{\text{crit}}$ in 2d, as can be seen in Fig. (5.1), and thus the criterion $|\beta|\gamma^2/\sigma^2 \ll 1$ for the validity of the linearization of Eqs. (5.4) and (5.5) is always met near $\beta_{\text{crit}}$. In contrast, for large $|\beta|$ the localization length $\sigma$ strongly deviates from the weak-coupling result. In particular, attractive impurities shrink to a point-like state and the density of the condensate $n(x_0)$ diverges as $\beta$ approaches a critical value $\beta^*$, which is in agreement with the scaling argument in the previous section. The behavior of $R_{\text{fit}}$ is similar to the 1d case.

For a 3d system we are able to obtain numerical results for $\beta > 0$ only, which in view of our scaling argument was to be expected. The localization length $\sigma$ and the density of the condensate $n(x_0)$ for repulsive impurities are shown in Fig. (5.5). We see that the weak-coupling approximation underestimates the exact value $\beta_{\text{crit}}$ since in 3d we have that $\sigma \sim 1$ even close to $\beta_{\text{crit}}$ and thus $\beta\gamma^3/\sigma^3$ is not necessarily small. As shown in the inset of Fig. (5.5) the transition from a sech-type to a Gaussian self-trapping state is slower than in 1d and 2d.

5.5 Discussion and conclusion

In our analytical and numerical investigation of the self-trapping problem we have shown, in particular, that an attractive impurity–BEC interaction leads to a strong deformation of the BEC in 1d and 2d and to a singular ground state of the impurity in 2d and 3d. However, both the high density of the BEC and the point-like state of the impurity entail additional physical effects, which were
initially small and not taken into account in our model.

The high density of the BEC near the impurity enhances inelastic collisions that lead to two- and three-body losses of the condensate atoms [62]. Specifically, the inelastic collisions might cause the loss of the impurity atom itself. However, provided that the impurity is not affected by inelastic collisions one can account for the loss of the condensate atoms by adding damping terms of the form $-i\Gamma_2|\psi(x)|^2\psi(x)$ and $-i\Gamma_3|\psi(x)|^4\psi(x)$ to Eq. (5.1), where the positive constants $\Gamma_2$ and $\Gamma_3$ are two- and three-body loss rates, respectively. We note that these additional terms would require the simulation of the full dynamics of the system [149] and may have a nontrivial effect on the self-trapping process.

Moreover, the contact potential approximation is valid as long as the various length scales of the system, e.g. the localization length $\ell_{\text{loc}}$, are large compared to the characteristic range of the exact interaction potential [143]. Thus the interaction between the condensate atoms and the impurity is no longer correctly described by the contact potential $\kappa\delta(x-x')$ in the limit $\ell_{\text{loc}} \to 0$ where the influence of higher partial waves becomes important. The resulting repulsion would of course lead to a finite width of the impurity wave-function. We note that with the above proviso our results are also valid for ionic impurities with positive charge [150, 151] in the regime where the ion–boson scattering is dominated by the s-wave contribution [152, 153].

Finally, we conclude with the remark that our model is also applicable if the BEC is confined to a harmonic trap [91] provided that the harmonic oscillator length of the potential is much larger than the localization length $\ell_{\text{loc}}$ of the impurity and the healing length $\xi$ of the BEC.
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Chapter 6

The motion of heavy impurities through a BEC

6.1 Introduction

In this chapter we study the dynamics of an impurity in the weak coupling regime, where the impurity–BEC coupling is smaller than the interaction between the BEC atoms. Our results will be relevant to both self-trapped impurities and atoms confined to an optical lattice, which correspond to the set-up considered in chapter 5 and chapters 3 & 4, respectively. On one hand, the weak-coupling approach allows us to calculate the effective mass of self-trapped impurities; on the other hand it will be possible to determine corrections to the phonon-induced impurity–impurity interaction and the polaronic level shift due to finite impurity hopping. These quantities were calculated in chapter 4, but only for static impurities. In addition, we briefly discuss the effect of incoherent scattering of supersonic impurities with the BEC background.

The model we consider is a variant of the well-known Fröhlich polaron model in solid state physics [28, 35, 63, 64, 154], where in the original problem the bosonic excitations correspond to dispersionless optical phonons which interact either with electrons or holes. The general importance of the model is due to its generic form describing the motion of a (non-relativistic) particle while it is linearly
coupled to a bosonic quantum field [155]. The Fröhlich polaron problem has been tackled with numerous mathematical techniques [28, 35, 64, 154], which were also applied to the motion of an impurity particle through liquid helium [118, 120, 156]. In this chapter we will apply standard Rayleigh–Schrödinger perturbation theory, which was found to work surprisingly well despite its simplicity [28], and treat the impurity–phonon interaction as a perturbation. This is in contrast to the strong-coupling approach in chapter 4, where the kinetic term was assumed to be negligible.

6.2 Model

Our starting point is the Hubbard–Holstein Hamiltonian [28, 105, 124] for impurities trapped in an optical potential and immersed in a homogeneous BEC. Explicitly, the Hamiltonian reads

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}^\dagger_i \hat{a}_j + \sum_q \hbar \omega_q \hat{b}^\dagger_q \hat{b}_q + \sum_{j,q} \hbar \omega_q \left[ M_{j,q} \hat{b}_q + M_{j,q}^* \hat{b}^\dagger_q \right] \hat{a}^\dagger_j \hat{a}_j, \quad (6.1)$$

where the operators $\hat{a}^\dagger_j$ ($\hat{a}_j$) create (annihilate) an impurity at lattice site $j$, and the operators $\hat{b}^\dagger_q$ ($\hat{b}_q$) create (annihilate) a Bogoliubov phonon about the ground state of the condensate $\psi_0(r)$ in absence of impurities. Moreover, $M_{j,q}$ are the matrix elements of the impurity–phonon coupling and $\hbar \omega_q = \sqrt{\varepsilon_q (\varepsilon_q + 2 gn_0)}$ is the phonon dispersion relation, where $g > 0$ is the repulsive coupling between the BEC atoms, $n_0$ is the density of the BEC and $\varepsilon_q = (\hbar q)^2 / 2 m_b$ is the free particle energy.

In order to treat self-trapped impurities and lattice atoms on the same footing we make the following assumptions. First, we consider a system at zero temperature, in which initially there are no phonons present. Second, we assume that the
impurities are non-interacting and that they can be described by the free-particle dispersion relation $(\hbar k)^2/2m_a$. The mass $m_a$ is either the mass of a self-trapped impurity or the effective mass $m_a = \hbar^2/2Ja^2$ of an impurity in an optical lattice, with hopping $J$ and lattice spacing $a$. This description, of course, relies on the assumption that $|k|a \ll 1$, i.e. the impurity momentum $k$ is close to the minimum of the lowest Bloch band. Finally, we consider impurities whose mass $m_a$ is larger than the mass $m_b$ of the BEC atoms and introduce the parameter $\alpha = m_b/m_a \leq 1$. We note that for the case of trapped impurities we have $\alpha \propto J$, and thus static impurities have an infinite effective mass.

The slightly simplified model is best analyzed in momentum space. To this end we introduce the creation (annihilation) operators $\hat{a}_k^\dagger$ ($\hat{a}_k$) defined by the relations
\[
\hat{a}_j^\dagger = \frac{1}{\sqrt{N_a}} \sum_k \hat{a}_k^\dagger e^{ikr_j} \quad \text{and} \quad \hat{a}_j = \frac{1}{\sqrt{N_a}} \sum_k \hat{a}_k e^{-ikr_j},
\]
where $N_a$ is the number of lattice sites and $r_j$ the position of the site $j$. By invoking the identities $\sum_j e^{-i(k-k')r_j} = N_a \delta_{kk'}$ and $\sum_j \hat{a}_j^\dagger \hat{a}_j = \sum_k \hat{a}_k^\dagger \hat{a}_k$ we find
that the immersed impurity is described by the Fröhlich-type Hamiltonian

$$\hat{H} = \sum_{k} E_k \hat{a}_k^\dagger \hat{a}_k + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \hat{b}_{\mathbf{q}}^\dagger \hat{b}_{\mathbf{q}} + \hat{H}_I, \quad (6.3)$$

with

$$\hat{H}_I = \sum_{k, \mathbf{q}} \hbar \omega_{\mathbf{q}} \left[ M_{\mathbf{q}} \hat{b}_{\mathbf{q}} \hat{a}_{k+\mathbf{q}}^\dagger + M_{\mathbf{q}}^* \hat{b}_{\mathbf{q}}^\dagger \hat{a}_{k-\mathbf{q}}^\dagger \hat{a}_{k} \right], \quad (6.4)$$

where the kinetic term is $E_k = (\hbar k)^2/2m_a$ and the matrix elements $M_{\mathbf{q}}$ are given by

$$M_{\mathbf{q}} = \kappa \sqrt{n_{\mathbf{q}} \epsilon_{\mathbf{q}}} f(\mathbf{q}) \quad \text{with} \quad f(\mathbf{q}) = \frac{1}{\sqrt{\Omega}} \int \mathrm{d}\mathbf{r} |\chi(\mathbf{r})|^2 \exp(i\mathbf{q} \cdot \mathbf{r}), \quad (6.5)$$

The interaction term $\hat{H}_I$ corresponds to a process in which the impurity is scattered from state $\mathbf{k}$ to $\mathbf{k} + \mathbf{q}$ by the emission or absorption of a phonon with momentum $\mathbf{q}$, as illustrated in Fig. 6.1.

For lattice atoms, the wave-function $\chi(\mathbf{r})$ corresponds to the Wannier states [107], whereas the state of a self-trapped impurity $\chi(\mathbf{r})$ was determined in chapter 5. In either case, the impurity state $\chi(\mathbf{r})$ is well approximated by a Gaussian wave-function and the factor $f(\mathbf{q})$ takes the simple form $f(\mathbf{q}) = \Omega^{-1/2} \exp(-\mathbf{q}^2 \sigma^2/4)$, where $\sigma$ is the harmonic oscillator length and $\Omega$ is the quantization volume. The value of $\sigma$ for lattice atoms is obtained by expanding the optical lattice potential around the minima of the potential wells. For the case of a self-trapped impurity the length $\sigma$ results from the variational ansatz discussed in chapter 5, which for sufficiently strong impurity–BEC coupling corresponds to a harmonic approximation of the effective self-trapping potential. In what follows, an impurity with $\sigma = 0$ will be referred to as a $\delta$-impurity.
It should be mentioned that $\hat{H}_I$ can be written in terms of the static structure factor $S(q)$ of the BEC [157], which has been directly determined in experiments by using two-photon optical Bragg spectroscopy [40, 158, 159]. Inserting the explicit expression for $M_q$ into $\hat{H}_I$ and invoking the Feynman–Bijl relation [31, 160] $\hbar \omega_q = \varepsilon_q / S(q)$ we obtain

$$\hat{H}_I = \kappa \sqrt{n_0} \sum_{k,q} f(q) \sqrt{S(q)} \left[ \hat{b}_q \hat{a}_{k+q} \hat{a}_k + \hat{b}_{q}^\dagger \hat{a}_{k-q} \hat{a}_k \right].$$  \hspace{1cm} (6.6)

The formulation in terms of $S(q)$ also makes it possible to generalize our results to the case of a nearly uniform BEC based on the local density approximation [40, 157].

6.3 Coherent coupling effects

The impurity–phonon coupling $\hat{H}_I$ implies that the bare impurity state $|k\rangle$ with no phonons cannot be an exact eigenstate of the system. The impurity will be a superposition of states of the form $|k, \{N_q\}\rangle$, where $\{N_q\}$ is the phonon configuration with phonon occupation numbers $N_q$. Thus, the particle is dressed by a cloud of virtual phonons and constitutes a so-called weak-coupling polaron. Now, for sufficiently weak coupling, only a very limited number of phonons will be involved; in this case one would expect that the polaron is accurately described by the first-order perturbed state

$$|k, 0\rangle^{(1)} = |k, 0\rangle + \sum_q \frac{\hbar \omega_q M_q}{E_k - E_{k-q} - \hbar \omega_q} |k - q, 1_q\rangle.$$  \hspace{1cm} (6.7)

In other words, this expansion in terms of single-phonon states is valid provided that the average phonon number $N_{av}$ is small. Let us therefore determine $N_{av}$ by taking the expectation value of the phonon number operator $\sum_q \hat{b}_q^\dagger \hat{b}_q$ over the
The motion of heavy impurities through a BEC state $|k,0\rangle^{(1)}$. We obtain

$$N_{av} = \sum_{q} \frac{|\hbar \omega_q M_q|^2}{\{E_k - E_{k-q} - \hbar \omega_q\}^2}, \quad (6.8)$$

where we ignored small corrections due to the fact that $|k,0\rangle^{(1)}$ is not normalized.

To determine the dependence of $N_{av}$ on the system parameters we consider, for simplicity, an impurity with momentum $k = 0$. In the bulk limit $\Omega^{-1} \sum_q \rightarrow (2\pi)^{-D} \int dq$, we find that the phonon number is

$$N_{av} = F'(\alpha, \sigma, y_0) \left( \frac{\kappa}{g} \right)^2 \left( \frac{d}{\xi} \right)^D, \quad (6.9)$$

where $D$ is the dimension of the system, $\xi = \hbar/\sqrt{g m_q m_b}$ is the healing length and $d$ is the average distance between the condensate atoms. The dimensionless function $F'(\alpha, \sigma, y_0)$ is defined by the integral

$$F'(\alpha, \sigma, y_0) = C_D \int_{y_0}^{\infty} dy \frac{y^{D+1} \exp \left[ -\frac{1}{2} y^2 (\sigma/\xi)^2 \right]}{\sqrt{y^2(y^2 + 4)} \left\{ \alpha y^2 + \sqrt{y^2(y^2 + 4)} \right\}^2}, \quad (6.10)$$

with $y = |q|\xi$ and $C_D$ being a constant*. The lower cut-off $y_0$ was introduced because the integral diverges logarithmically in one dimension in the limit $y_0 \rightarrow 0$, i.e. for an infinitely large condensate. In general, the function $F'(\alpha, \sigma, y_0)$ is slowly varying and of the order of unity for realistic values of $y_0$, as illustrated in Fig. 6.2(a). Thus, as a simple rule we can assume that $|k,0\rangle^{(1)}$ is an accurate polaron state for an impurity with zero momentum provided that $(\kappa/g)^2 (d/\xi)^D \ll 1$. However, in principle one would have to consider two-phonon states to verify that higher order terms are indeed small. We note that a similar calculation yields essentially the same result for the range of finite values of $k$ considered in

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*Explicitly, $C_1 = 4/\pi$, $C_2 = 2/\pi$ and $C_3 = 2/\pi^2$. 
6.3. Coherent coupling effects

Figure 6.2. (a) The dependence of the phonon number on the mass ratio \( \alpha \) and the impurity width \( \sigma \) for a one-dimensional system. The function \( F(\alpha, \sigma, y_0) \) is slowly varying and of the order of unity. (b) The normalized phonon distribution for a \( \delta \)-impurity. The distribution is peaked \( q \sim 1/\xi \) in 3D (solid line), whereas the impurity is mainly dressed by low-energy phonons in 2D (dashed line) and 1D (dotted line). The cut-off respectively the lowest value of \( y_0 \) was set to \( y_0 = 10^{-3} \) for plot (a) and (b).

The introduction of the lower cut-off \( y_0 \) allows us to investigate the distribution of the phonon states contributing to the dressed state \(|k, 0\rangle^{(1)}\). The function \( F(\alpha, \sigma, y_0) \) represents a (non-normalized) cumulative distribution for the number of virtual phonons with momenta \( |q| \geq y_0/\xi \), and \(-\partial F(\alpha, \sigma, y_0)/\partial y_0 \) is the corresponding phonon distribution. The normalized phonon distribution, shown in Fig. 6.2(b), is peaked around \( q \sim 1/\xi \) in 3D, whereas the impurity is mainly dressed by low-energy phonons in 1D and 2D systems. In particular, the phonon cloud contains an infinite number of phonons in one dimension in the limit \( y_0 \rightarrow 0 \). However, as we shall see, this does not affect the calculation of physical quantities since the corresponding phonon energies are vanishingly small.
6.3.1 Polaronic level shift and induced impurity mass

The dressing of the impurity state $|k,0\rangle$ by phonons results in a change of the energy of the impurity. More precisely, the total energy is lowered by the polaronic level shift\(^\dagger\) $\delta E_0$ and the kinetic energy of the impurity is altered by the induced impurity mass $\delta m$. The latter effect is equivalent to a reduction of the hopping $J$ in the context of an optical lattice. To lowest order we obtain that the energy of the impurity in state $|k,0\rangle^{(1)}$ is

$$E_{|k,0\rangle^{(1)}} = E_k - \delta E, \quad (6.11)$$

with the energy change

$$\delta E = \sum_q \frac{|\hbar \omega_q M_q|^2}{E_{k-q} + \hbar \omega_q - E_k}. \quad (6.12)$$

The expression for $\delta E$ represents second-order processes, in which a single virtual phonon is emitted and reabsorbed, as depicted in Fig. 6.3(a). The emission of a real phonon with momentum $q$ only occurs at resonance, i.e. if the denominator $E_q + \hbar \omega_q - \hbar^2 k \cdot q/m_a$ in $\delta E$ vanishes [35, 64, 154]. Considering phonons with small momenta $q$ and correspondent energies $\hbar \omega_q = \hbar c_s |q|$, with $c_s$ the speed of sound in the BEC, we find that the resonance condition is $\hbar |k|/m_a = c_s + \hbar |q|/m_a$. This can only be fulfilled for momenta $\hbar |k|/m_a \geq c_s$, and thus a phonon is emitted only if the group velocity of the impurity exceeds the speed of sound $c_s$, which is in agreement with Landau’s criterion [161, 162].

In what follows we restrict our attention to slow impurities with $\hbar |k|/m_a \ll c_s$, thereby neglecting the emission of real phonons. To evaluate the energy change $\delta E$ we expand the sum over $q$ as a power series in the impurity momentum $k$,

\(^\dagger\)The polaronic level shift $\delta E_0$ was denoted by $E_p$ in the previous chapters.
6.3. Coherent coupling effects

Figure 6.3. (a) The Feynman diagram for the process leading to the polaronic level shift $\delta E_0$ and the effective mass $\delta m$. The impurity with momentum $k$ emits and reabsorbs a virtual phonon with momentum $q$. (b) Two impurities with momenta $k$ and $k'$, respectively, exchange a virtual phonon with momentum $q$, which results in an attractive interaction between the impurities.

which yields

$$
\delta E = \sum_q \frac{|\hbar \omega_q M_q|^2}{E_q + \hbar \omega_q} \delta E_0 + \sum_q \frac{|\hbar \omega_q M_q|^2}{\left(\frac{E_q + \hbar \omega_q}{m_a}\right)^3} \left(\frac{\hbar^2 k \cdot q}{m_a}\right)^2 + O(k^3).
$$

The first term in Eq. (6.13) is the polaronic level shift $\delta E_0$, which does not depend on $k$, and the second term $\delta E_k$ is a correction to the kinetic energy of the impurity. We note that the result for $\delta E_0$ is consistent with the findings in chapter 4 since the additional energy term $E_q$ in the denominator vanishes for static impurities.

In the same way as the phonon number $N_{\text{av}}$, we have evaluated the polaronic level shift in the bulk limit. Unlike the level shift for static impurities, denoted by $\delta E_0^\text{st}$, the result depends on the mass ratio $\alpha$ and is conveniently expressed as

$$
\delta E_0 = G(\alpha, \sigma) \frac{\kappa^2}{g \xi_D}.
$$

Similarly to $F(\alpha, \sigma, y_0)$, the dimensionless function $G(\alpha, \sigma)$ changes only slowly
with varying $\alpha$ and $\sigma$ and is defined by the integral

$$G(\alpha, \sigma) = \frac{C_D}{2} \int_0^\infty dy \frac{y^{D-1} \exp \left[ -\frac{1}{2} \frac{y^2 (\sigma/\xi)^2}{y^2 + 4 + \alpha \sqrt{y^2 + 4}} \right]}{y^2 + 4 + \alpha \sqrt{y^2 + 4}}$$

(6.15)

with the same constant $C_D$ as in Eq. (6.10). Ignoring the exact form of $G(\sigma, R)$ for a moment, we see from Eq. (6.14) that the polaronic level shift $\delta E_0$ is closely related to the number of phonons $N_{av}$ in the polaron, namely

$$\delta E_0 \sim N_{av} g n_0$$

(6.16)

with $gn_0$ the typical energy scale of the BEC interactions.

Of particular interest is the effect of non-zero hopping on the level shift $\delta E_0$, which is specified by the function $G(\alpha, \sigma)$. Figure 6.4(a) shows the ratio of the dynamic ($J > 0$) level shift $\delta E_0$ and the static ($J = 0$) level shift $\delta E_0^{st}$ as a function of $\alpha \sim J$. We see that $\delta E_0$ decreases with increasing $J$, an effect which is almost independent of the dimension of the system. The dependence of $\delta E_0$ on the mass ratio $\alpha$ takes a particularly simple form for a $\delta$-impurity in a one-dimensional system. Introducing the angle $\cos \theta = \alpha$ we get

$$\frac{\delta E_0}{\delta E_0^{st}} = \frac{2}{\pi} \frac{\theta}{\sin \theta},$$

(6.17)

and hence $\delta E_0$ tends to $(2/\pi) \delta E_0^{st}$ as $\alpha \rightarrow 1$, which for reasonable physical parameters$^\dagger$ corresponds to $J \sim 1$kHz. We note in view of this result that the condition $J/\delta E_0 \ll 1$, defining the strong-coupling regime in which the impurities are described by small polarons, may already be violated for moderate $J$.

The second term in the expansion of $\delta E$ in Eq. (6.13) is quadratic in $k$ and therefore constitutes a correction $\delta E_k$ to the kinetic energy of the impurity, which

$^\dagger$For example, a BEC of $^{87}$Rb atoms and an optical lattice with $a = 500nm$. 
is conveniently expressed in terms of an induced mass $\delta m$, or equivalently an effective hopping $\tilde{J}$. Making the same assumptions as for the evaluation of the level shift $\delta E_0$ one obtains

$$\frac{\delta E_k}{E_k} = H(\alpha, \sigma) \alpha \left( \frac{\kappa}{g} \right)^2 \left( \frac{d}{\xi} \right)^D,$$

where the dimensionless function $H(\alpha, \sigma)$ is represented by the integral

$$H(\alpha, \sigma) = C_D \int_0^\infty dy \frac{y^{D+3} \exp\left[-\frac{1}{2} y^2 (\sigma/\xi)^2\right]}{\sqrt{y^2(y^2 + 4)} \left\{ \alpha y^2 + \sqrt{y^2(y^2 + 4)} \right\}^3},$$

with $C_D$ a constant.$^8$ The induced mass $\delta m$ is defined by the relation

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$^8$Explicitly, $C_1 = 16/\pi$, $C_2 = 4/\pi$ and $C_3 = 2/\pi$. 

---

Figure 6.4. (a) The ratio of the static and dynamic level shift $\delta E_0/\delta E_0^{\text{st}}$ as a function of $\alpha$ for a fixed width $\sigma/\xi = 0.1$. The decrease of $\delta E_0$ with increasing $J$ is almost the same in 3D (solid line), 2D (dashed line) and 1D (dotted line). (b) The effective interaction potential between two $\delta$-impurities in a 1D system for the mass ratio $\alpha = 0$ (solid line), $\alpha = 0.9$ (dashed line) and $\alpha = 0.99$ (dotted line). The range of the potential $\xi_\alpha = \xi \sqrt{1 - \alpha^2}$ shrinks with increasing $\alpha$, whereas the depth increases as $1/\xi_\alpha$. 
\[(\hbar k)^2/2(m_a + \delta m) = E_k - \delta E_k,\] from which we find

\[
\delta m = \frac{\delta E_k}{E_k} m_a \sim N_{av} m_b,
\]

where we neglected terms of order \((\delta m)^2\). Thus, the induced mass is proportional to number of phonons that are ‘dragged along’ in the virtual phonon cloud, weighted by the mass of the atoms in the BEC. We note that this result is in agreement with the findings of Astrakharchik and Pitaevskii [121] for the motion of a heavy \(\delta\)-impurity through a BEC. In terms of an effective hopping \(\tilde{J}\), which is defined by the relation \((\hbar k)^2/2\tilde{m}_a = E_k - \delta E_k\), with \(\tilde{m}_a = \hbar^2/2\tilde{J} a\), we get

\[
\tilde{J} = J \left(1 - \frac{\delta E_k}{E_k}\right).
\]

We see from Eq. (6.21) that the impurity–phonon coupling leads to a reduced hopping \(\tilde{J}\) as was already shown for small polarons in chapter 4. However, expression (6.21) is clearly a perturbative result in \(\kappa\), which is valid only for \(\delta E_k/E_k \ll 1\), whereas the reduced hopping \(\tilde{J}\) for small polarons included all orders of \(\kappa\) in the form of an exponential.

The expression (6.18) allows us to calculate the effective mass \(m_a + \delta m\), i.e. the mass that would be experimentally observed, of a self-trapped impurity. For fixed parameters of the BEC and a given coupling strength \(\kappa\) we first determine the width \(\sigma\) of the localized impurity by using the variational ansatz discussed in chapter 5, and subsequently calculate its effective mass based on Eq. (6.18). Figure 6.5 shows the localization length \(\sigma\) and the induced mass \(\delta m\) as a function of the coupling \(\kappa\) for a 1D and 2D system. We see that the induced mass \(\delta m\) increases with decreasing width \(\sigma\) of the impurity wave-function. The effect of the BEC background on the impurity is quite small in 2D, whereas the induced
6.3. Coherent coupling effects

Figure 6.5. (a) The localization length $\sigma$ as a function of the relative coupling strength $\kappa/g$ in 1D (solid line) and 2D (dashed line). The vertical dotted line indicates the self-trapping threshold in 2D. (b) The relative increase in mass $\delta m/m_a$ as a function of $\kappa/g$. The induced mass $\delta m$ is a sizeable fraction of $m_a$ in 1D (solid line), whereas the effective mass changes only slightly in 2D (dashed line). The system parameters were set to $\alpha = 0.1$ and $d/\xi = 0.5$ for both plots.

mass $\delta m$ is a sizable fraction of $m_a$ in 1D. However, one would expect that the change in mass should also be observable in 2D and 3D for stronger interactions, for which the weak-coupling approximation breaks down.

6.3.2 Effective impurity–impurity interaction

Next we study the effective impurity–impurity interaction potential mediated by the phonons in the BEC [32, 116, 117]. First, we recall that a generic two-body interaction term in momentum space reads

$$\hat{H}_{\text{int}} = \frac{1}{2\Omega} \sum_{k,k',q} W_{k,k',q} \hat{a}^{\dagger}_{k'+q} \hat{a}^{\dagger}_{k-q} \hat{a}_{k} \hat{a}_{k},$$  

(6.22)

where $W_{k,k',q}$ is the matrix element between the states $|k,k\rangle$ and $|k - q, k' + q\rangle$ of two particles. In the context of immersed impurities, the effective potential results from a virtual phonon exchange induced by $\hat{H}_I$ that connects the two
The motion of heavy impurities through a BEC states above. The lowest-order matrix element between the states $|k,k',0\rangle$ and $|k-q,k'+q,0\rangle$ is

$$W_{k,k',q} = \langle k-q,k'+q,0|\hat{H}_I|k,k',0\rangle^{(1)}$$

(6.23)

with the first-order perturbed state

$$|k,k',0\rangle^{(1)} = |k,k',0\rangle + \sum_q \frac{\hbar \omega_q M_q^*}{E_k - E_{k-q} - \hbar \omega_q} |k-q,k',1_q\rangle$$

$$+ \sum_q \frac{\hbar \omega_q M_q}{E_{k'} - E_{k'+q} - \hbar \omega_q} |k,k'+q,1-q\rangle,$$

(6.24)

where we used the identities $\hbar \omega_{-q} = \hbar \omega_q$ and $M_{-q}^* = M_q$. It can be seen from Eq. (6.24) that there are two processes contributing to $W_{k,k',q}$. In the first process an impurity in state $k$ emits a virtual phonon with momentum $q$, which is subsequently absorbed by the impurity in state $k'$, as depicted in Fig. 6.3(b). In the second process the impurity in state $k'$ emits a virtual phonon with momentum $-q$, which is subsequently absorbed by the impurity in state $k$.

By adding the two contributions to $W_{k,k',q}$ we obtain

$$W_{k,q} = \frac{2(\hbar \omega_q)^3 |M_q|^2}{(E_k - E_{k-q})^2 - (\hbar \omega_q)^2},$$

(6.25)

where we used the fact that $E_k + E_{k'} = E_{k-q} + E_{k'+q}$; i.e. the energy of the impurities is conserved*.

This result for the matrix elements $W_{k,q}$ is consistent with our findings for the effective potential in chapter 4 since the additional energy term $(E_k - E_{k-q})^2$ in the denominator vanishes for static impurities. In the general case, one has in principle to sum over all $W_{k,q}$ to find the exact shape of the potential and,

*We also used the identity $(a-b)^{-1} - (a+b)^{-1} = 2b(a^2 - b^2)^{-1}$. 

in particular, to determine if the potential is attractive or repulsive. However, a sufficient condition for the potential to be attractive is that all $W_{k,q}$ are negative, i.e. $(E_k - E_{k-q})^2 - (\hbar \omega q)^2 < 0$ for all $q$. Accordingly, an analysis of the individual terms yields that the interaction is attractive for momenta $\hbar|k|/m_a \ll c_s$ provided that the impurities are sufficiently heavy ($\alpha \ll 1$). The contributions of the matrix elements $W_{k,q}$ to the potential also depend on the width $\sigma$ since the coupling to phonons with $|q|\sigma \gg 1$ is highly suppressed. This effect slightly relaxes the conditions for the potential to be attractive.

The interaction potential is not only characterized by its sign but also by the range, which for static impurities is of the order of the healing length $\xi$. We now show that the range of the potential shrinks to the width $\sigma$ in the limit $\alpha \to 1$ for slow impurities with $k \approx 0$. In other words, the potential effectively vanishes as $J$ approaches a critical hopping $J_c = \hbar^2/2m_a^2$ since $\sigma \ll \xi, a$ for an optical lattice system. Setting $k = 0$ and inserting the explicit expression for $M_q$ into $W_{k,q}$ we obtain

$$W_q = -\frac{\kappa^2}{g} \left(\frac{2}{\xi}\right)^2 \frac{|f_0(q)|^2}{(1 - \alpha^2) q^2 + (2/\xi)^2},$$

(6.26)

which for $\alpha \ll 1$ results in a Yukawa-type potential with range $\xi$ ’modulated’ by the factor $|f_0(q)|^2$. However, if the hopping $J$ reaches the critical value $J_c$ then $|f_0(q)|^2$ is the only $q$-dependent term remaining in $W_q$, which yields a Gaussian potential with range $\sigma$. As an example, we find that for $\delta$-impurities in one dimension the potential is of the form

$$V(x) = -\frac{\kappa^2}{g\xi_\alpha} e^{-2|x|/\xi_\alpha},$$

(6.27)

with $\xi_\alpha = \xi \sqrt{1 - \alpha^2}$ being the contracted healing length\textsuperscript{1}. Figure 6.4(b) shows the potential $V(x)$ as a function of $x$ for different $\alpha$. The change in the potential

\textsuperscript{1}Equivalently, in terms of the angle $\theta$ we get $\xi_\theta = \xi \sin \theta$. 

is rather small for $J \ll J_c$, but becomes significant for $J$ close to the critical coupling $J_c$.

It should be pointed out that the vanishing interaction potential is a result of the interference of two amplitudes contributing to $W_{k,q}$, which is a genuine quantum effect. This example shows that the simple picture based on a mean-field deformation potential is not always adequate. Moreover, we note that the effect described above does not occur for electrons in a condensed matter system given that their momentum at the Fermi surface is never close to zero.

6.4 Incoherent coupling effects

It was argued that incoherent phonon scattering does not occur for slow impurities with $\hbar|\mathbf{k}|/m_a \ll c_s$ since energy and momentum cannot be simultaneously conserved in the collision process. We now consider the opposite limit, namely ‘supersonic’ impurities emitting and absorbing real phonons due to incoherent collisions. First, we briefly discuss the total scattering rate of the impurities with the BEC, which was measured in a notable experiment by Chikkatur et al. [65, 113], and subsequently determine the energy dissipation of a supersonic impurity due to ‘Cherenkov radiation’.

6.4.1 Suppression and enhancement of incoherent scattering

Quite generally, the scattering process is characterized by the probability $w$ per unit time that an impurity with momentum $\mathbf{k}$ emits or absorbs a phonon with momentum $\mathbf{q}$. The rate $w$ can be calculated by using Fermi’s golden rule

$$w = \frac{2\pi}{\hbar} |\langle f | \hat{H}_I | i \rangle|^2 \times \delta(E_i - E_f),$$

(6.28)
where $|i\rangle$ and $|f\rangle$ stand for the initial and final state, respectively, with the corresponding energies $E_i$ and $E_f$. Let us consider the emission of a phonon with the initial state $|i\rangle = |n_k, n_{k-q}; N_q\rangle$ and final state $|f\rangle = |n_k-1, n_{k-q}+1; N_q+1\rangle$, where $n_k$ denotes the number of impurities with momentum $k$. By using the explicit expression for $\hat{H}_I$ we get

$$w_E(k, q) = 2\pi \frac{\kappa^2 n_0}{\hbar \Omega} \frac{\varepsilon_q}{\hbar \omega_q} (N_q + 1)(n_{k-q} + 1) n_k \times \delta(E_k - E_{k-q} - \hbar \omega_q), \quad (6.29)$$

where we considered a $\delta$-impurity for simplicity. As an example for the absorption of a phonon we take $|i\rangle = |n_k, n_{k+q}; N_q\rangle$ and $|f\rangle = |n_k-1, n_{k+q}+1; N_q-1\rangle$ with the resulting rate

$$w_A(k, q) = 2\pi \frac{\kappa^2 n_0}{\hbar \Omega} \frac{\varepsilon_q}{\hbar \omega_q} N_q(n_{k+q} + 1) n_k \times \delta(E_k - E_{k+q} + \hbar \omega_q). \quad (6.30)$$

The most important difference between the rates $w_E(k, q)$ and $w_A(k, q)$ are the bosonic enhancement factors. For a BEC with temperature $T$ the phonon occupation numbers are given by $N_q = (e^{\hbar \omega_q/k_B T} - 1)^{-1}$, and thus phonon absorption is only possible at finite temperatures, whereas spontaneous emission of a phonon occurs even at absolute zero. The rates $w(k, q)$ allow us to determine the total collision rate $\Gamma(k) = \sum_q w(k, q)$ or equivalently the relaxation time $\tau_k = 1/\Gamma(k)$, i.e. the average time between two scattering events. Without calculating $\Gamma(k)$ explicitly it is readily verified that $\tau_k \propto \hbar / \delta E_0$, where the proportionality constant depends on the impurity momentum $k$ and the BEC temperature. In practice, $\tau_k \sim 1\text{ms}$ for moderate coupling $\kappa \sim g$ and the BEC at zero temperature.

In the experiment by Chikkatur et al. [65, 113] most of the finite temperature effects could be ignored and $\Gamma_E(k) = \sum_q w_E(k, q)$ was compared against the experimental results. To be specific, a fraction of the BEC atoms was transferred
The motion of heavy impurities through a BEC to a different internal state by a Raman transition [163] and the redistribution of their momenta due to collisions with the stationary BEC was observed. It was found that the collisions were significantly reduced for impurity momenta $\hbar k/m_a < c_s$, whereas the scattering was enhanced if a large number of impurities was produced.

These experimental findings can be explained based on $w_E(k, q)$ in Eq. (6.29). The suppression of collisions is related to the density of final states represented by the $\delta$-function. Since only energy conserving processes are allowed $w_E(k, q)$ vanishes for impurities with $\hbar |k|/m_a < c_s$. On the other hand, the enhancement of collisions is due to the factors $N_q$ and $n_{k-q}$, which increase the scattering rate once the final scattering states are already occupied. This argument has of course to be refined when the finite temperature of the BEC is taken into account [65, 164, 165].

6.4.2 Čerenkov radiation

On a timescale much longer than $\tau_k$, a supersonic impurity can be modelled by a particle emitting radiation with power $P = \sum_q \hbar \omega_q w_E(k, q)$, here called Čerenkov radiation. Our goal is to determine the emitted power $P$ as a function of the velocity of the impurity, which for a three-dimensional system in the bulk limit reads

$$P = \frac{\kappa^2 n_0}{4\pi^2 \hbar} \int d^D q \varepsilon_q \delta(E_k - E_{k-q} - \hbar \omega_q).$$

(6.31)

The evaluation of the integral can be done by first introducing the variables $z = q^2/2$ and $v = \hbar k/m_a c_s$ (the velocity of the impurity in units of $c_s$) and changing to spherical coordinates, which yields

$$16\pi \int_0^\infty dz \, z^4 \int_0^\pi d\theta \, \sin \theta \, \delta(vz \cos \theta - \sqrt{z^2(z^2+1)} - \alpha z^2),$$
Figure 6.6. (a) The emitted power $P$ in units of $\kappa^2n_0/\hbar\xi^3$ as function of the mass ratio $\alpha$ and the impurity speed $v$ in units of $c_s$. The dissipated energy increases with both the mass and the speed of the impurity. (b) The impurity energy $\varepsilon$ in units of $g n_0$ as a function of time $t$ for the mass ratio $\alpha = 0.1$ (solid line), $\alpha = 0.2$ (dashed line) and $\alpha = 1$ (dotted line). The system parameters were set to $\hbar\xi^3/\kappa^2n_0 = 1$ ms with the initial value $\varepsilon_0 = 10$.

where $\theta$ is the angle between $z$ and $v$. To proceed further, we make the substitution $u = v \cos \theta$ and rewrite the $\delta$-function as an explicit expression of $u$, to find

$$
\frac{16\pi}{v} \int_0^{\infty} dz \, z^3 \int_{-v}^{v} du \, \delta\left(\sqrt{z^2 + 1} - \alpha z - u\right).
$$

(6.32)

We note that the argument of the $\delta$-function reduces to $1 - u$ for the lowest possible excitations of the BEC. Thus, there is no energy dissipation unless $v > 1$, which was to be expected. It follows from the identity for the Heaviside step function $H(x) = \int_{-\infty}^{x} dt \, \delta(t)$ that the integral over $u$ is equivalent to $H(v - \sqrt{z^2 + 1} - \alpha z)$, which results in a new upper limit $z_0$ for the remaining integral since $H(x) = 0$ for $x < 0$. Explicitly, we have $z_0 = (\alpha v - \sqrt{v^2 - 1 + \alpha^2})/(1 - \alpha^2)$ for $\alpha \neq 1$ and
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The equation for $z_0 = (v^2 - 1)/2v$ for $\alpha = 1$, and hence after integration over $z$ we get

$$P = \frac{\kappa^2 n_0}{\pi \hbar \xi^3} \left(\sqrt{v^2 - 1 + \alpha^2} - \alpha v\right)^4 \frac{v}{v(1 - \alpha^2)^4} \quad \text{for} \quad \alpha \neq 1,$$

(6.33)

$$P = \frac{\kappa^2 n_0}{16\pi \hbar \xi^3} \frac{(v^2 - 1)^4}{v^5} \quad \text{for} \quad \alpha = 1.$$  

(6.34)

Our expression for $P$ reduces to the well-known result for the special case $\alpha = 0$ [121, 166, 167]. The dependence of $P$ on the impurity speed $v$ and the mass ratio $\alpha$ is shown in Fig. 6.6(a), where it can be seen that the dissipated energy increases with the mass and the velocity of the impurity. We note that for $v \gg 1$ the dissipated energy scales as $P \propto v^3$, which is reminiscent of the quadratic drag in a classical fluid. A similar calculation shows that the relation $P \propto v^D$ even holds for 2D and 1D systems.

The effect of the emitted radiation on the motion of the impurity can be determined by solving the equation $d\varepsilon/dt = -p(\varepsilon)$, where $\varepsilon$ and $p$ are the impurity energy and the emitted power, respectively, in units of $gn_0$. The resulting deceleration of the impurity with fixed initial energy $\varepsilon_0$ is most pronounced for impurities with $m_a \approx m_b$ as shown in Fig. 6.6(b). The asymptotic value for $\varepsilon$ in the limit $t \to \infty$ is given by $m_a/2m_b$, and thus the minimal energy that can be achieved by the impurity increases with its mass.

The deceleration of impurities cause by Čerenkov radiation suggests that the interaction with the bath can be exploited to cool foreign particles immersed in a BEC. Indeed, various cooling schemes based on this idea have been proposed [25, 66, 94, 168], of which sympathetic cooling has been demonstrated experimentally for bosons [169] and fermions [170]. By generalizing the single impurity result to an ensemble of impurities it can be shown that the efficiency of sympathetic cooling is limited by the superfluidity of the BEC [66]. However, it should be
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noted that impurities in an optical lattice can be efficiently cooled from higher to lower Bloch bands [25] and even to very low temperatures within the lowest Bloch band by using a more sophisticated dark-state cooling scheme [94, 168].
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Conclusion

We conclude the thesis with a summary of our findings, along with a discussion of the potential further directions for research related to impurities immersed in degenerate quantum gases. In the following we refer to the most relevant results in this thesis without repeating technical details.

Chapter 2 We have shown that the dephasing of the internal states of an impurity atom coupled to a BEC is directly related to the temporal phase fluctuations of the BEC at the location of the impurity. Under the assumption that we know the coherence properties of the BEC this relation allows us immediately to estimate the rate at which the internal states dephase. On the other hand, we have suggested a scheme based on this relation to probe a priori unknown phase fluctuations of the BEC (whatever be their cause) via a measurement of the coherences of the impurity in a Ramsey-type experiment. Our findings also indicate that the use of immersed impurities for quantum information processing may be constrained because of unfavorable coherence properties of the BEC.

Chapter 3 & 4 We have seen that the dynamics of impurities confined to a deep optical lattice is best understood in terms of polarons. This approach has not only allowed us to describe the impurities by an extended
Bose–Hubbard model, but has also provided some intuition about the consequences of immersion. We have found that spatial coherence of impurities is destroyed in hopping processes at high BEC temperatures while the main effect of the BEC at low temperatures is to reduce the coherent hopping rate. Notably, the incoherent hopping leads to the emergence of a net atomic current across a tilted optical lattice with an Esaki–Tsu-type dependence of the current on the lattice tilt. In addition, it was argued that the phonon-induced interactions lead to the formation of stable clusters that are resilient to loss due to inelastic collisions.

Chapter 5  Our analytical and numerical investigation of the self-trapping problem has shown that the perturbative approach may be too restrictive to take the nonlinearity of the BEC properly into account. Especially attractive impurity–BEC interactions can have a surprisingly strong effects, namely a pronounced deformation of the BEC and high localization of the impurity ground state. Notably, under the assumption of a state-independent, attractive impurity–BEC coupling the model suggested by Gross does not have a well-defined ground state in 3D. From an experimental standpoint, the high density of the BEC near the impurity might lead to a loss of the BEC atoms and the impurity atom itself due to inelastic collisions.

Chapter 6  We have analyzed the interaction between impurities and the BEC in the weak-coupling regime based on a variant of the well-known Fröhlich polaron model. It has been shown that phonon-induced corrections to the bare mass of the impurity are significant in a one-dimensional system and that finite impurity hopping reduces the effective impurity–impurity interaction. In addition, we have considered the effect of incoherent collisions of
impurities with the BEC background and have determined the deceleration of supersonic impurities due to the emission of phonons.

Let us now outline some future directions related to immersed impurities. We restrict ourselves to three topics which occur naturally when considering the results in this thesis.

In the last chapter we have found the effective mass of self-trapped impurities for the weakly interacting case. However, the effective mass for highly localized impurities has to our knowledge not yet been determined. As a starting point it would seem reasonable to use a variational ansatz [171] in order to obtain a lower limit on the effective mass [172]. A more technical problem is related to the self-trapping ground state of impurities in a 3D system, which was shown to become arbitrarily localized for attractive impurity–BEC coupling. We here point out again that a strong effective confinement of the impurity would lead to change in the scattering properties of the impurity and the atoms in the BEC [173–175]. Thus, for highly localized impurities one has, in principle, to consistently solve the coupled Hartree equations as well as the scattering problem for the impurity and the BEC, a task which seems to be quite demanding.

A major challenge with ultra-cold neutral atoms in optical lattices is the implementation of terms in the Hamiltonian corresponding to an external magnetic field [1]. A variety of proposals for realizing magnetic fields in optical lattices exist [176–178] as, for example, driving Raman transitions between internal states of the lattice atoms [179]. It turns out that immersing an optical lattice into a rotating BEC in a vortex state provides an elegant method for creating an effective magnetic field. The space-dependent phase of the BEC background leads to a position dependent phase of the impurities, i.e. to the desired Peierls phase factor in the hopping term. Whether or not this phase is sufficiently large to be of
practical use, for example, in order to observe the high-field fractional quantum Hall effect [180], is currently under investigation [181].

Due to the enormous developments over the past few years in experimental studies of ultra-cold fermionic atoms it is now also possible to cool down Fermi gases to a regime where effects of the quantum statistics become noticeable [170, 182, 183]. These degenerate Fermi gases have attracted a lot of attention of experimentalist and theorists [99, 183], partly because their quantum statistics has a fundamental effect on their many-body properties. In particular, the single-particle spectrum of Fermi gases is more complicated than that of a BEC and features gapped and gap-less excitations [183]. Therefore, it would be interesting to determine the effects of a Fermi gas on either the internal or external degrees of freedom of an immersed impurity and contrast them with those of a BEC.

Finally, we conclude with the remark that the proposals put forward in this thesis might be quite challenging from an experimental point of view and their realization, if it will occur, may take some time. Nonetheless, our description of impurities in terms of polarons has already been contemplated as a tentative explanation of recent experimental results related to degenerate Bose–Bose mixtures [24]. Above all, considering the tremendous experimental progress in atomic physics just during my doctorate, the prospects for an implementation of our ideas look very encouraging and there is no doubt that cold atoms will be an extremely valuable tool for providing insight into many-body quantum physics in the future.
Bibliography


